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Proceedings of the Advisory Committee on Nuclear Waste Working Group on NRC and DOE Performance Assessments: Assumptions and Differences

Presentations on the Proposed High-Level Nuclear Waste Site at Yucca Mountain, Nevada

March 25-26, 2003

U.S. Nuclear Regulatory Commission
Advisory Committee on Nuclear Waste
Washington, DC 20555-0001

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ABSTRACT

This report contains the information presented to the Working Group Meeting on NRC and DOE Performance Assessments: Assumptions and Differences. The U.S. Nuclear Regulatory Commission's (NRC) Advisory Committee on Nuclear Waste (ACNW) convened this Working Group on March 25–26, 2003 at the NRC Headquarters in Rockville, MD. This report includes summaries of the presentations given to the Committee, followed by the presentation materials and selected discussions among the participants. The working group included a panel of experts who observed and commented on the proceedings.

The purposes of the working group were (1) to increase the ACNW's technical knowledge of the performance assessment work being done for the proposed Yucca Mountain repository, (2) to identify "soft spots" in the analyses to date, particularly in regard to the issue of "model realism," (3) to compare the different approaches taken by the NRC and the U.S. Department of Energy, and (4) to provide a reference point to develop a follow-on working group on performance confirmation for Yucca Mountain.

In addition to the summaries and presentation materials, these proceedings contain selected discussions which were extracted from the working group transcripts. The discussions can be found immediately following each presentation. Discussions and summaries of the presentations made were edited from the meeting transcripts. Where practical, the participants were given an opportunity to review and edit their individual contributions. Meeting transcripts are available on the NRC web site (www.nrc.gov) and should be reviewed for actual statements made during the meetings.

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EXECUTIVE SUMMARY

Working Group on NRC and DOE Performance Assessments: Assumptions and Differences

The U.S. Nuclear Regulatory Commission (NRC), Advisory Committee on Nuclear Waste (ACNW or the Committee), held its 140th meeting on March 25–27, 2003, at Two White Flint North, 11545 Rockville Pike, Rockville, MD. The ACNW published a notice of this meeting in the *Federal Register* (68 FR 11879) on March 12, 2003. The entire meeting was open to the public and served as a forum for attendees to discuss and take appropriate action on the items listed in the agenda. The Working Group on NRC and DOE Performance Assessments was held during the first two days of the three-day meeting.

ACNW members who attended this meeting were Dr. George M. Hornberger, Chairman, Dr. B. John Garrick, Dr. Raymond Wymer, Mr. Milton Levenson, and Dr. Michael T. Ryan.

March 25, 2003

ACNW Member B. John Garrick noted that performance assessment is a vital part of the eventual license application for Yucca Mountain because it is the basis for the technical decisions. The purposes of the working group session were fourfold, (1) to increase ACNW's technical understanding and knowledge of the performance work done to date for the Yucca Mountain repository, (2) to identify areas in the analysis that may warrant increased realism, (3) to understand the different approaches taken by the NRC and the Department of Energy (DOE), and (4) to provide a reference or baseline for a follow-up working group session on performance confirmation. Dr. Garrick described how performance assessments ought to be modularized in such a way that they can be divided into visible expressions of the driving contributors to the performance or to the risk.

Dr. Garrick introduced the keynote speaker, Dr. Joe Payer, as a Professor of Materials Science and Engineering and Director of the Yeager Center for Electrochemical Sciences at Case Western Reserve University. Dr. Payer was a member of the 1999 Total System Performance Assessment (TSPA) Viability Assessment Peer Review Panel that provided the DOE with a formal independent critique of that report. In addition, he chaired the DOE's Waste Package Materials Performance Peer Review Panel and currently is serving part-time on a DOE Science and Technology Review Panel in support of DOE's Director of the Office of Civilian and Radioactive Waste Management.

Keynote Presentation

Dr. Joe Payer, of Case Western Reserve University, gave the keynote address entitled, "Realism in Simulating Long-Term Waste Package Corrosion and Radionuclide Source Term." He talked about the composition of the water that could drip onto waste packages, the hypothetical composition of water on metal surfaces and waste package barrier layers, and the composition of the water that may enter waste packages and how that composition may evolve until the water is released. Corrosion is clearly identified as the primary determinant of waste package lifetime. It is the most likely degradation process that will determine when packages get penetrations and what the form and distribution of those penetrations will be. Dr. Payer discussed penetration of waste packages, various degradation modes, stress corrosion, mechanical damage, and embrittlement.

Localized corrosion, pitting, crevice corrosion, and stress-corrosion cracking are the most likely degradation modes that can occur in the Yucca Mountain environment with materials that are being considered by the DOE. Basing materials selection and design on high crevice corrosion resistance is a prudent and well-accepted way to proceed. Corrosion processes and rates depend on the corrosion resistance of the material and the environment to which the material is exposed. The repository environment is changed in the thermal period by evaporation and concentration. In the beginning there is a very low concentration of salts, but as the water evaporates, the salts become more and more concentrated. One of the real challenges is to determine what kinds of concentrated solutions will likely evolve.

Dr. Payer noted that the flow of groundwater through Yucca Mountain is a key performance issue. The climatology and the amount of infiltration will determine how much water comes down through the unsaturated zone above the repository. At the repository level, infiltrating water can interact with waste packages and drift materials. If the water inside the waste packages goes through the cladding or if there are clad failures, the water will come in contact with the fuel: this is where the radionuclide mobilization release starts. The water could ultimately move out of that area through the invert material and on down to the saturated zone.

Dr. Payer said that the issue relates to the realistic range of environments at Yucca Mountain. What is the realistic range of materials susceptibility and the corrosion resistance of Alloy C-22 and titanium? What is the likelihood of overlap in these ranges? What is going to occur in that area of overlap? In an ideal world, there would be no overlap.

Another issue is the deliquescence of various salts that are on the surface. The deliquescence shows the relative humidity versus temperature and at what point an aqueous phase would occur if sodium nitrate, sodium chloride, or magnesium chloride crystals developed on the waste package. At what relative humidity would moisture start to form? Data are available to help us look at that.

The goal of looking at the source term is to define a set of models that capture reality. In other words, the models need to recognize the important processes, and the dependencies of those processes, and do so in terms that are relative and meaningful to Yucca Mountain.

Introduction to DOE's Total System Performance Assessment Model

Dr. Abraham Van Luik (DOE) talked about what the NRC requires of the DOE regarding realism and conservatism, as well as the requirements for the performance assessment (PA) used to generate compliance with the post-closure performance objectives. He mainly discussed the DOE's perspective on requirements under the NRC's regulations in Title 10, Part 63 of the *Code of Federal Regulations* (CFR). He noted that the use of conservatism to manage uncertainty has implications for risk-informed reviews. The DOE believes that realism is desirable, but not required. Adding realism where practicable is a prudent approach because it allows more meaningful safety margin evaluations and improved understanding of system performance. Dr. Rod Ewing asked Dr. Van Luik to clarify his comment that as realism has been added to DOE's PA, long-term safety estimates have improved. Does that mean that the dose always drops or that uncertainty decreases? Dr. Van Luik responded that dose does not always drop with every nuance of change made. But the DOE did three separate PAs during the site recommendation period. They all passed muster when it came to the 10,000-year requirements, but the peak doses kept stepping down. Peak dose is always well beyond 10,000 years. Dr. Garrick asked whether the license application date is still proposed for the end of 2004. Dr. Van Luik responded that the current schedule remains in effect, but that a "frantic" reassessment was presently underway to evaluate whether the schedule was still achievable.

Introduction to the NRC's Total-System Performance Assessment

Dr. Andrew Campbell (NRC) reviewed the background and role of the NRC's total-system performance assessment (TPA) computer code capability. The role of the NRC's TPA code is to enhance the NRC's independent review capability to evaluate the DOE's PA, to understand and evaluate the DOE's models, assumptions, and data, and to provide flexibility to evaluate the completeness of DOE's modeling approaches. The TPA code also provides risk insights to help establish priorities in technical reviews. Overall, the TPA code provides confirmatory analyses of the DOE's modeling approach and results.

Overview of the DOE's TSPA

Dr. Peter Swift (Sandia National Laboratories/Bechtel SAIC Company, LLC) reviewed the status of the DOE's TSPA and summarized the TSPA methodology and its major model components. The TSPA process includes (1) screening of features, events, and processes, (2) developing models and their scientific basis for each process, (3) identifying uncertainty in models and parameters, (4) constructing an integrated TSPA model using all retained processes, and (5) evaluating total system performance (individual protection, groundwater protection, and human intrusion) through Monte Carlo simulations.

Overview of the NRC's TPA

Mr. Christopher Grossman (NRC) gave an overview of approaches and assumptions for The TPA computer code version 4.1. The TPA performs probabilistic dose calculations for given time periods and accounts for (1) essential features of the engineered and natural barriers, (2) chemical and physical processes affecting waste package degradation and release to the biosphere, (3) uncertainties and spatial variability of model parameters and future states, and (4) lifestyle characteristics of the reasonably maximally exposed individual. The TPA analyzes scenarios including a nominal case with climate change and seismic activity and disruptive cases with faulting and igneous activity. The TPA uses approaches based on fundamental principles and available data.

Source Term Module Under the TSPA

Dr. Robert Andrews (Bechtel SAIC Company, LLC) reviewed elements of the DOE's source term model. He described the factors that can potentially affect emplacement drift environments, including coupled thermal-chemical effects on water chemistry, mechanical effects of rock fall, humidity, and groundwater seepage into drifts. Dr. Andrews discussed the degradation models for the drip shield and waste package, including processes of general corrosion and stress-corrosion cracking. The TSPA model includes juvenile failure of waste packages, but the DOE estimates that the expected number of improperly annealed waste packages is only ~0.26 out of ~12,000 waste packages. The first drip shield failures occur at about 20,000 years as a result of general corrosion. The TSPA models bulk chemistry within the waste package under well-mixed, oxidizing conditions. Dr. Andrews also described the possible degradation of fuel cladding via perforation and unzipping.

Source Term Module Under the TPA

Dr. David Esh (NRC) provided a review of the NRC's source-term modeling. This included conceptualizations of how groundwater could enter repository drifts and come into contact with drip shields and waste packages. The amounts of water that could actually enter corroded waste packages in the future appears to be affected by diversion around drifts caused by capillary barriers and by the tendency for water to run down walls rather than drip into openings. Two conceptual models for water contact are the "bathtub" and the "flow through" models. Dr. Esh reviewed processes of drip shield corrosion, uniform and localized corrosion of waste packages, and waste package stress-corrosion cracking. Dr. Esh then reviewed various models for dissolution of spent nuclear fuel within the waste form. The current TPA code version simulates advective transport of radionuclides out of waste packages. The TPA Version 5.0 will include transport by diffusion in films of water inside and outside of waste packages. Dr. Esh concluded that the NRC models are primarily data based, use simple concepts, and provide the NRC staff with the flexibility to evaluate data and model uncertainties for the proposed Yucca Mountain site.

March 26, 2003

Simplified Models of Key Contributors to Dose Traced Through Various Modules (DOE)

Dr. Peter Swift (DOE) gave a talk entitled, "Component Performance and Key Contributors to Nominal Scenario Class Dose in the U.S. Department of Energy Total System Performance Assessment." He reviewed the overall results for nominal repository performance, including the TSPA total dose, major contributors to dose over time, and the chronology of major events in nominal performance. Dr. Swift showed changes in radionuclide inventories over time. He showed estimates for major chronological events, such as stages in climate change, timing for peak waste package surface temperatures, first drip shield failures, waste package failures due to defects and general corrosion, and relative transport times in the natural system. He traced Np-237 and Tc-99 through the system, component by component (i.e., waste form, waste package, invert, and unsaturated and saturated zones). Dr. Swift noted that the TSPA models and analyses for the license application are currently under development.

Simplified Models of Key Contributors to Dose Traced Through Various Modules (NRC)

Mr. Tim McCartin (NRC) gave a talk entitled "Understanding Performance Assessment Results." He noted that estimated doses within 10,000 years are influenced by the very mobile nuclides, I-129 and Tc-99. Estimated doses beyond 10,000 years are strongly influenced by Np-237, which is somewhat mobile. He described how performance assessment results are complex and reflect nuclide-specific behavior, temperature dependence, and the "masking" effects of redundant barriers.

The NRC staff is currently studying sensitivities within and relationships between various attributes (e.g., waste package, water flow into waste packages, waste forms, and unsaturated and saturated zone transport). The results of these studies will provide the perspective to understand and interpret performance assessment results. Waste package performance is easy to explain and understand (breached vs. not breached), despite complexities in technical basis. Mr. McCartin described the performance sensitivities for waste forms and for water flow into waste packages. He discussed dissolution rates of spent fuel, solubility limits used for radionuclides of interest (within waste packages), rates of deep groundwater percolation, and the relative degrees of flow diversion or enhancement.

Mr. McCartin also discussed the sensitivity of retardation in the Calico Hills nonwelded vitric unit, which is below the repository and covers about 50 percent of the repository "footprint." Poorly mobile radionuclides, like Am-241 and Pu-240, are strongly retarded by the Calico Hills vitric unit. Neptunium-237 is also retarded by this unit. All three radionuclides can also be strongly retarded in saturated valley fill alluvium. In his summary, Mr. McCartin observed that a large number of waste package failures are needed for I-129 and Tc-99 to be important due to their limited inventory. Neptunium-237 is sensitive to solubility limit and water flow and to the presence of the Calico Hills nonwelded vitric unit. In the saturated zone, Np-237 is sensitive to variations in retardation, has limited sensitivity to matrix diffusion, and limited sensitivity to the extent of alluvium (assuming a minimum of 1 kilometer of alluvium in the flowpath).

Stakeholder Presentations

Dr. Don Shettel (Geosciences Management Institute, Inc., representing the State of Nevada) gave a talk entitled, "Near-Field Environments and Corrosion." The talk described various water environments within Yucca Mountain, and noted water types that include precipitation, unsaturated fracture flow, matrix pore water, and water in a thermal refluxing zone. Dr. Shettel described various in-drift chemical and physical processes, and focused on the processes of acid volatilization and hydrolysis of salts. He explained how residual salt solutions and condensates become acidic with thermal evaporative concentration. Deliquescence of salts causes accumulation of liquid on waste package canisters. During hydrolysis of salts, nitric acid vapor is given off. Dr. Shettel estimated a corrosion rate of 678 microns per year, which means that a hole could develop through 2 centimeters of alloy C-22 in less than 30 years. Dr. Shettel concluded that in-drift processes are more complicated than the DOE admits, that corrosion rates are significantly higher for evaporating solutions and their condensates (0.1 to 1.0 millimeter per year (mm/yr), up to 10 mm/yr), that subboiling immersion testing of engineered barrier materials in groundwater is unrealistic and nonconservative, and that the vadose zone is not a good environment for a high-level waste repository.

Dr. John Walton (University of Texas at El Paso, representing Nye County, Nevada) gave a talk entitled "Evaporation, Reconstitution, and Water Chemistry." The talk noted the importance of water chemistry in estimating corrosion for all engineered barrier materials. A theme of the talk was the concern that the DOE had not considered physical separation processes in its analyses. During evaporation, different minerals deposit at different locations. He showed salt separations in two examples—deposits from a sidewalk and deposits near a desert spring. Dr. Walton believes that natural air movements within Yucca Mountain have not been fully considered, that the construction effects increase the air permeability of the rock, that the climate could be dryer than anticipated, and that the period of evaporation may last well beyond current projections. Dr. Walton concluded that physical separation of minerals is certain to occur, that potentially aggressive environments could be created for titanium drip shields and Alloy C-22 waste packages, that these environs will have high spatial and temporal variability, and that biological and other chemical processes will also be important.

Mr. Engelbrecht von Tiesenhausen (representing Clark County, Nevada) gave a talk entitled "Clark County Comments—What Is Our Concern, and Why Are We Still Concerned: Temperature, Coupled Processes, and Corrosion." He referred to a letter to NRC Chairman Meserve (dated August 13, 2001) that recommended continued exploration of the chemical issues associated with repository design, such as a "hot" versus "cold" repository, or the use of backfill. Mr. von Tiesenhausen expressed concerns that the DOE has selected the "hot" repository option for the design to be proposed in a license application. He was also concerned that the DOE is still using concentrated J-13 well water for seepage brines. He noted that a previous State of Nevada presentation to the Board on Radioactive Waste Management (of the National Academies) indicated that evaporation of concentrated unsaturated zone pore waters will produce acidic environments, while evaporation of J-13 well waters will produce more benign alkaline environs. Rock dust, with its major and minor chemical constituents, will also influence the chemistry of evaporated solutions. Mr. von Tiesenhausen concluded that fully coupled thermo-hydro-chemical processes may be impossible to model at this time, that chemical environs of the waste packages are likely to be very complex, and that predicting long-term corrosion of Alloy C-22 using J-13-based waters is probably not realistic.

Dr. Atef Elzeftawy (representing the Las Vegas Paiute Tribe) read a statement into the record regarding tribal concerns. He stated that the Tribe should be allowed to play a major role in the Yucca Mountain program, and that the Tribe has major concerns about the policies and technical direction of the Yucca Mountain project, and the DOE, U.S. Environmental Protection Agency, and NRC roles in the program. For example, the Tribe believes that the DOE's TSPA should not be accepted as the method of testing and evaluating the suitability of the Yucca Mountain site. The Tribe seeks no adverse impact on the health of the tribal population or on the economic development of its Snow Mountain Reservation.

Dr. John Kessler (representing the Electric Power Research Institute) gave a talk entitled "When Realism Is and Is Not Needed in TSPAs." He pointed out that conservatism (as opposed to realism) is often easier to defend, especially during licensing proceedings. It serves to provide boundaries for license conditions and maintains a connection to performance confirmation. However, conservatism may distort the relative importance of individual barriers. Dr. Kessler gave an example of this from the diffusive release model in the Electric Power Research Institute's (EPRI) TSPA code. The EPRI model assumes excellent contact among all regions of the engineered barrier system, but in reality, spent fuel would not be in close contact with the rock walls of tunnels. The EPRI model also assumes continuous water pathways through the engineered barriers, but actual pathways would be much more limited. Dr. Kessler showed model results that illustrate how an estimated 10,000 year dose is strongly affected by the conservative diffusion model. He concluded that better relative unsaturated/saturated zone performance would be apparent if he had used a more realistic diffusive release model. Dr. Kessler said that it is reasonable to replace uncertainty with pessimistic assumptions to establish robustness for the adjudicatory process, to provide boundaries for license conditions, and to provide "reasonable expectation" levels of confidence for compliance with regulations.

Working Group Roundtable Panel Discussion on TSPA/TPA

The five expert panelists (Payer, Ewing, Bullen, Morgenstein, and Latanision) participated in a panel discussion that was moderated by ACNW member Garrick.

Dr. Ron Latanision (Massachusetts Institute of Technology) focused on temperature issues because all of the modes of corrosion degradation, including uniform corrosion rates and the rates of localized corrosion, are affected by temperature, as well as by the environmental chemistry and state of stress of the material.

Dr. Joe Payer (Case Western Reserve University) posed a number of questions about the importance of the environment when evaluating corrosion. Given a population of environments and a range of corrosion resistance for a material, the issue is where they overlap because that's where corrosion can occur. Can these conditions be correlated with a real repository? How, when, and where will the corrosive conditions occur? How much corrosion will there be? Will the adverse environments persist? Dr. Payer noted that one of the things lost in most testing and thermodynamic modeling is that researchers point to a given condition and describe what can happen under that condition. But in real systems, the aqueous solutions are not constant—they evolve. With respect to waste package environments, if they contain something that can consume the acidity, then the solution will become more alkaline. If something is consuming the hydroxyl ions, the environment will become more acidic. Dr. Payer observed that we know about these processes—it is just a matter of working them in. He asked, whether these environments will form. Will the environments persist? If they do not persist, or go away because the package becomes dry in that area, could they re-form and start again?

Dr. Maury Morgenstein (Geosciences Management Institute, Inc.) focused on the vadose zone environment. He said that it is a very complex area that we do not understand at present, including the very basics of the hydrogeochemistry. He noted that water entering the soil zones within the region could likely have highly variable chemistry in spatial terms. This water will evolve as it migrates down through the vadose zone and through the repository environment.

Dr. Morgenstein referred to a basic lack of understanding of the hydrochemical system, and noted that engineered barrier system items, such as Alloy C-22 and Titanium-7, can react with water that has been altered by the temperature of the system and the variations of the dynamics of the system as it changes through time. He believes that the project is probably moving too fast to be able to collect and acquire the needed information. He noted that there are obviously degrees of retardation offered by the natural system, but it is not clear that these degrees of retardation are sufficient to meet licensing requirements. He also noted the importance of using vadose zone pore water chemistry, rather than the chemistry found in the saturated zone.

Dr. Dan Bullen (Iowa State University) covered a broad range of issues, including evolution of waste package design and changes in the understanding of how much water moves through Yucca Mountain. He focused on thermal- and biosphere-related issues. Dr. Bullen noted the difficulty of dealing with uncertainties if the models do not include key processes that relate to those uncertainties. For example, the DOE Supplemental Science and Performance Analysis examines both high- and low-temperature operating modes. But dependence of corrosion on temperature is not included in some calculations, and this alone can have a significant effect. In some cases, there is no simulation of localized corrosion because the localized corrosion model was not used to support it at the time. Dr. Bullen feels that a cooler repository design may be desirable, not only because it is less difficult to model, but also because it is more closely related to the current ambient conditions at Yucca Mountain. In other words, the less the mountain is perturbed the better. Perhaps a cooler design would not produce the high chloride concentrations and high salt concentrations that have been discussed as a concern. Dr. Bullen expressed concern about the 3000 acre feet of water dilution factor because it might be masking some significant problems associated with the biosphere model. He felt that the model is not realistic and not conservative because a small source of water with a high concentration that is not significantly diluted may give a significantly greater dose than that which is predicted with a greater dilution factor.

Dr. Rod Ewing (University of Michigan) noted that if he had either DOE's or NRC's job, the very first thing he would do is a performance assessment because the performance assessment informs one about how things are connected. But although the exercise would be informative, the results would almost certainly be wrong. Dr. Ewing noted that the modeled system is quite nonlinear. The fact that the "one-off" and "one-on" analyses can be done so readily suggests that the modeled parameters are probably not coupled well enough. Dr. Ewing noted that evolution of repository boundary conditions over time would be challenging to model (e.g., water chemistry, temperature, porosity, permeability, etc.). He said that the chemistry of this system may be the dominant driving force in terms of the end result. Although the TSPA computer code has chemistry in the model, from a geochemical point of view it is at a somewhat primitive level. Further, the remarkable extrapolation over time of all the processes makes for a very tough problem.

How to deal with these problems? Dr. Ewing feels that if we both look at the TSPA and the TPA computer codes in a very natural and understandable way, in terms of modeling, "they've evolved into a corner, talking one to the other." What is missing, and it is not part of the license application process, is the broader context in terms of what can be done by modeling.
Dr. Ewing presented the analogous case of future climate modeling and the difficulties in that arena. A key question in climate modeling is how can we extrapolate results before the uncertainty hinders the ability to make a policy decision? In the waste arena, the question should be, "How far can results be extrapolated before the uncertainty is so large that we cannot reasonably determine compliance with the regulation?" Dr. Ewing suggested that it would be informative to look around at other systems, particularly complex systems, and ask what the limitations are to see if we are fooling ourselves. Dr. Ewing concluded that he does not understand how the uncertainty of long-term extrapolation will be handled, and he sees a need for better ways to judge the adequacy of models and modeling.

Public Comments

Dr. Atef Elzeftawy (representing the Las Vegas Paiute Tribe) discussed how the researchers in the Manhatten Project looked at uncertainty in their theoretical work and ultimately demonstrated the results. This was their equivalent of "performance assessment." He also mentioned quantum mechanics theory and that the physicist Feynman said that it was not clear what quantum mechanics is and that it was not understood in all details, but that it works. Dr. Elzeftawy observed that if we can come up with performance assessment models that work, that helps the decisionmaking process.

Ms. Judy Treichel (Nevada Nuclear Waste Task Force) observed that it was "refreshing" to hear the "knock down, drag out" discussions, but felt that they did not last long enough. She described the different perspectives of Yucca Mountain seen by farming families living in the Amargosa Valley, who get their water from wells and consume many of their own agricultural products ("they don't have to just eat tomatoes and cucumbers, they can eat pistachios, they can drink the milk from the cow who drinks out of the same tap").. From their perspective, their risks will be assigned by someone else. Ms. Treichel stated that her real fear relates to the biases of the various presenters and that she is worried that, "NRC is sort of pushing to make this thing [Yucca Mountain] okay." She feels that the NRC would like to have Yucca Mountain, and that people who do not have to live with Yucca Mountain would be "way more eager to have uncertainty or to feel that it can be accepted than other people." Ms. Treichel was skeptical that the process was "totally fair."

Dr. Roger Staehle described examples of mechanical failures that have made an impression on him, including helicopter rotor blades and nuclear reactor pipe failure. He noted the very complex nature of Yucca Mountain with regard to surface chemistry, temperature, and mathematics. He recommended a bounding approach to the problem to make predictions, taking into consideration a "reasonable" set of worst cases, but not a worst case. He further recommended that the DOE use this set of worst cases as a basis to make progress with modeling.

Mr. Steve Frishman (representing the State of Nevada) noted that John Kessler had a viewgraph that said pessimism can be replaced with more realism at a time when more confidence is required, perhaps at a later stage of repository development. Mr. Frishman said there is no room for this staging concept under the current regulation. The NRC's rule as it stands today is not a staged rule. The confidence that is necessary is the "confidence that can be elicited through demonstration at the time a construction authorization is issued, if it is to be issued." Mr. Frishman noted that the TSPA computer code is not just a useful tool for understanding what is known or not known. He stated that under the licensing rule the outcome of the performance assessment is the statement of compliance (or not). One of Mr. Frishman's concerns is that performance assessment results will be translated into a decision for reasonable expectation or reasonable assurance that can lead to another level of subjectivity.

Dr. Garrick noted that the ACNW "does its best to address the technical issues and is not the body that makes the decision about whether or not a licensee is in compliance. ACNW members are not license experts, are not regulation experts. ACNW is here to complement the regulatory process but be focused on what is going on from a technical standpoint."

Committee Actions

A letter documenting the ACNW's conclusions from the Working Group on Total System Performance Assessment was sent from G. Hornberger to N. Diaz on June 12, 2003.

A follow-up ACNW Working Group Session on Performance Confirmation for Yucca Mountain was held on July 29-30, 2003.

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B. John Garrick, Working Group Chairman, ACNW
Milton Levenson, Member, ACNW
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Joe Payer, Case Western Reserve University
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[1]Two of the panel members serve on the U.S. Nuclear Waste Technical Review Board (NWTRB). However, they represented themselves at the working group session as individual professionals from their respective universities, rather than as members of the NWTRB.

ACKNOWLEDGMENTS

We thank all the speakers and participants for their contributions, which collectively made this Working Group a success. We thank Neil Coleman, Michael Lee, Howard Larson, and the staff of the ACRS/ACNW Operations Support Branch for their efforts in assisting the Working Group.

George M. Hornberger, Chairman
ACNW

Raymond G. Wymer, Vice Chairman
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B. John Garrick, Member
ACNW

Milton Levenson, Member
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ACNW

ABBREVIATIONS

ACNW	Advisory Committee on Nuclear Waste
ACRS	Advisory Committee on Reactor Safeguards
CFR	*Code of Federal Regulations*
CNWRA	Center for Nuclear Waste Regulatory Analyses
CWRU	Case Western Reserve University
DOE	U.S. Department of Energy
EPRI	Electric Power Research Institute
FR	*Federal Register*
GMII	Geosciences Management Institute, Inc.
KTI	Key Technical Issue (for the proposed Yucca Mountain site)
MIT	Massachusetts Institute of Technology
NRC	U.S. Nuclear Regulatory Commission
PA	performance assessment
SNL	Sandia National Laboratories
TPA	NRC's Total-system Performance Assessment
TSPA	DOE's Total System Performance Assessment
UTEP	University of Texas at El Paso

INTRODUCTION

An Advisory Committee on Nuclear Waste (ACNW) working group session on Total System Performance of the Proposed Yucca Mountain High-Level Waste Repository was convened on March 25–26, 2003. This was a technical session on the quality of the performance assessment work conducted to date by the U.S. Nuclear Regulatory Commission (NRC) staff and the U.S. Department of Energy (DOE) staff. Performance assessment is a vital part of an eventual License Application because it provides a key basis for the technical decisions. This ACNW review is timely because, as currently planned, the DOE will submit a license application for Yucca Mountain to the NRC by December of 2004.

In Title 10, Part 63 of the *Code of Federal Regulations* (CFR) Performance assessment is defined as:

> . . .an analysis that:
>
> (1) Identifies the features, events, processes (except human intrusion), and sequences of events and processes (except human intrusion) that might affect the Yucca Mountain disposal system and their probabilities of occurring during 10,000 years after disposal;
>
> (2) Examines the effects of those features, events, processes, and sequences of events and processes upon the performance of the Yucca Mountain disposal system; and
>
> (3) Estimates the dose incurred by the reasonably maximally exposed individual, including the associated uncertainties, as a result of releases caused by all significant features, events, and processes, weighted by their probability of occurrence.

The theme of the working group session was how to achieve *appropriately credible and realistic* performance assessment models. While the working group discussed the total scope of the performance assessment, they emphasized the confidence of the source term work because the most important driver in the performance of the repository is the mobilization of the waste, which is what is meant by a source term.

Purpose

The purposes of the working group session were (1) to increase the ACNW's technical knowledge of the performance assessment work being done for the proposed Yucca Mountain repository, (2) to identify areas in the analyses that warrant increased realism, (3) to understand the different approaches taken by the NRC and DOE, and (4) to provide a reference point for developing a follow-on working group session on performance confirmation. Before the meeting, participants were asked to address various questions, including the following examples:

- What is the basis for the water chemistry assumptions inside the waste package in the current models?
- What is a realistic representation of the water pathway into the waste packages?

- How can the performance assessments be used to achieve a more realistic and balanced design of engineered and natural barriers?

- How should the performance assessments be used to facilitate performance confirmation?

General Approach

The format of the working group session included a keynote talk by a distinguished scientist or engineer that set the tone for the meaning of a realistic performance assessment, a series of expert presentations from senior practitioners of the performance assessment work itself, additional talks from stakeholders having varied opinions about the technical quality of the work, a panel discussion of issues and results presented, public comments, and a wrap-up of the session.

A "pinch point" approach was used as the format for the "practitioner" papers. Total system performance assessment was discussed in modules. The suggested modules were (1) infiltration, (2) source term, (3) nearfield, (4) unsaturated zone, (5) saturated zone, and (6) biosphere and dose. To illustrate the pinch point idea, consider the first module, infiltration. The input to this module, rainfall, is determined by climate conditions and the output is determined by different water infiltration rates and compositions reaching the drip shield/waste package region. Similarly, the input to the source term module is discrete water composition from the infiltration model and the output is release fractions and compositions of radionuclides. The idea was to divide the total system into "pinch points" of inputs and outputs that allow individual modules to be analyzed independent of pre- and post-modules.

Stakeholders and other investigators presented their views on the general approach and technical quality of the performance assessment work, with a special focus on waste package, waste mobilization, and source term. Following the presentations, a panel of experts, moderated by the chairman of the working group, reviewed the material presented and offered their expert opinions on the technical breadth, depth, and quality of the work. These experts emphasized identifying areas in the models that would benefit from increased realism. The ACNW gave the participants, including those in the audience, several opportunities to make comments consistent with the purpose and objectives of the working group session.

Letter to

The Honorable Nils J. Diaz, Chairman
U. S. Nuclear Regulatory Commission

from

George Hornberger, Chairman
Advisory Committee on Nuclear Waste

Comments on the Total System Performance Assessment Working Group Session
March 25-26, 2003

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June 12, 2003

The Honorable Nils J. Diaz
Chairman
U. S. Nuclear Regulatory Commission
Washington, D.C. 20555-0001

SUBJECT: TOTAL SYSTEM PERFORMANCE ASSESSMENT WORKING GROUP SESSION, MARCH 25-26, 2003

Dear Chairman Diaz:

At its 140th meeting on March 25–26, 2003, the Advisory Committee on Nuclear Waste (ACNW or the Committee) held a working group session (WGS) on performance assessment for the proposed high-level waste repository at Yucca Mountain, Nevada. The session included a panel of five distinguished scientists and engineers from academia and research institutions renowned in the fields of geosciences, corrosion science, and engineering.[1] Representatives of the U. S. Department of Energy (DOE), the U. S. Nuclear Regulatory Commission (NRC), and the State of Nevada made presentations, as did various other stakeholders.

The primary purposes of the working group session were to (1) better understand the principal issues of performance assessment that might affect the licensing process, (2) review the NRC staff readiness to evaluate a total system performance assessment, and (3) assess the level of realism in the modeling of the repository. The principal bases of the discussions were the performance assessment models of the NRC and DOE identified as Total-system Performance Assessment (TPA) and Total System Performance Assessment (TSPA), respectively. While the TSPA was part of the discussions, the focus of the session was on the "near-field," by which is meant the drip shield, the waste package, the radionuclide source term, and the geosphere in the immediate vicinity of the repository drifts. In particular, the discussion emphasized the "source term" and "source term uncertainty."

The rationale for the emphasis on the source term is that it is the principal boundary condition for assessing the performance of the natural setting. One view is that if a strong scientific basis can be established for the argument that not much radioactive material escapes from the waste, any impact of uncertainties about the performance of the geosphere may be of limited concern. Thus, a better understanding of the near-field containment capability may reduce the need for additional characterization of the site.

The focus on uncertainty and realism relates to the issue of risk-informing the performance assessment. The Committee has long held the view that to comply with regulations that are

[1]Two of the panel members serve on the Nuclear Waste Technical Review Board (NWTRB). However, they represented themselves at the working group session as individual professionals from their respective universities, rather than as members of the NWTRB.

designed to be risk-informed, a license applicant must provide analyses that include an answer to the question, "what is the risk?" Of course the answer is expected to include the applicant's best estimate of what is the real risk, not some other assessment such as an extreme over- or under-estimate of the risk. Our point has always been that it is best to estimate the real risk, including its uncertainty, as a baseline against which to determine how much safety margin actually exists and to better aid the decisionmaking process as to what seems to be a "reasonable" safety margin.

The Committee was very pleased with the depth and breadth of the technical discussions and the opportunity to hear the different views and exchanges of the participants. We anticipate that the record and insights provided will enhance our ability to effectively offer advice to the Commission as the Yucca Mountain project moves into the licensing phase. While there was sharp and in-depth discussion of several technical issues, the Committee heard no issues and received no information that would establish a basis for major changes in the positions we have taken in reports to the Commission on past performance assessment work.

The technical discussions centered on the (1) chemical and temperature environment of the drip shield and waste package and their effects on degradation mechanisms, (2) uncertainties and realism of the performance assessment models, and (3) NRC staff readiness to perform a comprehensive review of the performance assessment that will be submitted as a part of the DOE license application. The discussions also included the following highlights:

- The State of Nevada has a concern that severe corrosive environments might be possible in the vicinity of the drip shield and waste package. This concern arises from their opinion that the performance assessments have failed to properly represent the appropriate water chemistries. They believe that water composition is important and that vadose zone water ought to be the basis for the water chemistry, rather than well water as presently assumed. The state representatives presented no evidence concerning the effect of different water chemistries on the overall performance of the repository.

- Two members of the expert panel shared their views about temperature effects on the performance of the repository. They pointed out that exceeding certain temperature thresholds can lead to the activation of specific corrosion processes in the presence of some environments. They have concerns that those conditions exist in the temperature regime of the current design and such temperature data have not been adequately employed in the assessments. For example, DOE's calculations of high- and low-temperature repository designs showed essentially no difference between the two in terms of the dose calculations. Using the TPA, the NRC staff should be able to conduct an independent analysis of different repository temperature profiles to verify the effect on the dose calculations.

- Another participant posed a question, "Do the models simulate all the processes that are major sources of uncertainty?" The large margins of safety in the current dose calculations accommodate considerable uncertainty, but only if the uncertainties are properly represented. Primary sources of uncertainty associated with the near-field are the specific chemical environment of the corrosion models and key parameters and assumptions in the source term calculation. Examples of important parameters and assumptions are temperature, chemical form and phase, humidity, and solubilities, including in-package chemistry effects on those solubilities. Work is in progress by both DOE and the NRC staff to quantify the important uncertainties, and it appears that they are making considerable progress.

- Other participants challenged the realism of some of the source term modeling. Each successive performance assessment has made progress toward making the models more realistic with respect to both conservative and nonconservative assumptions. Areas of improvement have included the climate process model, treatment of coupled effects (thermal, hydrological, and chemical), use of more realistic solubilities for important radionuclides, treatment of thermal effects, and chemical environment of the drip shield and waste package. A specific example of addressing nonconservatism has been a more realistic representation of the amount of water accessing the near-field. As a result, the infiltration rates in the current models are considerably higher than in the early models. An example of increased conservatism is the radionuclide release model of the DOE TSPA with respect to the assumption of a fully water-saturated environment inside the waste package in the absence of dripping water. Recognizing these inconsistent assumptions and basing the calculations more on the supporting evidence has resulted in the performance assessments moving in the direction of greatly improved realism.

- The WGS provided the opportunity to challenge the NRC staff on their progress toward a capability to perform a comprehensive review of the complex TSPA expected in DOE's license application. The staff did an outstanding job of demonstrating that they are well-positioned for that effort. They recognize that their role is to review the TSPA, rather than simply performing independent analyses, and they manifest that recognition in the way in which they have specialized their performance assessment code. The staff's ongoing investigations of important contributors to the performance of the proposed Yucca Mountain repository are creative and insightful. The Committee strongly recommends that they continue this work.

A more detailed discussion of the WGS follows.

Principal Technical Issues

The principal technical issues discussed during the WGS included the chemical environments for initiating and sustaining corrosion, the temperature at which those environments occur, and the uncertainties and realism associated with the corrosion and radionuclide mobilization and transport models in the near-field. The representatives from the State of Nevada focused primarily on the chemical environment, while two members of the five-member panel emphasized the temperature issue and several participants, including the Committee, contributed to the discussion concerning model uncertainties.

Chemical Environment

Some WGS participants, primarily the representatives from the State of Nevada, were skeptical that sufficient data exist to exclude extreme corrosive environments for the drip shield and waste package. They believe that there is a need for additional data on water chemistries before they can be convinced that extreme environments cannot exist. They consider water composition to be a major chemical environmental factor and expressed concern at the project's use of well water, rather than vadose (unsaturated) zone water. The Committee has not seen evidence that such changes in water chemistry will lead to changes in the dose calculations of sufficient magnitude to represent a significant compliance issue, but we will follow this issue as the performance assessments evolve.

Temperature Effects

Temperature is an environmental parameter, but it is often discussed as a specific issue because of its high profile in the performance assessment debate. The Nuclear Waste Technical Review Board (NWTRB) has raised this issue for some time and panel members from that Board (participating as individuals, not as representatives of the Board) introduced the topic into the WGS. Their specific concern is that exceeding certain temperature thresholds can lead to the activation of specific corrosion processes in some environments. In particular, they do not believe that the corrosion models are based on realistic temperature data. DOE has analyzed so-called hot and cold temperature profiles in supplemental performance assessment work, but the results did not show any significant difference in the safety performance of the repository. If the phenomena are properly captured, however, differences may arise in both the results and their uncertainties; this will require careful review. The ACNW has not reviewed the details of these differences to form an opinion concerning the effect they may have on the dose calculations. The safety margins of the calculations that DOE has performed are such that it would be surprising if these differences threatened compliance with the dose standard. We are confident that the NRC staff has the capability to determine the sensitivity of the dose calculations to different temperature profiles.

Uncertainties in the Analyses

Uncertainties in the source term parameters were extensively discussed during the WGS. The uncertainties include water composition, because of how it affects the mineral phases inside the waste package, the solubility limits for some of the radionuclides involved, and the details of the corrosion process. The primary parameter and phenomena uncertainties are temperature, chemical form and phase, humidity, and solubilities, including in-package chemistry effects on those solubilities. How much water exists in thin films for diffusive transport or in droplets by advective flow continues to be an issue in the respective DOE/NRC performance assessment models.

DOE's TSPA model treats the release of radionuclides from the engineered barrier system (the source term) by both diffusion and advection from "cracks" associated with stress-corrosion cracking and general corrosion "patches." The NRC's TPA model treats releases from the waste package as being primarily driven by advection, rather than by diffusion. While the models differ, some of the WGS panel members expressed the opinion that the DOE and NRC models have identified most of the relevant processes.

The issues are the rationale for the differences in the details of the corrosion and release mechanisms more than the results obtained. How important are source term uncertainties? The importance of these uncertainties is diminished if (1) they are adequately quantified and (2) in the presence of the uncertainties, there is still a reasonable safety margin in terms of meeting the radiation dose standard. DOE and the NRC staff are currently involved in work to quantify the important uncertainties.

For calculated doses within the first 10,000 years following closure of the repository, uncertainties continue to exist with regard to the assumptions made in the performance assessments about early failures of waste packages as a result of manufacturing flaws. The flaws of greatest interest are improper heat treatment of waste package lid welds. Assumptions about such flaws and the uncertainties therein account for the appearance of a calculated dose in the most recent versions of the TSPA model for the first 10,000 years. The calculated doses are extremely small. The issue discussed at the WGS was the lack of supporting evidence for the calculations of manufacturing flaws and the fact that such flaws could be the most significant cause of early failures of the waste packages.

NRC Staff Readiness

One of the clear benefits of the WGS was that it gave all those in attendance, including the Committee, a chance to see how the NRC staff is progressing in their capability to review a very complex performance assessment. In general, the Committee was very impressed with the staff's progress. We are confident that the necessary technical tools and staff will be in place to perform a competent review when DOE submits its license application (LA). Other factors that contribute to our confidence are (1) the NRC staff's experience base (~25 years) in developing and performing performance assessments (2) specialization of the tools, especially the TPA code, to assess the LA performance assessment, and (3) a capability to map the results of the DOE performance assessment into the NRC's key technical issues.

The centerpiece of the staff's analytical tools is the TPA code. The Committee has followed the TPA work since its inception and has urged the staff to risk inform the code as much as practicable, including the ability to quantify uncertainties. We have especially encouraged the staff to develop the ability to rank the importance of contributors to repository performance, including the contribution of individual barriers. While much of the importance-ranking capability is not yet automated, the offline use of the code to make such assessments is impressive. One advantage of the TPA code is that its development and application involve very few individuals and organizational entities. By comparison, DOE does not have such a simple computational management structure, and must rely on many different contributions from several different contractors with their ability to make the proper linkages. The TPA code should be a powerful tool for challenging the completeness of the TSPA in terms of its scope and the degree to which it is fully integrated.

Realism of the Performance Assessment Models

DOE and the NRC staff are making progress toward more realistic performance assessment models. The three scenarios to consider in the TSPA are (1) nominal performance, (2) disruptive events, and (3) a stylized human intrusion scenario that is specified by regulation. Examples of improvements in the realism of the TSPA models include the climate process model, treatment of coupled effects (thermal, hydrological, chemical), use of more realistic solubilities for important radionuclides, accounting for retardation of selected radionuclides, treatment of igneous events, and the uncertainty analysis of selected contributors to risk.

The progress in the TPA code is illustrated by its ability to account for uncertainties including variability of system attributes, the treatment of thermal effects for calculating temperatures at critical locations such as the drift wall and the waste package surface, and improvements in the ability to model groundwater flow and the near-field chemical environment. To assist in reviewing DOE's TSPA, the next version of the TPA code will incorporate a diffusion model—a release mechanism that figures prominently in DOE's TSPA model. The staff is also considering evaluating cladding protection of the fuel in the next version of the TPA code.

The Committee continues to question the realism of the release model in DOE's TSPA. Much of the skepticism centers on the assumptions about the in-package environment and the supporting data. For example, the TSPA assumes that the waste package is fully saturated, even in the absence of any dripping water, and the analysis includes calculating the cladding and waste reaction rates and chemical concentrations for these conditions. The conditions may be bounding in terms of the source term, but the evidence does not support the need for such an extreme model for mobilizing the waste. We continue to question the extent to which diffusive transport is the basis for radionuclides to exit the waste package. We also need to better understand the effect of different mineral phases on the mobilization of the waste. This issue was discussed at length during the WGS. Again, it is not so much a concern that the dose standard cannot be met, as it is a matter of having a realistic baseline for the level of risk involved.

As previously noted, there are other barriers to complete realism in the models such as the somewhat prescriptive human intrusion model and the biosphere dose model. The result is the possible masking of either conservative or nonconservative contributors to risk. The degree of this masking is difficult to assess at this time, but it is a possibility the Committee will follow.

Of the various activities concerning realism, the Committee strongly supports backtracking from the final results of the performance assessment, where few radionuclides dominate the performance, into the internals of the model. As discussed in previous letters to the Commission, the Committee believes this approach will enable the staff to ferret out the contributing factors and the basis for their respective contributions. The NRC staff is doing just that with their own TPA model and the insights are extremely valuable in exposing what is really important. In fact, they have taken the concept further by seeking answers regarding why other radionuclides do not contribute to the risk. Some of the important insights are the effect of different engineered and natural barriers, the impact of modeling assumptions, and the importance ranking of contributors to performance. As we have in other reports to the Commission, we strongly recommend that this work continue.

Other Points of Discussion

In addition to the key points regarding technical issues, staff readiness, and realism, two other important observations arose from the WGS. One involved the debate over whether Yucca Mountain is a research project or an engineering project. This debate centered on the meaning of "reasonable expectation." Some participants expressed the opinion that given that it is a first-of-a-kind project, it requires a far greater depth of scientific activity than other large-scale projects. Other participants argued that the evidence does not support that view, noting that the analyses performed so far, which many WGS participants consider very conservative, have indicated a trivial safety issue in comparison to other risk issues facing our society. This debate turned out to be an excellent illustration of the value of uncertainty analysis in determining the "adequate" amount of scientific investigation. The Committee has always advocated that the best way to know how much additional scientific work is needed is to quantify the uncertainties of the important contributors to risk. If the contributors, with all of their uncertainties, make little difference to the bottom-line risk measure, there is evidence that further work is not necessary. This is a primary benefit of risk-informing the analyses.

Finally, in terms of model structure, the participants expressed strong support for staging performance assessment models along the lines of modules that represent "pinch points," that is, structuring the model according to inputs and outputs of specific stages that facilitate the transparency of the total system. Such a structure permits a detailed examination of the initial conditions of the model, and also identifies the boundary conditions for the different stages. Such discretization better portrays the dynamics of the repository. Also, a staged structure allows clear exposition of the assumptions made on critical parameters as material moves through the repository region. Both DOE and the NRC have incorporated relevant modules in their models, but the interfaces between the modules lack definition in terms of specific inputs and outputs in a pinch point sense.

Summary

This outstanding WGS met the goals to (1) better understand the principal issues of performance assessment that might affect the licensing process, (2) review the readiness of the NRC staff to evaluate a total system performance assessment, and (3) assess the level of realism in the modeling of the repository. The WGS provided an excellent forum in which to exchange views on the technical issues associated with the performance assessment process and the particular issues surrounding the definition of the source term for the proposed Yucca Mountain repository.

Sincerely,

/R/

George M. Hornberger
Chairman

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3. KEYNOTE PRESENTATION

Realism in Simulating Long-Term Waste Package Corrosion and Radionuclide Source Term

Presentation by Dr. Joe H. Payer
Case Western Reserve University
Cleveland, OH
March 25, 2003

[Note the slide numbers refer to slides from Dr. Payer's presentation]

My goal is to give an overview starting with relevant conditions at Yucca Mountain. (Slide 1) I think it's worthwhile to note some unique and important conditions at Yucca Mountain. We do a lot of testing in beakers, fully immersed, because that is the way to do those tests. We do a lot of short-term testing, even when we test for a number of years and try to apply that to 10,000 years. Another important message is when we talk about a corrosion process or an alteration product of spent fuel, we tend to use whatever the experimental or modeling information we have to determine the kinetics or the rate of reaction that is going on under these conditions. Then, we can intuitively, or by mistake, predict what will happen over 10,000 years or 100,000 years. I think it is important to recognize what conditions are relevant to the repository at 500 years, or at 5,000 years, or at 50,000 years because the conditions change over that period. Some processes will rise in importance with time, while others will decrease.

As John Garrick mentioned in the introduction, I come from a materials science background. I did my thesis work at Ohio State University in the area of corrosion and electrochemistry. Basically, I have spent my career in the field of corrosion, materials selection, failure analysis, and determining how materials behave. This is the bias I bring to this presentation. Having said that, my primary expertise has been on the types of processes that will penetrate the package, for example, the corrosion processes. What I will say about the performance of the waste form and radionuclide release processes is based on having sat through many sessions like this listening to Rod Ewing and others who have worked very closely in this field. I am trying to capture what they say. So Rod Ewing certainly will have an opportunity to put the right spin on it if I miss the perspective here.

Yucca Mountain Perspective: Background and Conditions

<u>Background</u>

We are going to talk about the conditions at Yucca Mountain just to provide some background and perspective. (Slide 2) Then I will present the three important aspects of the source term. John, I agree very much with the way you try to modularize this overall process. It is important to know the overall outcome of these things. But I think we need competence and to strive for understanding at each of the modules. The three modules I would like to talk to you about are (1) What is the composition of the water that's on the metal surfaces and waste package barrier layers? (2) What is the composition of the water entering the waste packages? and (3) What happens to the water once it is in the package and released from the waste package? We are going to spend time here talking about the composition of water. Corrosion is clearly the primary determiner of waste package delay time for radionuclide transport from the waste package. It is the most likely and the most probable degradation process that will determine when packages get penetrations, and what the form and distribution of those penetrations will be. I want to talk about the waste form degradation and radionuclide mobilization, and I think that gets to the essence of the source term.

So let me say a little bit about the Yucca Mountain conditions. (Slide 3) Start at the top level. What do we want a repository to do? (Slide 4) There are two things we are interested in here. First and foremost, we would like to completely isolate the radionuclides in the waste. Secondly, when they are released, we would like to retard egress of radionuclides from penetrated packages.

One of the things that makes this very difficult is to identify the relevant failure modes and possible penetrations of waste packages. What are the different degradation modes (e.g., stress corrosion, mechanical damage, embrittlement) that could cause penetrations? When will they occur, what is the likelihood that they will occur, and what would they look like? That is at the core of what materials scientists do in this field, that is, in the topic of degradation process and assessment of materials performance.

What is special about Yucca Mountain is the extremely long time frame of interest. (Slide 5) We are interested in regulatory periods of 10,000 years, but that is not enough. People are asking what happens even at much longer times than that. But again, to reiterate a point I made in the introduction, I think it is important to consider the conditions and analyze what is going on in the waste package at different time frames, from 50 to 100,000 years. These could be time frames of interest.

Why is localized corrosion a major issue for waste packages in a Yucca Mountain repository? (Slide 6) Several groups have looked at this since the very early days and it has been revalidated and revisited. Long-lived waste packages are essential for long-term isolation. Localized corrosion processes (i.e., pitting, crevice corrosion, stress-corrosion cracking) are the most likely degradation modes that can occur in these environments with the materials that are being selected. So basing materials selection and design on high crevice corrosion resistance is a prudent and well-accepted way to proceed. It makes sense.

The general issues in corrosion science and engineering and materials science in electrochemistry are well developed—we know a lot about localized corrosion processes. We understand the breakdown of passive films in many ways. These are not new concepts to us. Having said that, corrosion science is advancing. We understand more about these all the time, and there is a very solid scientific base for these concepts. The challenge is to apply this understanding of corrosion science to the conditions that occur at Yucca Mountain. The rate of damage due to corrosion will depend on two things. First, it will depend upon the corrosion resistance of the material (i.e., the strength of the material to resist corrosion damage). Second, it will depend on the environment to which it will be exposed. If you ask how corrosive are the conditions at Yucca Mountain, you've got to think about the material in that environment. How corrosive is it to a ceramic, to a nickel-chrome alloy, to a titanium alloy, to carbon steel? If you ask how corrosion resistant is titanium, Alloy 22, carbon steel, or fiberglass, the question is under what conditions? And for any material, there are environments where it will act more like Alka Seltzer than a structural material. It will certainly be attacked in these long time frames. So the question is, how do you define where those environments are and how do you determine the materials' corrosion resistance in those environments? What you're striving for is to select a material for waste packages that is resistant to corrosion for a very long time in the environments that will occur in a Yucca Mountain repository.

What do we want to know about the environment? (Slide 7) We want to know the temperature and the time of wetness. It is well accepted that dry metals, without the presence of an aqueous phase, are not going to corrode at an appreciable rate in this environment. So for dry environments, we do not have to worry about corrosion. However, when we say time of wetness, we don't have to fully immerse the metal in a water. We don't have to put the waste package in a swimming pool. If there is a condensed layer of several monolayers of water, that amount of moisture can be sufficient to promote corrosion. I lived in Houston in 1983 and there was a thin layer of moisture on everything all the time. That is sufficient moisture, or a sufficient aqueous environment, to support electrochemical dissolution. Anodes, cathodes, and the electrochemical corrosion cell can operate in that very thin moisture layer.

The pH of the environment is a very important property for the stability of passive films, the corrosion rate, and so forth. The oxidizing and reducing power of the environment, which we refer to as the Eh, is the oxidizing potential of the environment. We go from very reducing environments, that do not have a great propensity to take materials into solution, to highly oxidizing environments. Oxygen is one oxidizing material, but there are other oxidants. Ferric ions, cupric ions, and others will increase the oxidizing power.

There are detrimental species for the stability of passive films. High on the list are chloride ions, reduced sulfur species, and other ionic materials in the environment that can affect the stability and corrosion resistance. There are some beneficial species that will make the stability of the passive films more likely, and these include nitrates and silicates. The other important thing to consider is that in almost all cases we are dealing with aqueous solutions—wet environments that have multiple species in them. Seldom will the environment contain only sulphate or chloride. We are dealing with chloride, plus nitrate, plus sulfates, plus this long menu of other materials. This is important because it can change the behavior of passive films.

The ambient waters at Yucca Mountain are essentially innocuous. (Slide 8) We are talking about neutral sodium bicarbonate waters with very low amounts, parts per million, of dissolved solids and mixed salts. There are a number of anions, cations, and salts that are available, but they are at quite dilute concentrations. It is an aerated environment. The mountain is open to air and so it is oxygenated. There is a higher partial pressure of carbon dioxide in the atmosphere than in air at ground level. That is the ambient condition out there. Those environments, both the gas and the liquid phase, are changed during the thermal period by evaporation and concentration. So if you start with a very low concentration of salts, and you evaporate the water, it becomes more and more concentrated. One of the real challenges here is to determine what solution is obtained as the dilute solutions become more and more concentrated.

The modulations of these waters (and I am going to talk about waters in a general sense, i.e., the environment and water) that can occur on the metal surface, or when that thin film of water or droplets of water are in contact with the waste form, can be very significant. I would say they overwhelm the changes that can occur out in the rock. There are changes that can occur in hot rock and exchange of this sort, but when that water sits on a metal surface, if corrosion starts, that environment can be modulated much more. Certainly, the corrosion products and the interaction of the electrochemical reactions can modulate water sitting on the waste form much more.

For the waste form mobilization, we are discussing primarily the behavior of the uranium oxide matrix of the spent fuel. (Slide 9) It's very important whether the spent fuel matrix is exposed to oxidizing or reducing conditions. Under reducing conditions, the dissolution rate, the corrosion rate, of the uranium matrix, is quite low. But under oxidizing conditions, the rates are much higher. Therefore, it is important to consider the local oxidizing potential.

The composition and amounts of water going into a waste package, and changes caused by contact with the waste form and its alteration products, are important. There may be droplets of water and thin films of water. The amount of water is limited, and the water composition will undergo significant water composition changes due to the corrosion and the oxidation and reduction processes, the precipitation of salts and minerals, and the dissolution of salts and minerals. The interaction with the degraded waste form produces many alteration products and corrosion products. I will show a table later. In addition, there are other materials inside the waste packages. We have got a significant amount of steel. We've got some aluminum and some zirconium cladding. There are other materials that are all going to be potentially reacting in this stew that we are boiling up. Interactions with the invert and the drift support materials need to be considered. The key to this whole thing is that the water composition tells us what processes occur and what the transport processes into and from the waste package are.

An earlier repository design concept called for a very hot repository where the entire area would be heated (intentionally) to fairly high temperatures, and the packages would be dry for long periods of time. Designers are also considering a low temperature repository. The idea in this design is to never exceed boiling at the drift wall; therefore, you will not get any dry rock around the drifts. One of the things to keep in mind is that the design has evolved over a number of years. (Slides 10–11) It will continue to evolve. A design needs to be specified for a license application, and that specific design will be evaluated. But it is unrealistic to think that the design will be constant. I have picked these numbers at random, but the 100th package, the 1,000th package, the 10,000th package, I can guarantee are not going to look like package number 1. Because a design evolves, we are talking about a period of many years. The performance can get better, the confidence can get better, and the waste packages can become less expensive, if the performance can be justified along the way.

The natural system out there is a series of layers of geologic formations. (Slide 12) The repository is placed at about 300 meters below the rock. It is about another 300 meters to the saturated water table. The importance of that is that the repository sits in an unsaturated zone. It is porous rock, and the porosity is only partially filled with water. The repository is at atmospheric pressure which is an important consideration. There are no processes by which we can go to 10 atmospheres of over pressure or more as you could if you were inside a metal package or an impermeable barrier and generating gases.

The water flow through this mountain is the critical issue. (Slide 13) The climatology and the amount of infiltration will determine how much water comes down through the unsaturated zone above the repository. At the repository level, that water can react and interact with waste package materials and drift materials. That will eventually determine the penetration of the waste packages. The water inside the waste packages, after it goes through the cladding, or if there are clad failures, will come in contact with the spent fuel. This is where the radionuclide mobilization release starts. There can be interactions of waters at that location, and the waters can move out and through the invert material and on down to the saturated zone.

And so water is very important. You ask why we spend so much time thinking about water. Water is the first material or instrument by which we're going to penetrate the packages. It is going to be the material or the instrument by which we mobilize and release radionuclides, and it is going to be the medium, the instrument by which those radionuclides move into the rock and down to the water table. Almost all the slides I have shown here have been taken from DOE project reports because they have much better figures than I can draw. I want to acknowledge those sources which are from publicly available documents.

I want to bring home another fact. We are talking about corrosion and degradation and radionuclide mobilization on a wide range of scales. (Slide 14) Sometimes we are talking about mountain scale, where the measurement of interest is tens or hundreds of meters. Other times, at the drift scale, we are talking about processes and phenomena that go on over centimeter to meter scales. We can go all the way down to discuss the stability of passive films or the development of very thin layers on spent fuel that are measured in nanometers or micrometers.

Conditions at Yucca Mountain

Consider the various parts of the engineered barriers, including the steel invert support and various types of waste packages that hold spent fuel rods from pressurized-water reactors. (Slides 15 and 16) There is other spent fuel from boiling-water reactors. Titanium drip shields will apparently be placed over the waste packages. It is the integrity of these, and the release of radionuclides within these, that are of interest. We are also talking about a waste package that has an outer layer of a highly corrosion resistant material. Alloy 22, a nickel-chrome molybdenum alloy, is highly corrosion resistant in a wide range of environments, but any material will corrode in very aggressive environments. The trick is, where's the boundary? The inner layer gives structural integrity and structural strength. This material is a 316 stainless steel. The fuel rods are inside the waste package canisters. There are a lot of materials—more than we have discussed here. The package will be back flushed and filled with helium when it is put in place. There is steel, zirconium cladding, and spent fuel in this structure. We must consider how these materials will interact with the waters that enter the structure.

There are various types of waste form. (Slide 15-16) There is commercial spent fuel. There's material from other sources. These will be put in similar packages, not identical, but similar packages. That defines the inventory, or the menu of materials that goes into waste packages. Then, by fission and reaction processes, and radioactive decay, we will get a whole series of materials of interest. (Slide 17) These are the radionuclides of interest that we are trying to control and hold back. They go from the fission products, things like cesium and iodine, to all of the actinide and lanthanide series. The half-lives of several of these materials are measured in 1,000, 10,000 years–very long times. Some of them drop off in a matter of years; some in hundreds of years. Others are going to be around for tens of thousands and hundreds of thousands of years.

When we talk about "source term" we are talking about the source of radionuclides. But it might be interesting to remind ourselves that the spent fuel is the thermal source term, as well. (Slide 18) We start with heat that is generated at the fuel pellet and fuel bundle area. That heat is then transferred to the waste package surfaces, and the waste package transfers heat to the drift wall. That heats the rock and water locally around the drift. You can then follow this to the mountain scale. The heat from the spent fuel transfers to the waste package, and then goes to the drift wall in the rock. There are design and operational factors that can control heat flow and resulting temperature profiles (e.g., the drift spacing, the package spacing, and the size and geometry of the packages). What is their diameter and length? What type of fuel do you put in them, and how much do you load in the packages? So there is some control of this thermal source term. Consider some modeling examples. If you have got a hot package here, you can get a dry out zone where the rock is heated above the boiling point. You push the water back. At some point, you get back to an ambient, basically saturated moisture level of 100 percent relative humidity. For a cool package, you would not have any complete dry out zone. That is a controllable thing.

Now we look at temperatures from the mountain-scale modeling over a time scale of 500 to 2000 years. (Slide 19) For the areas above the boiling point of water, the dry out zone is localized around 5 to 10 meters from the repository drifts. You heat the repository up above and below the drifts, and a thermal cycle is observed that goes out and then comes back after thousands or tens of thousands of years. In looking at the response for the hot cycle, when the repository is closed, ventilation stops, and the waste package surface heats up, perhaps to as much 160 to 180°. (Slide 20) Over a long period, it cools down. If you go to a lower temperature operation, with a ventilation period of 300 years to keep the packages cool, you also build up heat, but here it is controlled so it does not heat above the boiling point. Then you get a long slow cool down. The temperature profiles depend on the type and location of the waste package.

If you look at the relative humidity as a function of time, what is the amount of moisture that's in the atmosphere around the waste packages? (Slide 21) In the high temperature mode, during the ventilation, the water is driven away from the waste packages. Then, as the cooling occurs, the relative humidity continues to increase, and eventually after tens of thousands or a hundred thousand years, you come back to ambient temperatures and 100 percent relative humidity. Well, why is that important? People would suggest that if the relative humidity is below 20 percent or so, the packages are dry. There is no moisture. You do not have this thin film of moisture on the metal surfaces, and corrosion processes do not occur. Then, as the relative humidity rises, there will be a relative humidity level at which moisture forms. Observations show that around 20 or 30 percent, and on up to 60 percent, depending on the condition of the surface, it may be dry or it may be wet. If there are deliquescent salts on that surface, moisture will form sooner. Without those salts, the surface will remain dry. So we are in an area where it may be dry or may be wet, and we need more information.

Most folks would suggest that if we were up around 70 to 80 percent relative humidity, that the surface, even with just some particles of an inert dust material, would form a condensed layer. Therefore, over this time period, we can know and we can gather information about when it is dry, when it gets wet, and what type of moisture forms on the metal surfaces.

For a high temperature-operating mode (Slide 22), the outer surface of the waste packages would be at 120° C around 500 years. After a thousand years, the surfaces would cool to 100°, after 3000 years to 80°, and after 10,000 years to 60°. The temperature returns to ambient after very long times. The lower temperature curves shown never get above the 100 to 120° range. They are at about 80° at closure for about 1000 years; then at 5000 years they are at 60°. (Slide 22) So again, it is important to keep in mind what the temperature and relative humidity are various times.

I would suggest that the emphasis from an engineering standpoint certainly is the first several thousand years. We've got to be very confident that waste packages will perform well over that time period. Longer periods are still quite important, but the conditions start becoming more benign. The radiation fields drop as the fuel degrades, temperature drops, and the corrosion conditions become less aggressive.

There are a lot of chemistry and thermal-coupled processes that are going on when you put hot packages into this mountain. (Slide 23) If we get the boiling zone, we get dry-out periods; there is condensation and interaction with the water and the rock. I again would point out the combination of chemical processes and electrochemical processes that can occur at the package level.

In the DOE performance assessment model, there are aspects that deal with water contacting the waste package (Slide 24) and there are aspects that deal with the waste package lifetime. There are aspects that work with the release from the waste packages, as well as the radionuclide concentrations as they move out toward the biosphere. So there are pieces of this model and, as John Garrick showed earlier in his presentation, there are modules that are appropriate for looking at these various levels.

Looking at models for the source term, one of the big issues is water. (Slide 25) Water is the accessor. It is what will cause the penetrations by the corrosion that will allow water to get access to the fuel. Water is the mobilizer due to chemistry and access and mobilization within the package. Water is the mobilizer for getting through the cladding and penetrations in the waste package and the cladding to the fuel to mobilize radionuclides. Water is also the transporter, that is, the primary medium for transport. I think we need apply realism throughout these issues.

What are some of the characteristics of a source term. (Slide 26) Composition of these waters is critical. When will the penetrations occur? What are those penetrations going to look like? How many? Where are they? What is the distribution? How much water will enter the package through those penetrations? What will be the waste form alteration products? How are we going to mobilize these? What is the interaction of the radionuclides with corrosion products, waste form alteration products, and invert materials and how are they transported away from the waste packages and emplacement drifts? You can come up with your list, but some place somebody has to talk about our understanding of these processes.

Water Contacting Waste Packages

Earlier in this talk, two crucial issues were identified—the realistic range of environments at Yucca Mountain and the realistic range of materials susceptibility, (i.e., the corrosion resistance of Alloy 22 and titanium). (Slide 27) In order for localized corrosion to occur, there must be an intersection of these two fields (Slide 28). You are looking for where and how large that level of overlap is. What is the likelihood of overlap? What is going to occur in that area of overlap? In an ideal world you would have no overlap at all. You would like to separate these fields so that for realistic environments you'd see no damage because there would be no intersection with the field of susceptibility for the metal. If there is an overlap of fields, it does not mean that damage necessarily need occur. In order for damage to occur, there has to be water at that time and place. The water has to remain in the "damaging range" while the degradation is occurring. In other words, there has to be corrosive water, and the water must have a composition in the corrosive range of environments. The material has to be susceptible to corrosion in these waters. Further, those conditions have to persist. If it is an on again/off again situation, then the damaging conditions must persist for a cumulative time that is long enough to result in a penetration.

We are interested in water on the package (Slide 29), water on the waste form, water coming off of the waste form, and water coming from the waste package. The water is going to be in a couple of different forms, including condensation of moist layers and dust layers on surfaces, and drippage and seepage into the drift from the environment. We have a science base for understanding and predicting behavior in these types of materials. One of the useful treatments in the water chemistry issue is to take a dilute solution and predict, as you concentrate the solution, as you drive the water out of that solution, what are you going to have left in the beaker? What will be left in the drop on the waste package surface or the thin film? The chemical divide concept for water composition evolution is widely used and applies to these considerations. (Slide 30) What it says is you start with a dilute mixture and you reach several chemical divides. Depending upon the relative amount of calcium versus carbonate species in the dilute water, if there is an excess of calcium, you will go one path. You then go through several divides. If you've got excess carbonate and lower amounts of calcium, you will go another path.

There are ways to deal with water chemistry, geochemistry, and solution chemistry that will tell you what types of brines will evolve. There is a logic and procedure for dealing with the evolution of concentrated waters (brines) from dilute solutions. Let's discuss the issue of deliquescence of various salts that are on the surface. (Slide 31) On a plot of relative humidity versus temperature, at some point, you would get an aqueous phase forming if you had sodium nitrate crystals sitting on the package or if you had sodium chloride on the package or if you had magnesium chloride sitting on the surface. At what relative humidity would you start to form moisture? There is a data set that is available to help us look at these phenomena. One of the important aspects is mixtures of salts–such as sodium chloride and sodium nitrate. Mixtures of those salts can have a lower deliquescence point than any of the pure substances. (Slide 31) So again, we have got to come back and remind ourselves of what's going on when we have multiple constituents.

Silica, SiO_2, is readily available at Yucca Mountain. At high pH, silica is very soluble, and some solubility is observed even at lower pHs. (Slide 31) The amount of silica in solution, in parts per million, varies with temperature. When we have got a crevice material where there is a restricted geometry, a solution could get back in there. Due to the chemical and electrochemical processes back in the crevice, the solution that is in the crevice or underneath a deposit can become significantly different in composition than the bulk environment. (Slide 31) In addition, there can be buildup of species in the crevice. It can become more acidic. There are many processes that are fairly well understood that occur underneath deposits or in metal-to-metal contact.

Corrosion: The Primary Determinant of Waste Package Lifetime

(Slide 32) The natural water composition in Yucca Mountain is the major source of water and ionic species and dissolved minerals. (Slide 33) It is the aqueous environment on the metal surfaces and on the spent fuel that is of primary interest to us. The waste packages will not be fully immersed in water. The full immersion of the metal surfaces is highly unlikely. The two likely conditions are condensed water from the air and water seeping and dripping on to those metal surfaces, causing deposits to form on the metal surfaces. But it is unlikely that we will see fully immersed conditions.

Nickel-based alloys and titanium are the primary materials of construction in which we are interested. These materials have excellent corrosion resistance. (Slide 34) However, they are susceptible to corrosion in extremely aggressive environments. The question is, Do those environments have a chance of occurring over reasonable amounts of time at Yucca Mountain? Two of the major considerations are fabrication processes and welding. How the packages are fabricated, as well as the temperature, can have a significant effect on these materials.

Temperatures are kept low during the ventilation period and prior to closure. When the repository is closed, the temperatures rise and there is a long slow cooldown period. (Slide 35) If there is backfill, temperatures will get quite hot. If you ventilate for longer periods of time, up to 300 years for example, and then close, you can keep the package surfaces at lower temperatures. Important performance factors are waste package temperature, the form and composition of the water, and the interaction with the cladding and internal temperature.

Consider a series of nickel-chrome molybdenum alloys–these are all in the same environment after a given corrosion test. (Slide 36) The materials that are less corrosion resistant can undergo very significant attack. Notice it is localized attack; the dark spots are pits into the metal surface. The more corrosion resistant materials in these experiments, Alloy 22, Alloy C-4, and titanium, basically show no attack at all. The difference between the Alloy 22 behavior and the Alloy 825 behavior is that the Alloy 22 has more chrome, more nickel, and more molybdenum. It has a more stable passive film.

We know a lot about the chemistry and treatment of localized corrosion processes, and corrosion science provides a basis for understanding these behaviors. We can measure the polarization behavior, and the potential versus log current of these processes to obtain various polarization curves that give us a rationale to determine the corrosion resistance of the material. (Slide 36) We can compare the corrosion potential to the potential at and above which damage occurs, and we can determine the expected corrosion behavior. The rationale is if this corrosion potential never gets more positive than the potential at which damage occurs, we could then expect long-term passive behavior.

That is in terms of potential. Potential is not the easiest thing to measure on an operating waste package. One of the things that would be easier to measure would be temperature, and there are temperature analogs to those critical potentials. (Slide 37) We can determine the temperature at which aqueous corrosion occurs, and we can determine the temperature at which crevice corrosion occurs. If the temperature for moisture formation is below the temperature at which crevice corrosion occurs, there is no corrosion, and thus, there is no vulnerability.

If the temperature of aqueous corrosion is greater than the temperature at which crevice corrosion could occur, then that temperature difference defines a range of vulnerability. It doesn't mean that corrosion will occur in there, but corrosion could occur. The important qualifier of this is that these temperatures are sensitive to the environment. As the environment changes, the critical temperatures change. If you have the temperature ranges of vulnerability, you could go back to plots of temperature versus time and you could determine periods of vulnerability for the waste packages.

Regarding passive film formation, we are talking about very thin films. (Slide 38) These films are measured in nanometers. If the films remain stable and if the passivity persists, then it is very likely that the packages could last longer than 10,000 years without any penetration. That is the trick. Why would they break down? They are going to break down primarily because of chemical attack. We have laboratory methods to measure the composition, structure, and so forth of those films.

Stress-corrosion cracking is an issue, because stress-corrosion cracking is a potential failure mode. (Slide 39) In the presence of a mechanical (tensile stress) and a corrosive environment (a particular environment), you can get very rapid failure. This phenomenon has been dealt with empirically. You load up specimens and see if they fail or not. There is theory behind why stress corrosion occurs. The theory for stress-corrosion cracking is an evolutionary thing in corrosion science. But there is a basis to understand these processes. One of the primary ways of controlling stress-corrosion cracking is to use treatments that will put compressive stresses on the surface of the material. Welds are of particular interest for these phenomena, and important factors for stress-corrosion cracking are the residual stresses that might occur around welds and composition of the corrosive environment.

We know some things about long-term stabilities of alloys. (Slide 40) The challenge is to determine the very long-time aging as a function of temperature. An approach is to take information at 400°, 500°C and higher, and project that over long times at lower temperatures.

The design and fabrication processes are also crucial. (Slide 41) There are lots of design details and just how the waste packages and other structures are fabricated and put together can greatly affect durability and performance. There are lots of structural details around the drift, including what materials are used and how they are used. Those things can have significant effects. For example, for the materials of construction, what is the metallurgy of those materials, and what is the residual stress of those materials? Again, when we are looking at waste package components, the welds are critical items.

Some of the special aspects of waste packages include their exposure to one long, slow cycle. (Slides 42–43) There are no moving parts. It is a static exposure. We do not have cyclic loads. The heat fluxes are low, and waste packages would be dry in a higher temperature mode. Materials give off heat and radiation that decrease with time. Radiation effects, after a few hundred years, on the package surfaces are not important. Thermal effects at the repository level diminish after several thousands and tens of thousands of years.

Waste Form Degradation and Radionuclide Mobilization

(Slide 44) Once you get a penetration in a waste package, depending on where it is and whether there is seepage and dripping water that can impact it, the question is, How is the penetrated package going to behave? There are two different ways of dealing with this. You can either accept that you are going to have penetrations at the top, or wherever the penetration is, knowing that the water will start to fill the package which will act like a bathtub. (Slide 45) The alternative concept is to have a package that has a penetration at the top and a penetration in the bottom. This would allow the moisture to move through and out of the system. If you cannot get advective transport, then diffusion processes will control the transport. The movement of moisture in and the movement of materials through penetrations, and the movement of radionuclides, which are of primary interest, are all going to happen by diffusive processes as opposed to advective flow processes.

Consider the fuel bundle. (Slide 46) For the zirconium fuel rods, if there is a fracture in a rod, the moisture can go through that fracture and access the spent fuel. If it accesses the spent fuel, it can then start breaking down, dissolving that fuel, and mobilizing the radionuclides which can then move back out through those packages.

There is a science to understanding those processes. (Slide 47) It is an area of continued corrosion research; in this case, it is dissolution-type study. Consider the grains within the fuel and the fuel cladding. The grains are a couple microns to tens of microns in diameter. The question is, What happens when moisture comes through and contacts the spent fuel? Anything like the cesium that would be built up in the gap between cladding and fuel would essentially become mobilized right away, in a very short time.

Materials that were on the surface of the fuel grains or in the grain boundaries, if the moisture had access to them, would mobilize very quickly. The radionuclides that are incorporated within the structure, within the matrix, or bound within these particles, could be retarded and could be held back, that is, they could be slowed down in their release. So we would like to know about the dissolution processes. Under oxidizing conditions, the dissolution can be very high; under reducing conditions, the dissolution is not very high. (Slide 48) We understand these chemical interactions; the challenge is to apply this understanding to the conditions relevant to the spent fuel at Yucca Mountain.

The pH in the environment and the oxygen content are critical for the corrosion rate. (Slide 48) Radiation levels vary over time. Radiolysis products can be important here. After 100 years or so, the gamma and beta radiation have fallen off dramatically. Those radiolysis effects are critical early on but less important later. There is a pH effect on the dissolution—the corrosion rate of the spent fuel grains. Under reducing conditions they are fairly stable, and they would provide a significant retardation to radionuclide release. Under oxidizing conditions, they dissolve; they corrode much more rapidly, releasing radionuclides. These processes are fairly well understood. We can use thermodynamic calculations to look at the stability of the various films. Important factors here are oxidizing versus reducing conditions. We can measure that as an Eh or describe it as an Eh, and the acidity/alkalinity of the environment is very important. I refer you to an excellent review article by David Shoesmith, as well as an article by Burns, Ewing, and Miller. Rod Ewing is sitting here on this panel.

There is some complex mineralogy to describe the waste form. (Slide 49) There are lots of different phases that can form when we have silicates and uranites and various other materials. We understand some of these materials and structures at the atomic level, and so we can use crystal chemistry to predict the various tetrahedra and how they will be put together to get some of these sheet-type or interlocked-type products. In addition, thermodynamics provides an excellent basis for what phases will be stable in various chemistries. Where is the uranium dioxide stable? Where is uranophane, and so forth, stable? Important factors here are the crystal chemistry, chemical analysis, and thermodynamics. We are interested in how the fission products and actinides might be incorporated and held within these types of materials in an alteration product.

Consider a transport mechanism for radionuclides. (Slide 50–52) With colloids forming and the radionuclides sorbing or desorbing from these products, the colloids may provide a mechanism by which radionuclides can be carried on and transported. How do the radionuclides interact with the degraded fuel and the alteration products from that fuel? How do the radionuclides interact with the corrosion products, the iron oxides that are developed, and other corrosion waste package and internal materials? How do they interact with the dripping water and influence what is being transported in the water? If radionuclides are sorbed on the colloids and move through the fracture, how will those radionuclides being transported interact with the matrix, or will they stay in the fractures and move?

Closing Remarks

(Slide 53) Let me finish by saying that the goal of looking at the repository performance from the perspective of the source term is useful. I would suggest that there be a set of models that capture reality. What that means is that the models recognize the important processes and the dependencies of those processes. Further, the models capture reality in terms of the conditions that pertain to Yucca Mountain.

If you go back to the modules that we might want to consider, what do we know about the water contacting waste packages? How is that captured in these performance models? What's the waste package lifetime, the types of penetrations, and the form of penetrations? What is the release or the incorporation of radionuclides from the waste form? Finally, how do the radionuclides mobilize and transport?

Thank you very much.

Realism in Simulating Long-Term Waste Package Corrosion and Radionuclide Source Term

Presented by
Dr. Joe H. Payer
Case Western Reserve University

Presented to
Advisory Committee on Nuclear Waste
140th ACNW Meeting
March 25, 2003
Rockville, MD

Slide 1

Outline

- Yucca Mountain Conditions
    - Background and Perspective
- Composition of Waters
    - Contacting Waste Package and Entering Waste Packages
- Corrosion
    - The Primary Determinant of Waste Package Lifetime
- Waste Form Degradation and Radionuclide Mobilization
    - The Source Term

Slide 2

Yucca Mountain Conditions: Background and Perspective

Slide 3

140th ACNW Meeting March 25, 2003

Realism in Long Term Corrosion and Source Term; J.H. Payer

Perspective on Proposed Yucca Mountain Repository

- A geologic repository for the disposal of high-level radioactive waste and spent nuclear fuel
- Containment strategy for the disposal site is twofold
  - First and foremost, complete isolation of the waste
  - Subsequent retardation of the egress of radionuclides from the penetrated waste package

Slide 4

Repository Conditions: Overview of Time, Temperature, Environment

A particular challenge for the analysis is the extraordinarily long time period required for performance.

> **Operational phase of 50 years for emplacement of waste packages.**
> **Monitoring phase out to 300 years.**
> **Closure phase when the repository is closed. Regulatory period of 10,000 years. Projected performance to 100,000 yrs and more.**

In the analysis, it is important to consider not only the conditions that could initiate a process, but also the time period over which those conditions persist.

Consider conditions at 50, 500, 1000, 3000, 10,000, 50,000, 100,000

Slide 5

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Localized Corrosion: Waste Package Materials and Water Chemistry Determine Performance

- **Long-lived Waste Packages** (WP) are essential for long-term isolation of radionuclides
- **Localized corrosion** is the greatest, realistic threat to WP performance, i.e. pitting, crevice corrosion and stress corrosion cracking
- **Materials selection and design** based on crevice corrosion resistance is prudent and sound engineering
- **General key issues and processes** are reasonably well understood in corrosion science and technology
- **Corrosion Performance at Yucca Mountain** is under active study and can benefit from further experiments and analysis

Slide 6

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Waters on and in Waste Packages: Important water chemistry and properties

- Temperature & Time-of-Wetness
- Acidity-alkalinity (pH)
- Oxidizing-reducing (Eh)
  e.g. oxygen, ferric ion
- Detrimental ionic species, e.g. chloride, reduced sulfur
- Beneficial species, e.g. nitrate, silicate
- Complexing species

- Important to consider the ***mixed species*** effects and not species in isolation

Slide 7

Ambient waters innocuous for waste package corrosion

- Neutral, sodium bicarbonate water with low dissolved solids and mixed salts
  - (ppm): Si-30, Na-50, Ca-10, K-5, Mg-2, Li-0.1, Fe-0.1
  - (ppm): HCO_3^- 150, $SO_4^=$ 20, NO_3^- 10, Cl^- 8, F^- 2
- Aerated and higher P_{CO2} than atmospheric
- Modulation processes during thermal period are evaporation, concentration, dissolution/precipitation of solids

- *Modulations to waters on metal and waste form surfaces are likely greater than those outside of drift*

Slide 8

Waste Form Degradation and Radionuclide Mobilization

- Oxidizing or reducing (Eh) is major effect for UO_2 corrosion
- Amount of waters and composition: into, in, and from
- Alteration of Spent Fuel and Incorporation Mechanisms
- Interaction with degraded waste form; alteration products; and corrosion products (internals and waste package)
- Interactions with invert and drift support
- Transport processes: into, in, and from

Slide 9

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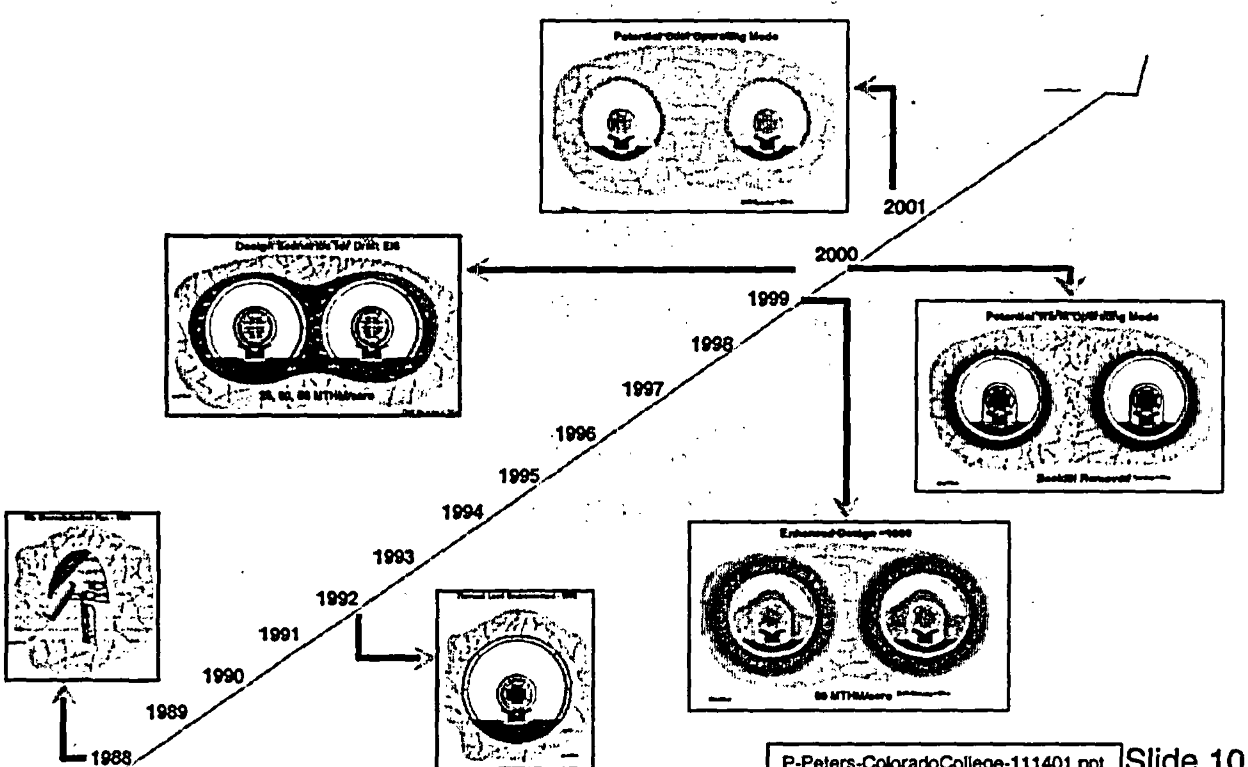
Evolution of Repository and Waste Package Design and Operating Mode



P-Peters-ColoradoCollege-111401.ppt Slide 10

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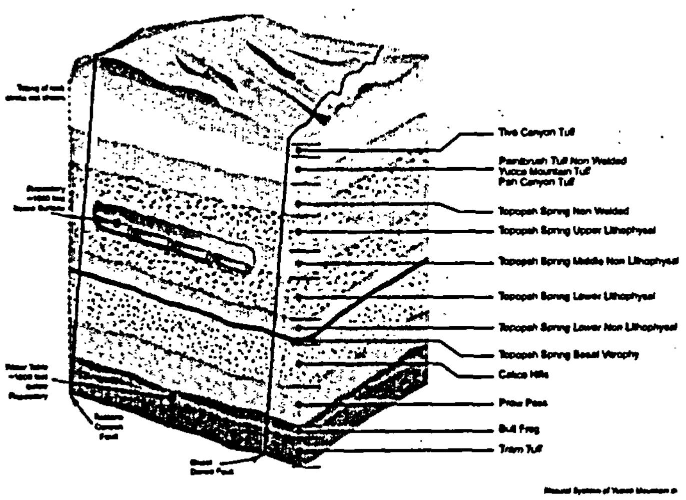
Evolution of Repository Design

- Design has evolved over last 15-20 years
- Will continue to evolve
  - Initial design must be safe, suitable and reasonable
  - Unrealistic to think that waste package #108, #1017 or #10,054 will be same as #1.
  - Better performance, more confidence, less expensive

Slide 11

Natural System of Yucca Mountain



__Important Factors__

Repository in Unsaturated Zone

- Porous Rock
- Pores partially filled with water

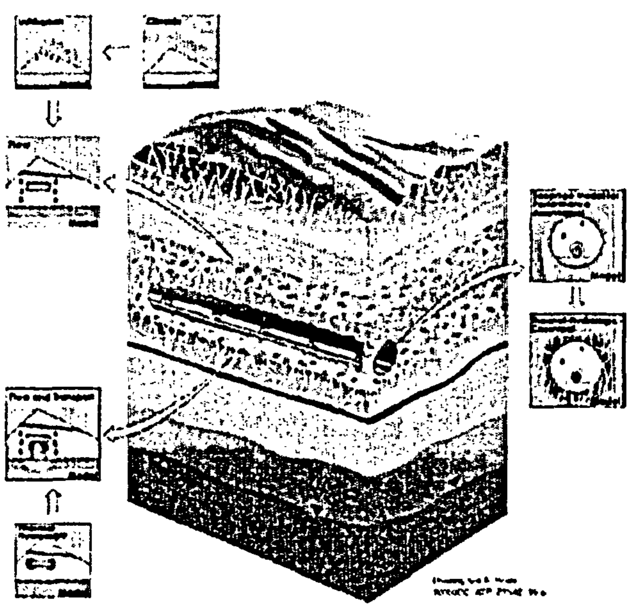
Atmospheric pressure

High Relative Humidity

Ambient waters are dilute and near neutral

Slide 12

Water Flow through Yucca Mountain



Important Factors

Limited amount of water enters soil (mm's/year)

Water movement through fractures and matrix (pores)

Limited and variable seepage and drips into drifts

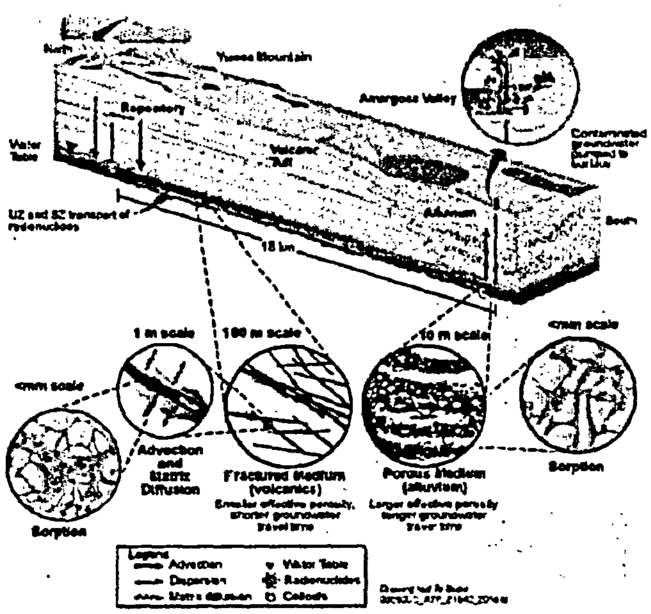
Transport into, in and from waste packages is crucial

Large thermal effects

Episodic flow behavior

Slide 13

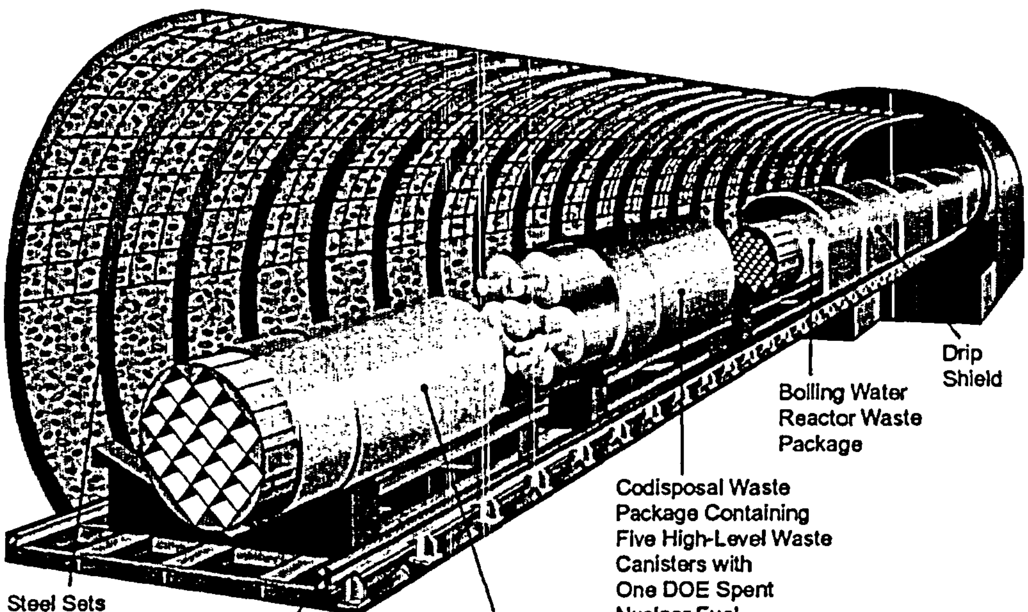
Processes Occur on Many Scales



- Mountain scale (macro)
  - 10's – 100's meter
- Drift scale (meso)
  - cm – meter
- Particles and Droplets (micro)
  - μm-mm
- Films and molecules (nano)
  - nm-μm

Slide 14

Cutaway of a Drift with Three Types of Waste Packages



Drawing Not to Scale
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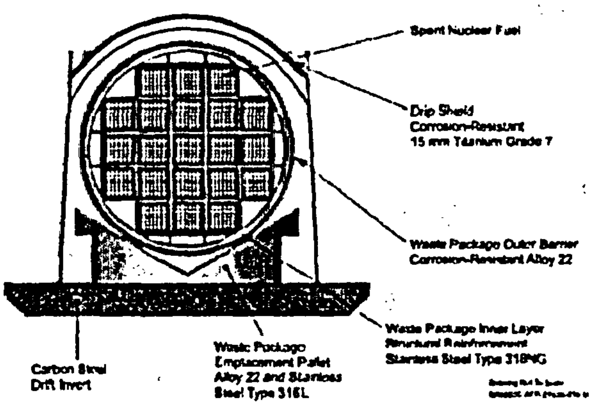

Figure 3-1. Cross-Sectional Illustration of an Alloy 22 and Stainless Steel Emplaced Dual-Metal Waste Package

The figure illustrates a waste package supported on an emplacement pallet and covered by a titanium drip shield, showing multiple engineered barriers that provide defense in depth. The use of engineered barriers of different materials protects against common mode failures.

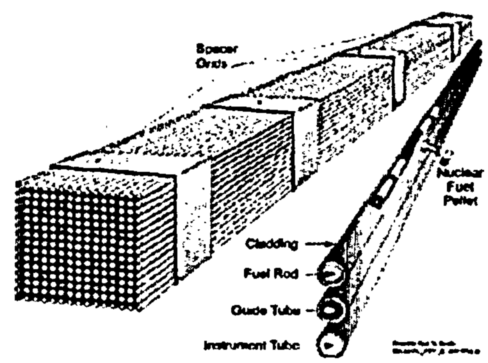

Table 3-8. Waste Package Design Component Materials

Component	Material
Dual-layer design Inner structural shell Outer corrosion-resistant barrier	 Stainless Steel Type 316NG Alloy 22 (SB 575 N06022)
WP fill gas	Helium
Fuel tubes for commercial SNF WP basket design	Carbon steel (SA 516 Grade 70)
Neutron absorber interlocking plates for commercial SNF WP	Neutronit A 978 (borated 316 stainless steel)
Interlocking plates for 21-PWR Control Rod design	Carbon steel (SA 516 Grade 70)
Structural guides for commercial SNF WP basket design	Carbon steel (SA 516 Grade 70)
Canister guides for 5-DHLW/DOE SNF designs	Carbon steel (SA 516 Grade 70)
Thermal shunts for commercial SNF WP basket design	Aluminum plate (SB 209 6061 T4)

NOTES: SNF = spent nuclear fuel, WP = waste package

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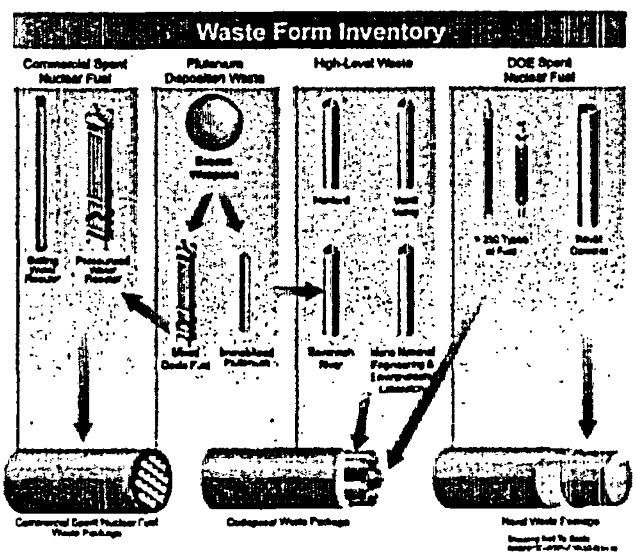
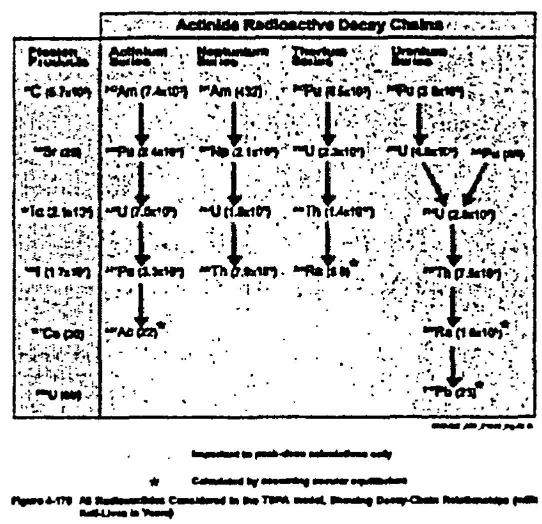
Waste Forms and Radionuclides





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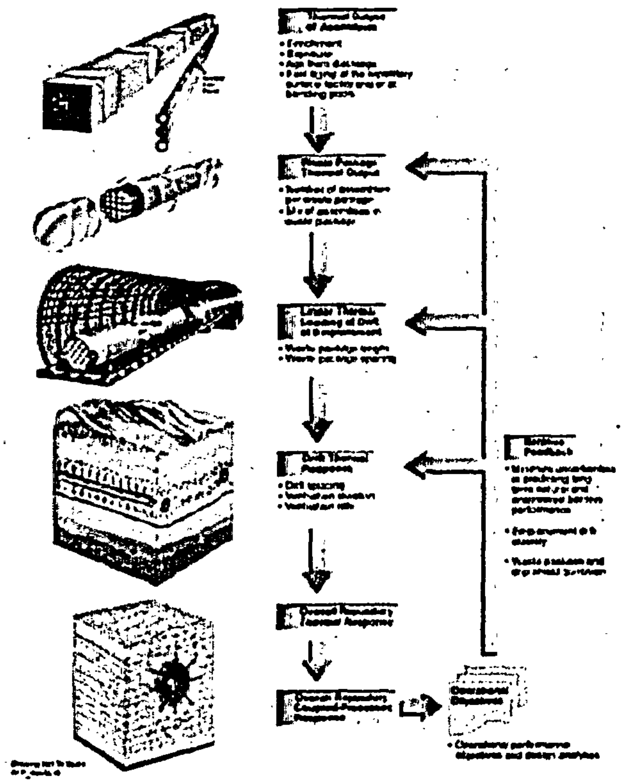
Source Term: Thermal Performance of Repository



- Heat from spent fuel
- Heat transfer within and from waste package
- Heat transfer to drift walls and into rock

Design and Operation Factors

- Drift spacing
- Package spacing
- Package size/length
- Fuel type and age
- Package loading
- Ventilation

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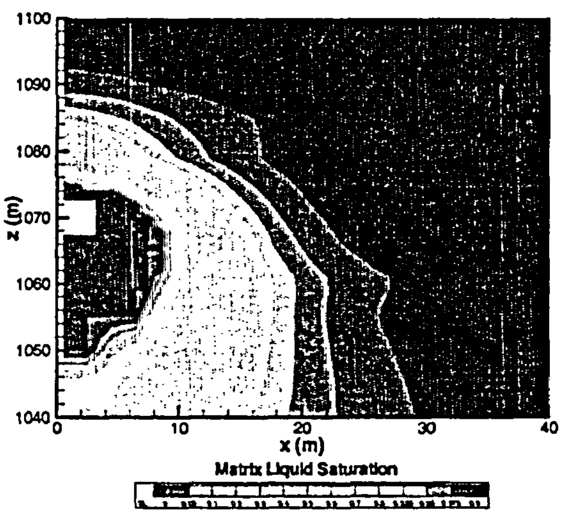
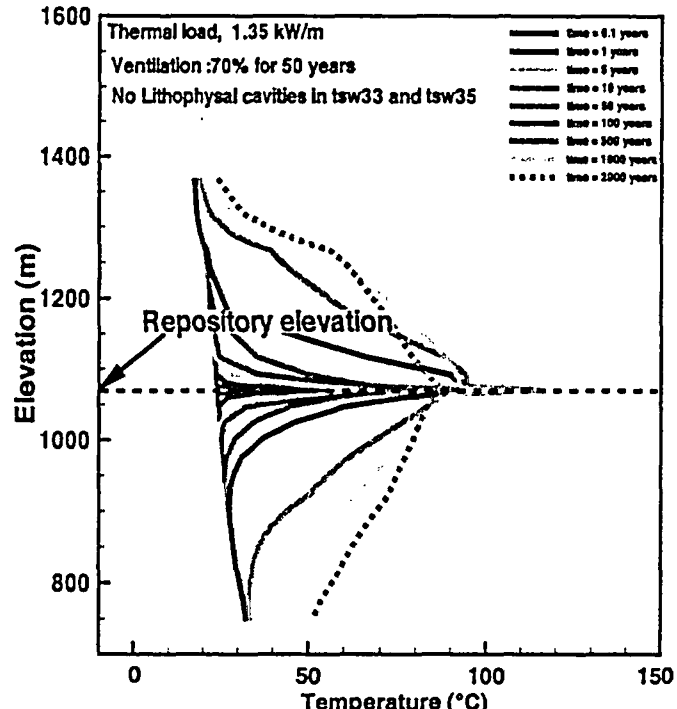
Dry Condition around Hot Waste Packages





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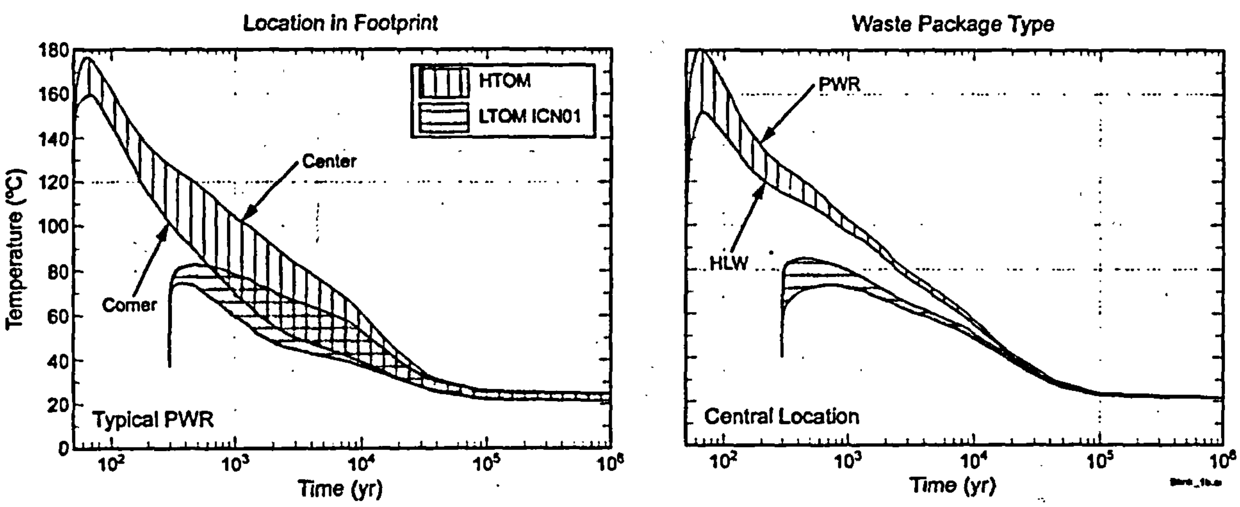
Example Thermal Load Time Profiles



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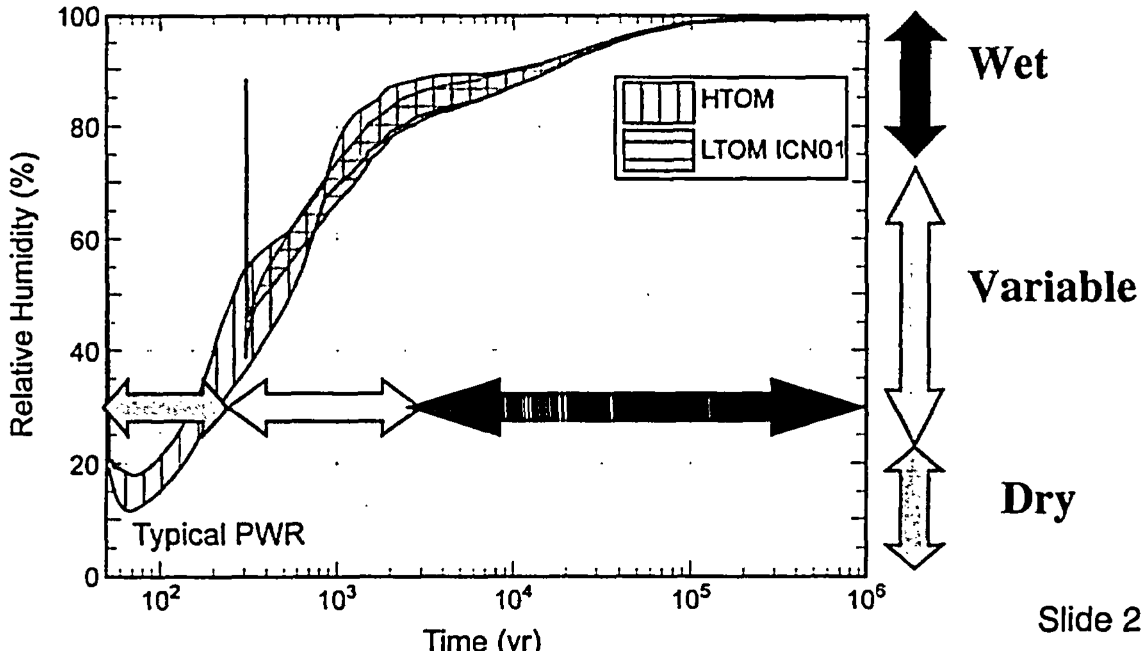
Example of Equilibrium Humidity and Its Connection to Moisture on Surfaces



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Repository Conditions: Time-Temperature-Relative Humidity

Waste Package Temp, °C	Higher Temp Conditions	Lower Temp Conditions
120 C	At 500 yrs	Not applicable
100 C	At 1000 yrs	Not applicable
80 C	At 3000 yrs	At closure to 1000 yrs
60 C	At 10,000 yrs	At 5000 yrs
40 C	At 25,000 yrs	At 25,000 yrs
Ambient (~25 C)	At 100,000 yrs	At 100,000 yrs

- **Crucial to get the first several hundred to one thousand years correct, that is have high confidence that the waste packages are durable for this time period.**
- **Conditions become more benign during this period: gamma radiation level drops, temperature decreased**
- **Likelihood of localized corrosion and stress corrosion cracking decrease, and the uniform corrosion rates decrease.**

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Thermal-Hydrological-Chemical Processes

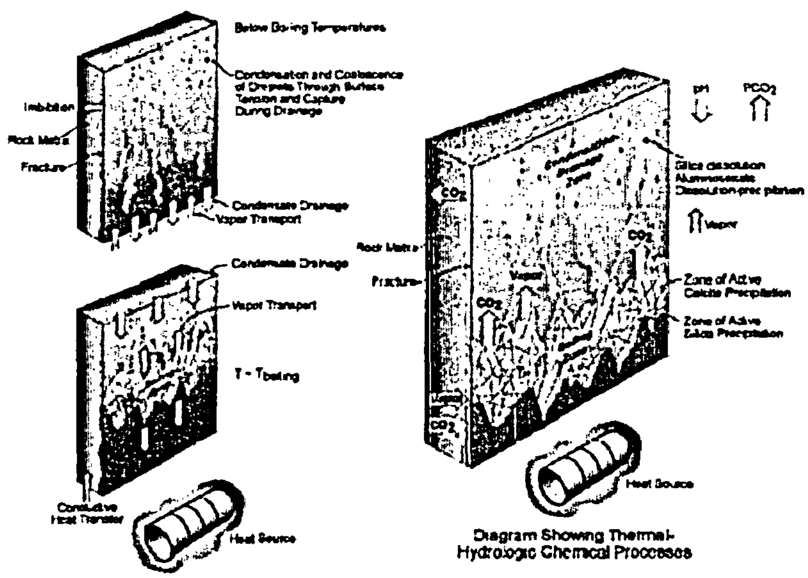

Diagram Showing Thermal Hydrologic Processes

Figure 4-40. Schematic Diagram Showing Relation between Thermal-Hydrologic Processes and Geochemical Processes

Source: CRWMS M&O 2000c, Figure 3.10-2.

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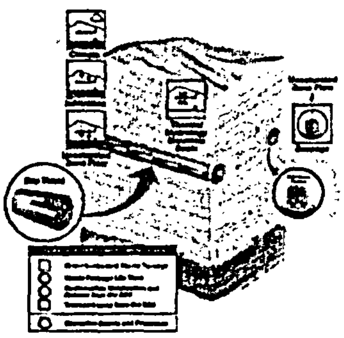
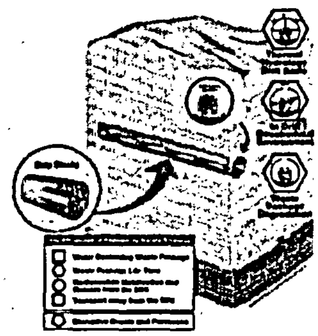
Sequence of Events (*from TSPA Model Components*)

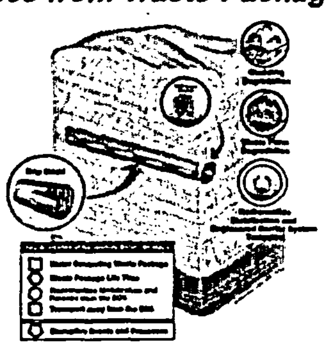
Water Contacting Waste Package



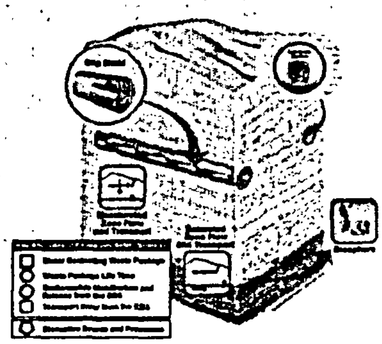
Waste Package Lifetime



Releases from Waste Package



Radionuclide Concentration in Groundwater



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Key Components of Models of Source Term

Water is the primary accesser, mobilizer and transporter

Waters on waste package surface (access)
- -when, how much, chemistry
- -determines corrosion behavior

Waters into waste package (access/mobilize)
- -when, how much, chemistry
- -form, frequency and distribution of penetrations

Waters in waste package (mobilize)
- -on clad, waste form and internals
- -determines radionuclide mobilization

Waters from waste package and drift (transport)
- -when, how much, chemistry
- -determines radionuclide transport

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Characteristics of Reality for Source Term

- Composition (corrosivity) of waters on waste package surface
- When penetrations of waste packages occur
- Form, number and distribution of any penetrations
- Amount of water entering packages through penetrations
- Waste form degradation and radionuclides mobilization
- Interaction (retardation) of radionuclides with corrosion products, waste form alterations, invert
- Transport of radionuclides from drift

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Water Contacting Waste Package and Entering Waste Packages

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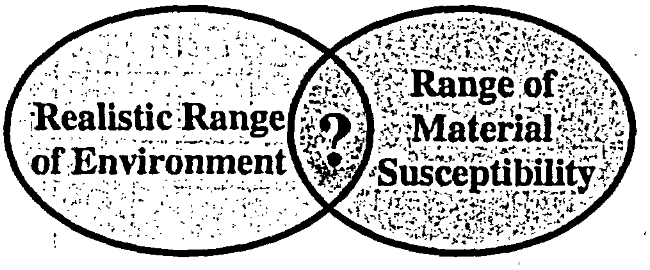
Necessary Conditions for Significant Corrosion to Occur on Waste Packages

- Water must contact WP
- Water must remain on WP
- Corrosive species must be present to form electrolyte
- Material must be susceptible to corrosion under these conditions
- Conditions must persist over sufficiently long time



After Kelly 3-25-2002

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Composition of Waters

Primary Controlling Factors

ON- Waste Package Surface

ON-Waste Form

From-Waste Package/Drift

Three Important Conditions

➢**Condensation leads to moist dust**

➢**Dripping seepage water forms mineral scale**

➢**Crevice areas entrap environments**

- **Ambient Waters:**
  Dilute solutions
  $Na-Ca-Mg-HCO_3-CO_3-Cl-NO_3-SO_4$
  pH 5.6-7.4
- **Waters can be concentrated**
  modified during movement
  thermal-chemical processes
- **Modifications on waste package and waste form**
  Can be greater effect than in rock
  Chemical and electrochemical processes

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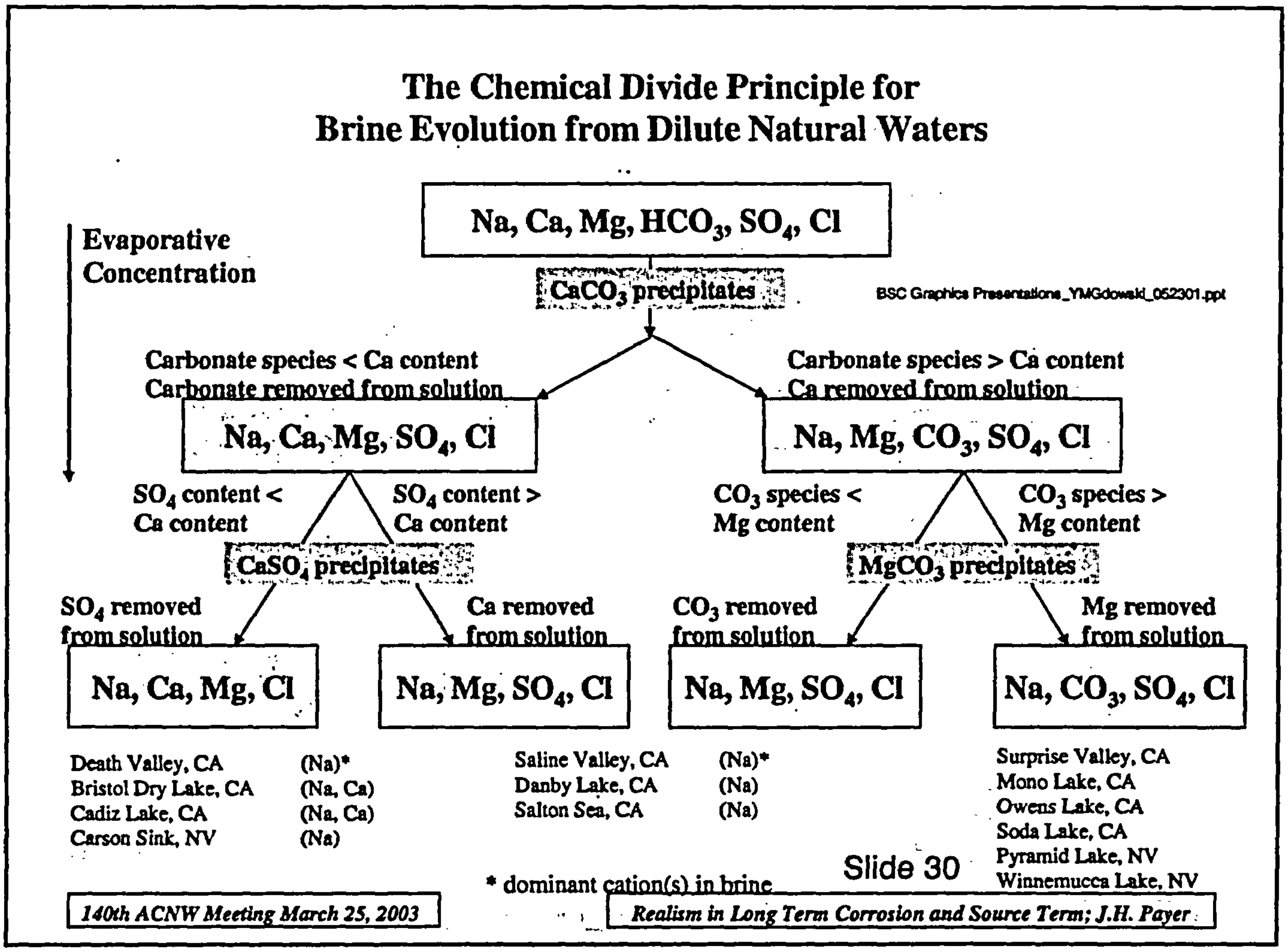
The Chemical Divide Principle for
Brine Evolution from Dilute Natural Waters
Evaporative Concentration
Na, Ca, Mg, HCO3, SO4, Cl
CaCO3 precipitates
BSC Graphics Presentations_YMGdowski_052301.ppt
Carbonate species < Ca content
Carbonate removed from solution
Carbonate species > Ca content
Ca removed from solution
Na, Ca, Mg, SO4, Cl
Na, Mg, CO3, SO4, Cl
SO4 content < Ca content
SO4 content > Ca content
CO3 species < Mg content
CO3 species > Mg content
CaSO4 precipitates
MgCO3 precipitates
SO4 removed from solution
Ca removed from solution
CO3 removed from solution
Mg removed from solution
Na, Ca, Mg, Cl
Na, Mg, SO4, Cl
Na, Mg, SO4, Cl
Na, CO3, SO4, Cl
Death Valley, CA (Na)*
Bristol Dry Lake, CA (Na, Ca)
Cadiz Lake, CA (Na, Ca)
Carson Sink, NV (Na)
Saline Valley, CA (Na)*
Danby Lake, CA (Na)
Salton Sea, CA (Na)
Surprise Valley, CA
Mono Lake, CA
Owens Lake, CA
Soda Lake, CA
Pyramid Lake, NV
Winnemucca Lake, NV
* dominant cation(s) in brine
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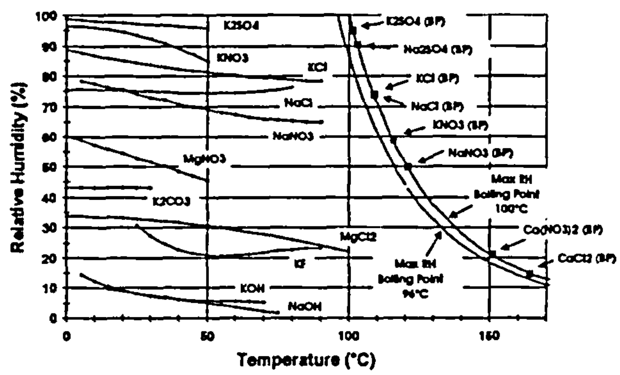
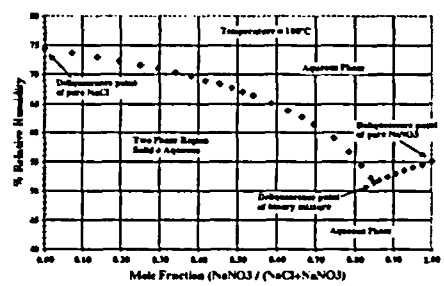
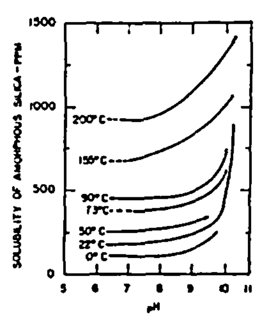
Deliquescence Points for Salts



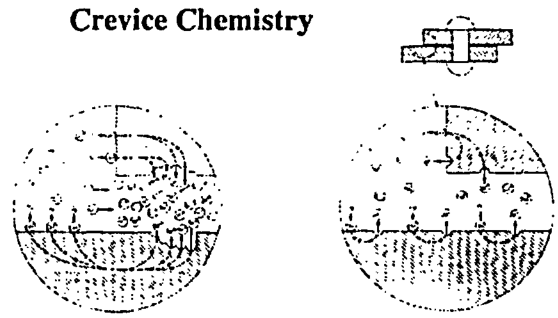
Phase Diagram for Mixture of NaCl + $NaNO_3$



Silica Solubility vs. pH



Crevice Chemistry



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Corrosion the Primary Determinant of Waste Package Lifetime

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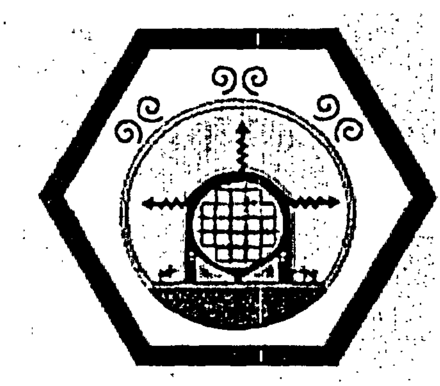
Waters at Yucca Mountain

Water composition in Yucca Mountain

- –naturally occurring
- –major source of water and ionic species

Aqueous environments on metal surfaces and on spent fuel

- –alteration of waters due to thermal and chemical conditions



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- Full immersion of metal surfaces highly unlikely condition
- Two sources of water:
  Condensation from the air
  Seepage from the rock

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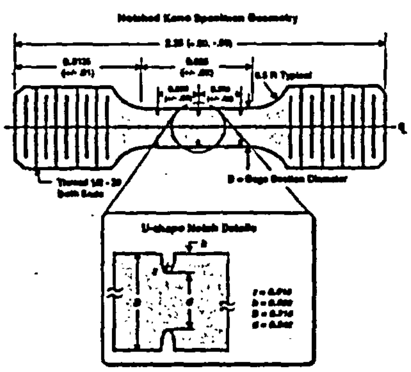
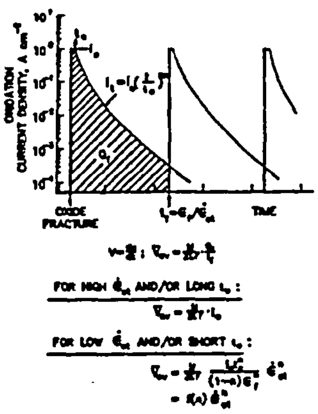
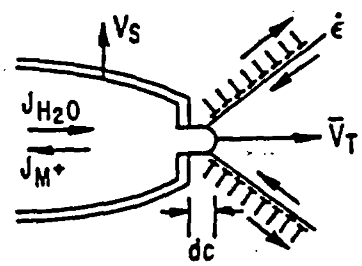
Stress Corrosion Cracking







Important Factors

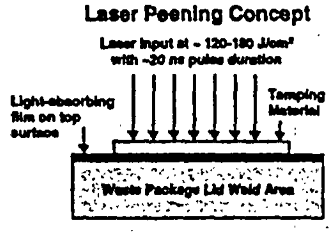
Residual stresses

Corrosive environment

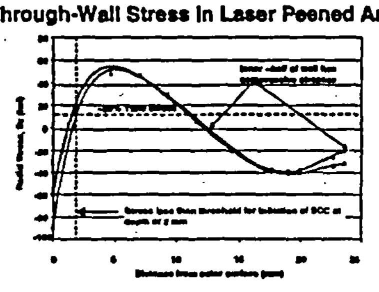
Alloy stability: aging

Welds of particular interest

Laser Peening Concept



Through-Wall Stress In Laser Peened Areas



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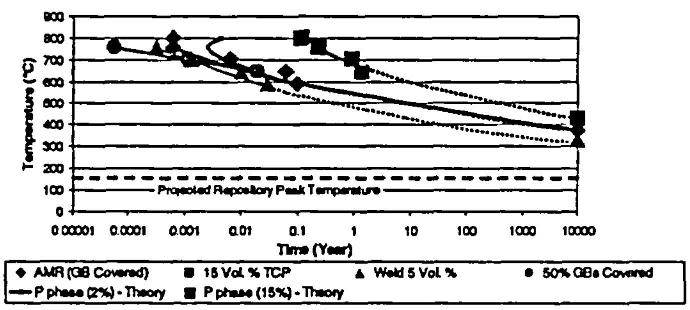
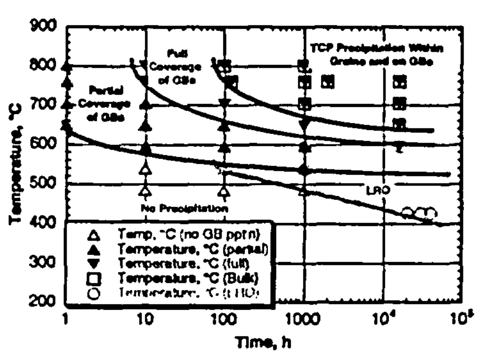
Long Term Stability of Alloys





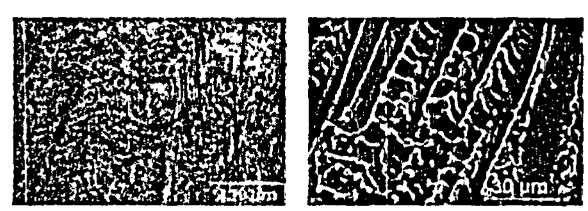
Important Factors

Aging and long range ordering can affect corrosion resistance

Time-temperature-composition

Bulk alloy and welds

As-welded Alloy 22 (Gas-Tungsten-Arc-Weld, GTAW)



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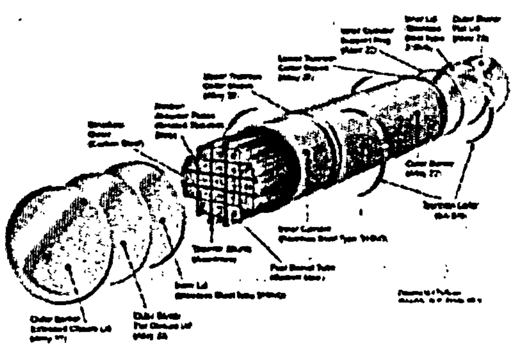
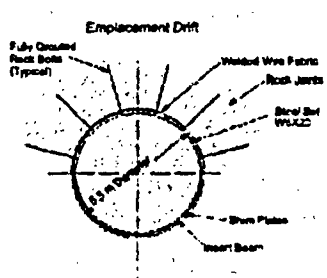
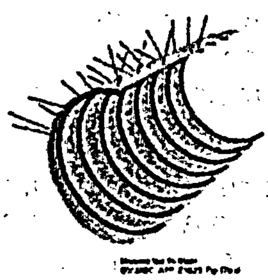
Design and Fabrication Processes

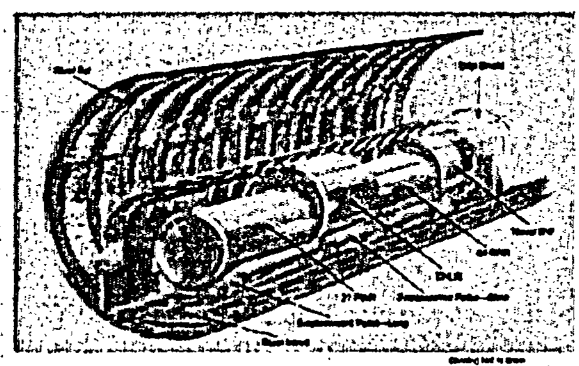


Some Important Factors

- Materials of construction
- Metallurgical structure
- Residual stresses
- Welds-Welds-Welds







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Corrosion: Long-Term Materials Performance

- Nickel-base Alloy 22 and Titanium Grade 7
  - Principal alloys of interest for waste package and drip shield
  - Excellent corrosion resistance over a wide range of aqueous solution compositions and temperatures
- Nickel-base Alloy 22 and titanium Grade 7 are extremely resistant to localized corrosion
  - Nevertheless, these alloys are susceptible to crevice corrosion under extreme conditions of environment and potential
  - It is necessary to perform experiments under conditions beyond those thought to be relevant to Yucca Mountain in order to examine the margins of corrosion resistance.
- Two major considerations
  - Fabrication processes, particularly welding, can have a major impact on corrosion resistance and performance
  - Temperature has major effects on the composition of the environment and the behavior of materials.

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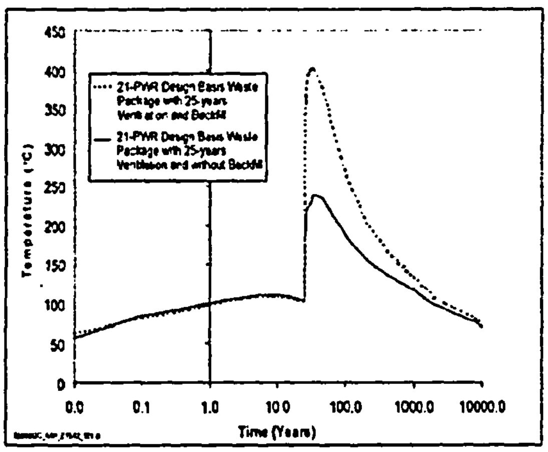
Repository Heat-up and Cool-down Cycle



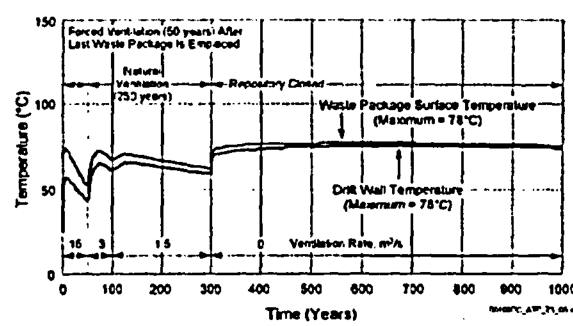
One long and slow thermal cycle

Rise in temperature at end of ventilation period

Long, slow cooling period

Important Performance Factors

- Waste package surface temperature
- Form and amount of water
- Clad and internal temperature



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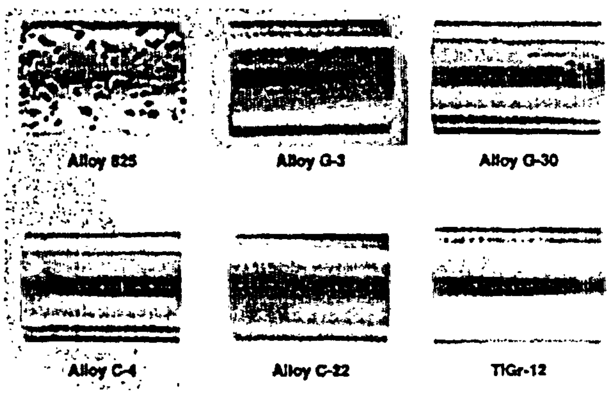
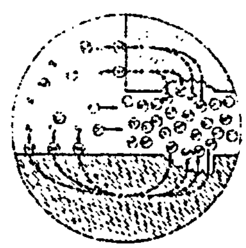
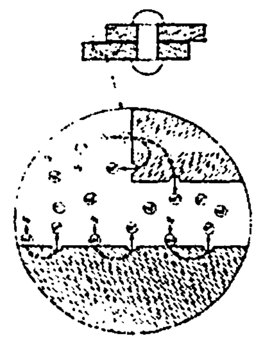
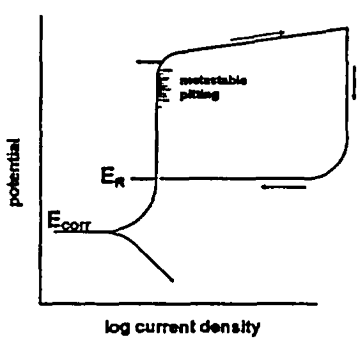
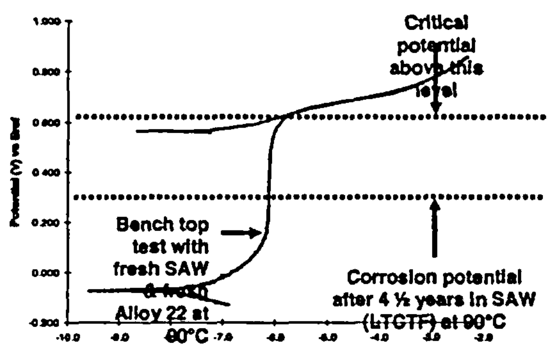
Localized Corrosion











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Vulnerable Temperature Range for Corrosion of Corrosion Resistant Metal (CRM)

Alternative perspective on crevice corrosion

CRM (C-22, Ti, ...) vulnerable to crevice corrosion

Vulnerable temp range, below which no crevice corrosion

$\Delta T_{VULN} = T_{AQS} - T_{CREV}$

T_{AQS}: highest temp for aqueous solution

Eqm boiling or droplet on hot surface

T_{CREV}: lowest temp to sustain crevice corrosion

For given alloy is function of pH, Eh, X^{-n}, Y^{+m},

Where $T_{AQS} < T_{CREV}$ $\Delta T_{VULN} = 0$

Where $T_{AQS} > T_{CREV}$ $\Delta T_{VULN} = T_{AQS} - T_{CREV}$

Vulnerable time: $\Delta t_{VULN} = t_{AQS} - t_{CREV}$

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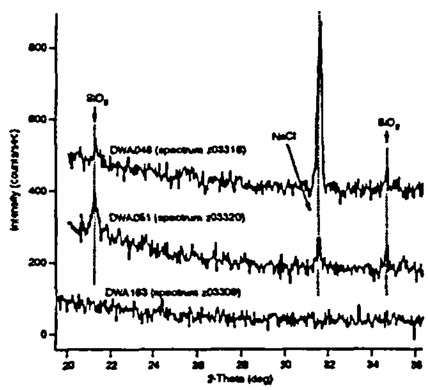
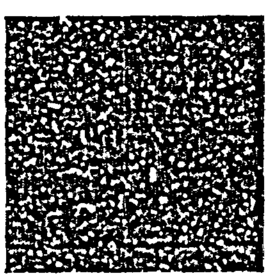
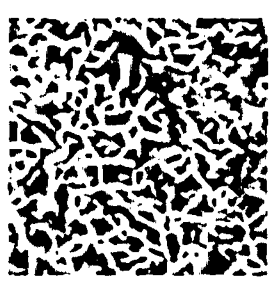
Passive Film: Formation and Stability







Important Factors

Stability of passive film is crucial to performance

Long lives (10,000's) of waste packages with stable films

Boundaries of performance defined by localized corrosion processes

Thin films (nm's) examined for composition and structure

Models for passivity current area of corrosion research

Slide 38

Repository Conditions: Relevant to Waste Packages

- Several important aspects of the long-term storage.
  - Waste packages are exposed to one, long and slow, temperature cycle.
  - No moving parts.
  - Static exposure does not subject the waste packages to potentially detrimental, cyclic loads.
  - Low heat fluxes and extremely slow heating and cooling do not expose the waste packages to large thermal gradients or rapid thermal expansion and contraction.
  - In a higher temperature operating mode, the waste packages are exposed to dry conditions for long times (several hundred years) before the surfaces are wetted.

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Repository Conditions: Relevant to Waste Packages

- The waste material gives off heat and radiation at rates that decrease with time.
  - Thermal effects diminish over several thousands of years
  - Radiation effects diminish over a few hundred years.
- At the repository level, the waste packages are isolated beneath 300 meters of rock and are a few hundred meters above the water table.
- The waste packages sit in air on support pallets.
  - Ambient air is saturated with water equivalent to 100% relative humidity.
  - While the amounts of moisture will be small, there is sufficient water for corrosion, therefore corrosion resistant metals are required.

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Waste Form Degradation and Radionuclide Mobilization

Slide 44

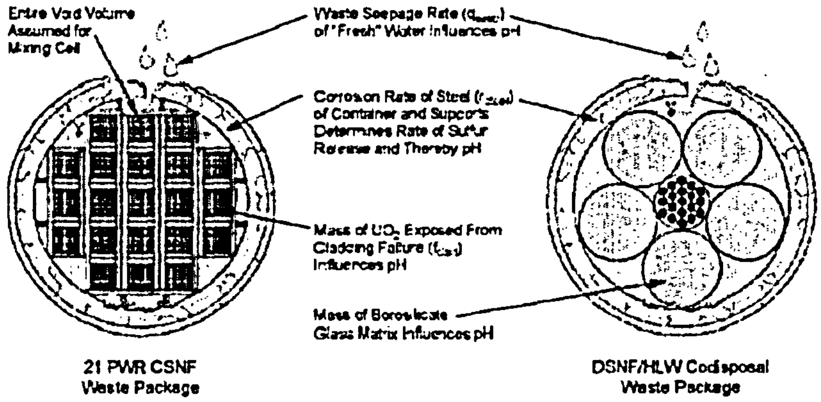

Figure 4-98. Conceptual Model of In-Package Chemistry
DSNF = DOE spent nuclear fuel; HLW = high-level radioactive waste. CSNF = commercial spent nuclear fuel.
Source. CRWMS M&O 2000bm, Figure 3.2-1.

Bath-tub mode

Flow-through mode

Slide 45

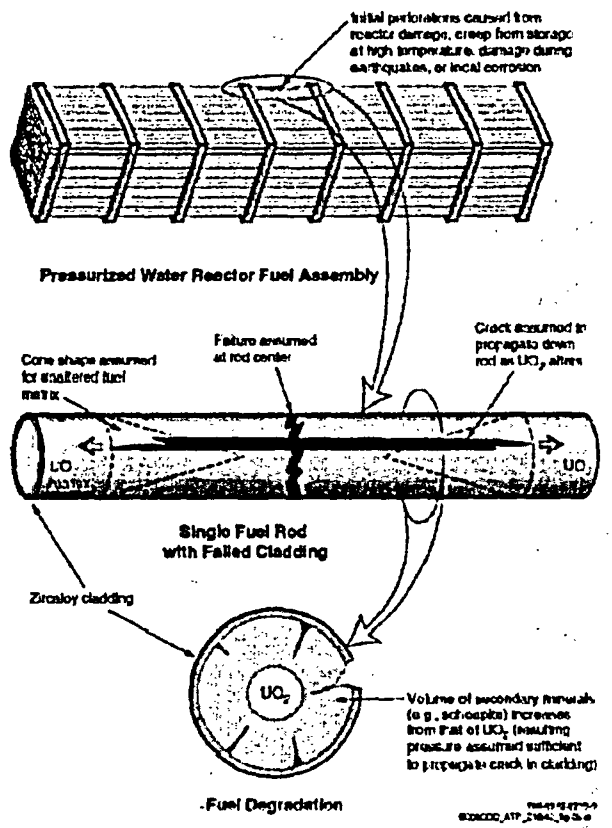

Figure 4-102. Conceptual Model of Commercial Spent Nuclear Fuel Cladding Degradation
Source: CRWMS M&O 2000m, Figure 3.8-2

Important Factors

Water transport into waste package

Water composition: pH, Eh, chemistry

Degradation of Zr clad

UO_2 corrosion and alteration

Radionuclide mobilization

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Corrosion of UO_2 Spent Fuel Matrix

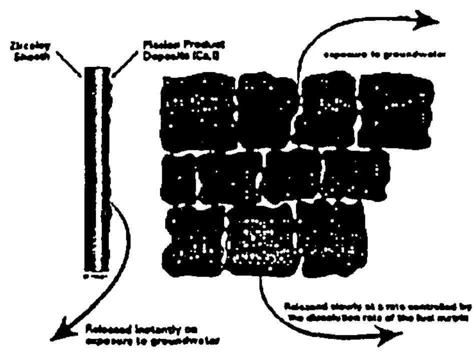
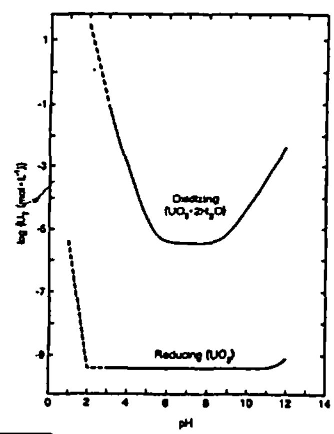


Fig. 1. Schematic diagram showing the distribution of radionuclides in used fuel. Radionuclides located at the fuel-Zircaloy cladding gap and at grain boundaries within the fuel are assumed to be instantly released.

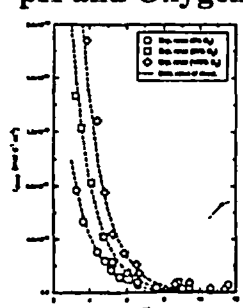
Oxidizing vs. Reducing

Eh and pH



after Shoesmith, J Nucl Matls, 282 (2000)

pH and Oxygen



Complexes/Alteration

$UO_2^{2+} + 2CO_3^{2-} \Leftrightarrow UO_2CO_3(aq)$

$\log K_1 = 9.5 \pm 0.4$

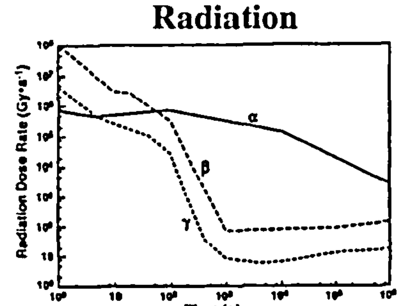
$UO_2^{2+} + 2CO_3^{2-} \Leftrightarrow UO_2(CO_3)_2^{2-}$

$\log \beta_2 = 16.6 \pm 0.3$

$UO_2^{2+} + 3CO_3^{2-} \Leftrightarrow UO_2(CO_3)_3^{4-}$

$\log \beta_3 = 21.6 \pm 0.6$

Radiation



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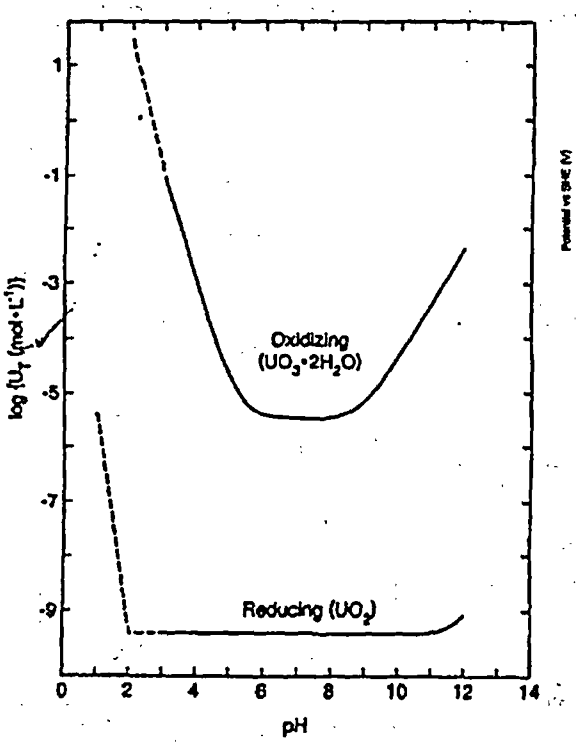
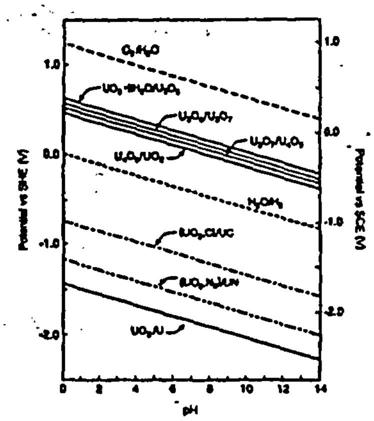
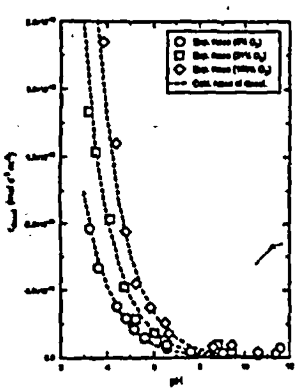


Fig. 3. Solubilities of uranium dioxide (UO_2) and schoepite ($UO_3 \cdot 2H_2O$) as a function of pH at 25°C [4].





Important Factors

Oxidizing vs. Reducing

Oxidizing potential (Eh)

Acidity (pH)

after Shoesmith, J Nucl Matls, 282 (2000)

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Alteration of Spent Fuel and Incorporation Mechanisms

Table 1
Uranyl phases found as alteration products of UO_2

Structure known	
schoepite	$[(UO_2)_8O_2(OH)_{12}](H_2O)_{12}$
becquerelite	$Ca[(UO_2)_3O_2(OH)_3]_2(H_2O)_8$
compreignacite	$K_2[(UO_2)_3O_2(OH)_3]_2(H_2O)_8$
billietite	$Ba[(UO_2)_3O_2(OH)_3]_2(H_2O)_4$
soddyite	$(UO_2)_2(SiO_4)(H_2O)_2$
Na-boltwoodite	$(Na,K)(H_3O)[(UO_2)(SiO_4)]$
sklodowskite	$Mg[(UO_2)(SiO_3OH)]_2(H_2O)_6$
uranophane	$Ca[(UO_2)(SiO_3OH)]_2(H_2O)_5$
haiweeite	$Ca(UO_2)_2Si_6O_{15}(H_2O)_5$
Structure not known	
Dehydrated schoepite	$UO_3(H_2O)_{0.8-1.0}$

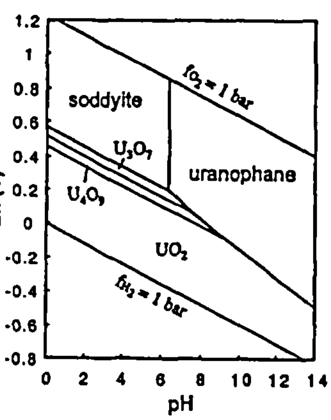
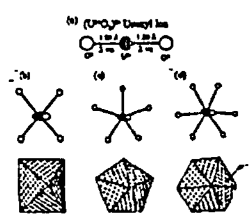
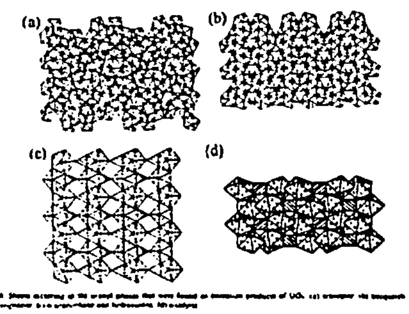


Fig. 2. Eh-pH diagram showing the stability relations among uranium phases equilibrated with Yucca mountain J-13 groundwater. The thermodynamic data for the uranyl phases are from [17]; those for the uranium oxides are from [18].





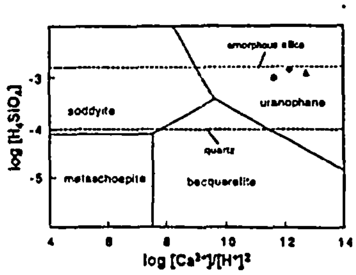


Fig. 1. Activity-activity diagram for SiO_2-CaO-UO_3-H_2O

after Burns, Ewing, Miller, J Nucl Matls, 245, 1997

Important Factors

Crystal chemistry

Chemical analysis

Thermodynamics

Fission product and actinide incorporation??

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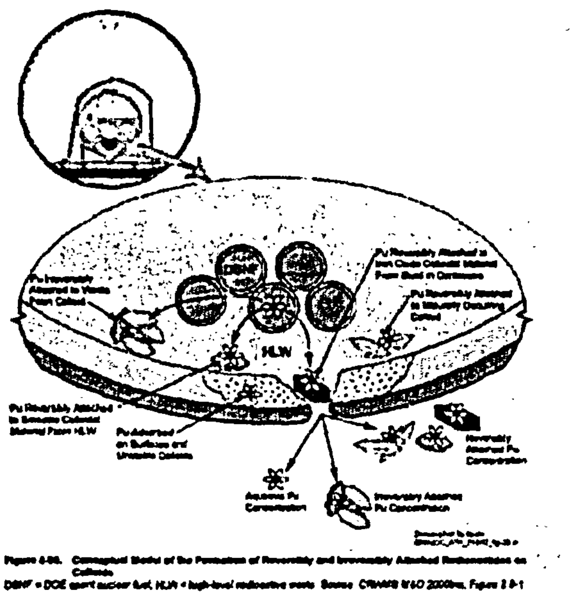
Radionuclide Transport



Important Factors

Interaction with degraded waste form-alteration products

Interaction with corrosion products: internals and waste package

Interactions with invert and drift support

Transport processes

Slide 50

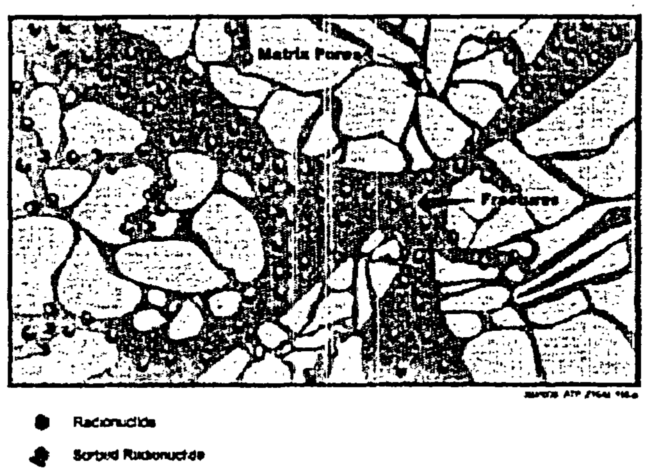


Figure 4-134. Conceptualization of Solute and Colloid Transport in a Fracture with Sorption in the Rock Matrix

Sorption in the fracture rock is conservatively ignored in TSPA-SR calculations. After diffusing into the matrix solutes are sorbed into the rock matrix. Source: CRWMS M&O 2000a, Figure 3.7-4

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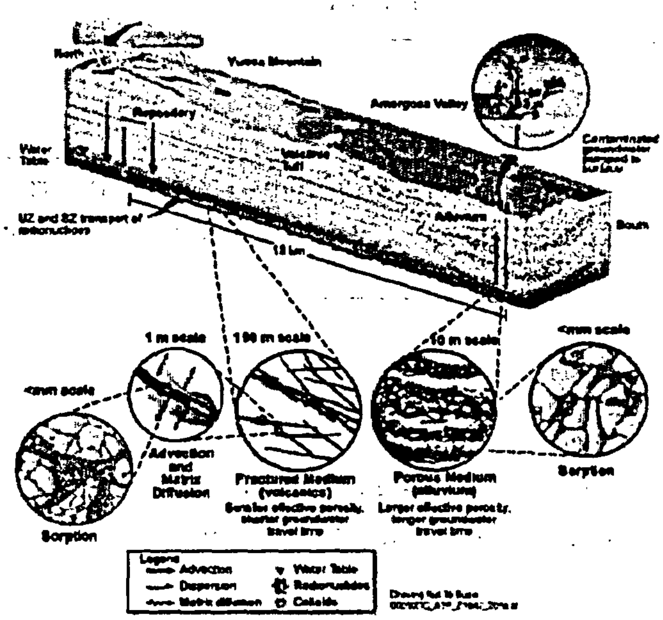

Figure 4-128. Conceptualization of Features and Processes Important to Saturated Zone Transport
This schematic illustration presents transport processes in fractured and porous media flow at Yucca Mountain, providing a conceptualization of transport through the saturated zone to the location of the reasonably maximally exposed individual in the Amargosa Valley. Moving groundwater carries (advects) dissolved or suspended radionuclides in fractures in the volcanic rocks and in pores between individual rock grains in the alluvium. The processes of diffusion and sorption slow the transport of radionuclides to the accessible environment. Radionuclides diffuse into and out of the unfractured portion (matrix) of the volcanic rocks. In the alluvium, radionuclides diffuse into and out of regions where water is stagnant or flows very slowly. UZ = unsaturated zone; SZ = saturated zone

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Summary

Goal is for a set of models that capture reality—important processes, controlling factors and performance relevant to conditions at Yucca Mountain.

Water Contacting Waste Package

Waste Package Lifetime

Releases from Waste Form and Alteration

Mobilization and transport of Radionuclides

Slide 53

4. PRESENTATIONS BY PERFORMANCE ASSESSMENT PRACTITIONERS

4.1 Introduction to the DOE's Total System Performance Assessment (TSPA) Model

Total System Performance Assessment for the License Application–Credibility and Realism Issues

Abraham E. Van Luik
U.S. Department of Energy

Dr. Abraham Van Luik talked about what U.S. Nuclear Regulatory Commission (NRC) requires of the U.S. Department of Energy (DOE) regarding realism and conservatism, as well as the requirements for the performance assessment (PA) used to generate compliance with the post-closure performance objectives.. He mainly discussed the DOE's perspective on requirements under the NRC's regulations in Title 10, Part 63 of the *Code of Federal Regulations* (CFR). He noted that the use of conservatism to manage uncertainty has implications for risk-informed reviews. The DOE believes that realism is desirable, but not required. Adding realism where practicable is a prudent approach because it allows more meaningful safety margin evaluations and improved understanding of system performance. Dr. Rod Ewing asked Dr. Van Luik to clarify his comment that as realism has been added to DOE's PA, long-term safety estimates have improved. Does that mean that the dose always drops or that uncertainty decreases? Dr. Van Luik responded that dose does not always drop with every nuance of change made. But the DOE did three separate PAs during the site recommendation period. They all passed muster when it came to the 10,000-year requirements, but the peak doses kept stepping down. Peak dose is always well beyond 10,000 years. Dr. Garrick asked whether the license application date is still proposed for the end of 2004. Dr. Van Luik responded that the current schedule remains in effect, but that a "frantic" reassessment was presently underway to evaluate whether the schedule was still achievable.

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

YUCCA MOUNTAIN PROJECT

Total System Performance Assessment for the License Application - Credibility and Realism Issues

Presented to:
Advisory Committee on Nuclear Waste

Presented by:
Abraham E. Van Luik
Senior Policy Advisor - Performance Assessment
Office of License Application and Strategy
Office of Repository Development
U.S. Department of Energy

March 25, 2003
Rockville, Maryland

Overview

- **NRC requirements and guidance - treatment of uncertainty**
  - **10 CFR Part 63**
  - **Yucca Mountain Review Plan**
- **Summary of DOE's approach to realism and conservatism**
- **Total System Performance Assessment - License Application development schedule**

Meeting Nuclear Regulatory Commission Requirements

- 10 CFR Part 63 specifies requirements for the performance assessment used to demonstrate compliance with 63.113 (b and c) postclosure performance objectives
- The Yucca Mountain Review Plan, Rev. 2, specifies the approach to judging adequacy of the performance assessment in terms of meeting 10 CFR Part 63 requirements

10 CFR 63 Requirements

§63.304–Reasonable Expectation

- *Reasonable expectation* means that the Commission is satisfied that compliance will be achieved based upon the full record before it. Characteristics of reasonable expectation include that it:
  - Requires less than absolute proof because absolute proof is impossible to attain for disposal due to the uncertainty of projecting long-term performance
  - Accounts for the inherently greater uncertainties in making long-term projections of the performance of the Yucca Mountain disposal system
  - Does not exclude important parameters from assessments and analyses simply because they are difficult to precisely quantify to a high degree of confidence
  - Focuses performance assessments and analyses on the full range of defensible and reasonable parameter distributions rather than only upon extreme physical situations and parameter values

§63.304 Implications for DOE's Performance Assessments

- The DOE should:
  - Evaluate uncertainties
  - Include parameters of importance even if not precisely known
  - Evaluate full range of distributions but be reasonable (goal is likely performance, not unlikely performance for tails of distributions–see next slide)

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5

10 CFR 63 Requirements

§63. 303–Implementation of Subpart L

DOE must demonstrate that there is reasonable expectation of compliance with this subpart before a license may be issued. In the case of the specific numerical requirements in § 63.311 this subpart, and if performance assessment is used to demonstrate compliance with the specific numerical requirements in §§ 63.321 and 63.331 this subpart, compliance is based upon the mean of the distribution of projected doses of DOE's performance assessments which project the performance of the Yucca Mountain disposal system for 10,000 years after disposal.

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§63.303 Implications for DOE's Performance Assessments

The mean dose is to be evaluated using full range of distributions as discussed in §63.303.

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10 CFR 63 Requirements

§63. 342–Limits on Performance Assessments

DOE's performance assessments shall not include consideration of very unlikely features, events, or processes, i.e., those that are estimated to have less than one chance in 10,000 of occurring within 10,000 years of disposal. DOE's assessments for the human-intrusion and ground-water protection standards shall not include consideration of unlikely features, events, and processes, or sequences of events and processes, i.e., those that are estimated to have less than one chance in 10 and at least one chance in 10,000 of occurring within 10,000 years of disposal. In addition, DOE's performance assessments need not evaluate the impacts resulting from any features, events, and processes or sequences of events and processes with a higher chance of occurrence if the results of the performance assessments would not be changed significantly.

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§63.342 Implications for DOE's Performance Assessments

- Performance assessments not to consider very unlikely features, events, or processes
- Assessments for human-intrusion and groundwater protection not to consider unlikely features, events, and processes

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10 CFR 63 Requirements

§63.114–Requirements for Performance Assessment

- Any performance assessment used to demonstrate compliance with § 63.113 must:
  - Include data related to the geology, hydrology, and geochemistry (including disruptive processes and events) of the Yucca Mountain site, and the surrounding region to the extent necessary, and information on the design of the engineered barrier system used to define parameters and conceptual models used in the assessment
  - Account for uncertainties and variabilities in parameter values and provide for the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment
  - Consider alternative conceptual models of features and processes that are consistent with available data and current scientific understanding and evaluate the effects that alternative conceptual models have on the performance of the geologic repository
  - Consider only events that have at least one chance in 10,000 of occurring over 10,000 years

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10 CFR 63 Requirements

§63.114–Requirements for Performance Assessment

(Continued)

- Provide the technical basis for either inclusion or exclusion of specific features, events, and processes in the performance assessment. Specific features, events, and processes must be evaluated in detail if the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission
- Provide the technical basis for either inclusion or exclusion of degradation, deterioration, or alteration processes of engineered barriers in the performance assessment, including those processes that would adversely affect the performance of natural barriers. Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission
- Provide the technical basis for models used in the performance assessment such as comparisons made with outputs of detailed process-level models and/or empirical observations (e.g., laboratory testing, field investigations, and natural analogs)

§63.114 Implications for DOE's Performance Assessments

- DOE's performance assessments must:
  - Provide basis for models selected and the features, events and processes evaluated and excluded
  - Provide basis for data used and for derived parameter ranges
  - Provide basis for judging adequacy of modeling

Yucca Mountain Review Plan Criteria

4.2.1 Performance Assessment Risk-Informed Review Process for Performance Assessment

- Conservative approach can be used
  - To decrease need to collect information
  - To justify simplified modeling approach
- Conservative estimates for dose may be used to demonstrate compliance
  - Caution: conservatism in one process may not mean conservatism in dose projection
  - Technical basis needed for claimed conservatism

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Yucca Mountain Review Plan Criteria

4.2.1 Performance Assessment Risk-Informed Review Process for Performance Assessment

(Continued)

- Use of conservatism to manage uncertainty has implications for risk-informed review
  - Staff to evaluate assertions of conservatism from perspective of overall system performance
  - Staff will use any available information to risk-inform its review
- The Yucca Mountain Review Plan's review methods and acceptance criteria emphasize staff intent to thoroughly review potential nonconservatisms at subsystem and system levels

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Realism Desirable, Not Required

- DOE believes that adding in realism where practicable is a prudent approach because it allows:
  - More meaningful safety-margin evaluations
  - Taking a more informed, less conservative approach to barrier design
  - More straightforward communication of the case for system safety
  - Improved understanding of system performance

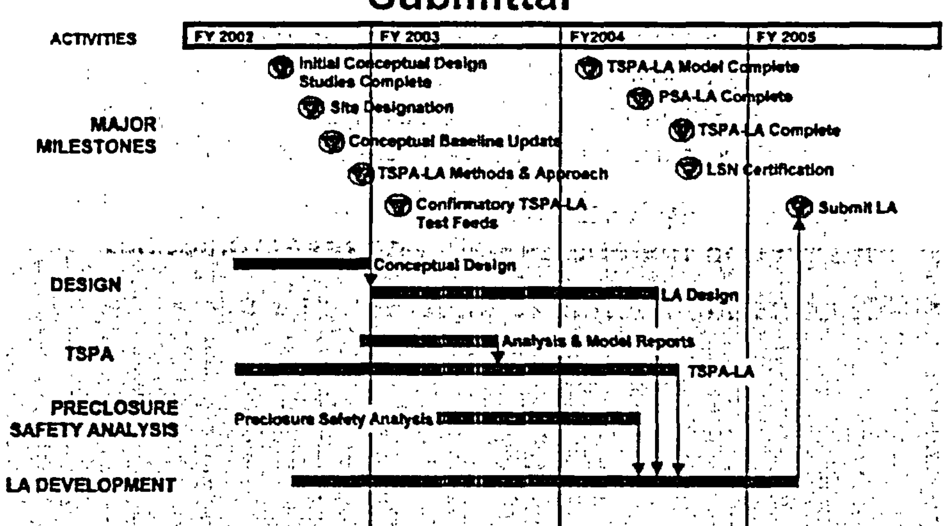
Conservatism Has Advantages, Disadvantages

- As recognized in the Yucca Mountain Review Plan, conservatism may allow assurance of safety with lesser time and other resource expenditures
- Pragmatically it can become a tradeoff issue between design and materials costs and research costs
- Conservatism tends to understate safety

Use of Pragmatic Realism

- Advisory Committee on Nuclear Waste and Nuclear Waste Technical Review Board comments–realism allows more meaningful uncertainty and safety-margin evaluations; DOE agrees
- Realism has improved as Total System Performance Assessment has evolved
  - As realism has been added, long-term safety estimates improved
  - Realism has improved understanding of system performance to the level needed to demonstrate safety in a regulatory context

Summary Schedule to License Application Submittal



NOTE: PSA-LA - Preclosure Safety Analysis - License Application
LSN - Licensing Support Network

Summary

- Total System Performance Assessment - License Application will have a mix of conservative and realistic models that meet 10 CFR Part 63 requirements
- Performance Confirmation Program to enhance confidence in key process models
- Long-Term Test and Evaluation Program to add understanding and realism for modeling
- Science and Technology Program to evaluate new science and technology for enhancing safety, efficiency and understanding

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BSC Presentations_ACNW_YM/Van Luik_03/26/03 19

R. Ewing, Univ. of Michigan: Abe, just a clarification. You made the point that as realism has been added to the TSPA, the long-term safety estimates improved. What did you mean exactly? Does that mean the dose always drops, or that uncertainty decreases?

A. Van Luik (DOE): The dose does not always drop with every nuance of change that we have made. For example, we did three separate TSPAs during the site recommendation period. They all passed muster when it came to the 10,000-year requirements, but the peak doses kept stepping down. If you look in between two of those cases, there was actually a time that they turned back up. But peak doses are of interest to me, and I am very pleased that every time that we've added realism into the modeling they have come down in size. Now, whether that's a trend that continues or not would be–

R. Ewing, Univ. of Michigan: And the peak dose is always beyond 10,000 years.

A. van Luik, DOE: Way beyond 10,000 years. It's about 500,000 years now.

R. Ewing, Univ. of Michigan: Does that seem strange that in a complicated system as you get more data and know more about the various parts, you always get a desirable answer--that is, the peak dose drops?

A. Van Luik, DOE: I think it is not strange if you recognize that we have made a concerted effort that, where there was uncertainty, we manage that uncertainty by (exactly what the ACNW is criticizing us for) going in an unrealistic, but conservative direction. It kind of verifies our major assumptions. As we get more data, especially in the waste package materials area, we add more realism to that model. In addition, as the waste package life extends out in time, the failure rates slow down.

R. Ewing, Univ. of Michigan: So, if I followed through this series of TSPAs and looked at the parameter ranges and values generally used, I would see that from point A to point C you were more conservative in C, and it became less conservative with realism?

A. Van Luik, DOE: Yes, I think for certain aspects of things.

R. Ewing, Univ. of Michigan: Right.

A. Van Luik, DOE: There were other things, for example, the very first cut at TSPA-SR, we had not updated the climate model yet. When we updated it, the peak doses actually went up.

R. Ewing, Univ. of Michigan: But that does not necessarily mean you added realism to the analysis, right?

A. van Luik, DOE: There is an argument that what we have added is informed speculation. That is better than the speculation we had before, I think.

4.2 Introduction to the NRC's Total-System Performance Assessment (TPA)

Background and Role of the NRC's Total-System Performance Assessment Capability

Andrew C. Campbell
U.S. Nuclear Regulatory Commission

Dr. Andrew Campbell reviewed the background and role of NRC's total-system performance assessment (TPA) computer code capability. The role of the NRC's TPA code is to enhance the NRC's independent review capability to evaluate the DOE's PA, to understand and evaluate the DOE's models, assumptions, and data, and to provide flexibility to evaluate the completeness of the DOE's modeling approaches. The TPA code also provides risk insights to help establish priorities in technical reviews. Overall, the TPA code provides confirmatory analyses of the DOE's modeling approach and results.

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United States Nuclear Regulatory Commission

Background and Role of NRC's Total-System Performance Assessment Capability

Andrew C. Campbell
Section Leader
Performance Assessment and Integration
Division of Waste Management
US Nuclear Regulatory Commission
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United States Nuclear Regulatory Commission

NRC's ROLE

- Pre-licensing Activities
  - Developing staff review capabilities
  - Understanding important features, events, and processes
  - Understanding Barriers
  - Interactions with DOE
  - Identifying information necessary to review a license application (agreements)
- Reviewing DOE license application

2

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Historical Background

- Integrated performance assessment (IPA) modeling activities
- Development of Total-system Performance Assessment (TPA) code
- Interactions with DOE on TSPA
- Development of Key Technical Issue (KTI) framework

3

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Role of NRC's TPA Code

- Independent review capability
  - Evaluate DOE's TSPA
  - Understand and evaluate DOE's models, assumptions, and data
  - Flexibility to evaluate completeness of DOE modeling approaches
- Enhance staff understanding
  - Identify key elements of repository system
  - Provide risk insights to help establish priorities
  - Integration of Evaluations of sub-system performance

4

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Applications of TPA code

- Confirmatory analyses of DOE modeling approach and results
- Simplified calculations to support system performance analyses
- Uncertainty and sensitivity analyses
  - Identify uncertainties important to performance
  - Test relative importance of parameters, alternative conceptual models, and key assumptions
- Integration of processes and models into a comprehensive understanding of repository system
- Identify uncertainties in abstraction process
- Understanding importance of certain scenarios

5

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Key Aspects of Estimating Nominal Performance

- Infiltration
- Near field
  - Engineered Barrier Degradation
  - Source Term
- Radionuclide Transport Through Geosphere
  - Unsaturated zone
  - Saturated zone
- Biosphere and Dose

6

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Confidence Building for Performance Assessment

- Peer review of TPA 3.2
  - Areas evaluated
  - Key recommendations
  - Staff follow-up
- Verification Testing of TPA 5.0
  - Purpose
  - Approach

7

United States Nuclear Regulatory Commission

Ongoing NRC Staff Activities and Path Forward in PA

- Risk Insights
  - Risk insights baseline
  - Risk Insights Report
  - Provide feedback to staff on agreements
- Interactions on DOE Risk Prioritization Approach
- Finalize development of TPA 5.0 prior to LA
- Developing IPA 4
- Update Risk Insights Baseline

8

B. J. Garrick, ACNW Member: I have one question, Andy. I notice that the Electric Power Research Institute was strongly urging you to do what evidently you are going to do—use your risk model to prioritize the agreements. Can you tell us a little bit about how you are going to do that, and to what extent you are going to importance-rank the agreements?

A. Campbell, NRC Staff: Right now we are developing and essentially redrafting what we call a risk insights baseline. This will really lay out an issue-level approach, at the integrated subissue level, the key areas of repository performance. Then we plan to align that information with specific agreement areas that are based upon the long history of analyses and specific work that we've been doing in the last few years. The agreements will be aligned with our fundamental understanding of the key features of repository performance. The idea is not to necessarily rule things out, but to really understand, what are the key elements of all those agreements that we feel are needed for our review of the license application.

B. J. Garrick, ACNW Member: Now, of course, the agreements are not completely decoupled from the subissue, or the key technical issues (KTIs). But they are not necessarily the same either.

A. Campbell, NRC Staff: That is right.

B. J. Garrick, ACNW Member: Are you going to do any kind of mapping of the importance ranking of the agreements with the subissues of the KTIs? As you know, the committee has been urging for a long time that there be more of a PA template put on the KTIs. It is probably not reasonable to think in terms of the KTIs themselves, but rather the subissues of the KTIs. Are you going to sort that out a little bit between the agreements and the subissues of the KTIs?

A. Campbell, NRC Staff: Well, one of the things we have done is that we have mapped the agreements to what are called the integrated subissues. These are the 14 key areas of the Yucca Mountain Review Plan. We are really focusing on how those agreements map to the 14 integrated subissues because that then leads into our ability to review the license application. So that kind of mapping is taking place.

Consider, for example, a KTI like CLST, container life and source term. There are something like 53 or 56 agreements there. Not all of those agreements are the most important. There are some that will rise to the top in terms of importance to long-term performance, certainly over the 10,000-year period, and others may fall down.

We are, of course, mapping to the integrated subissues rather than to the KTIs. We hope to be able to identify within the context of those integrated subissues, those particular agreements that are really key.

4.3 Overview of the DOE's TSPA

Overview of the U. S. Department of Energy Total System Performance Assessment Model

Peter Swift
Sandia National Laboratories/Bechtel SAIC Company, LLC

Dr. Peter Swift reviewed the status of the DOE's TSPA and summarized the TSPA methodology and its major model components. The TSPA process includes (1) screening of features, events, and processes, (2) developing models and their scientific basis for each process, (3) identifying uncertainty in models and parameters, (4) constructing an integrated TSPA model using all retained processes, and (5) evaluating total system performance (individual protection, groundwater protection, and human intrusion) through Monte Carlo simulations.

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

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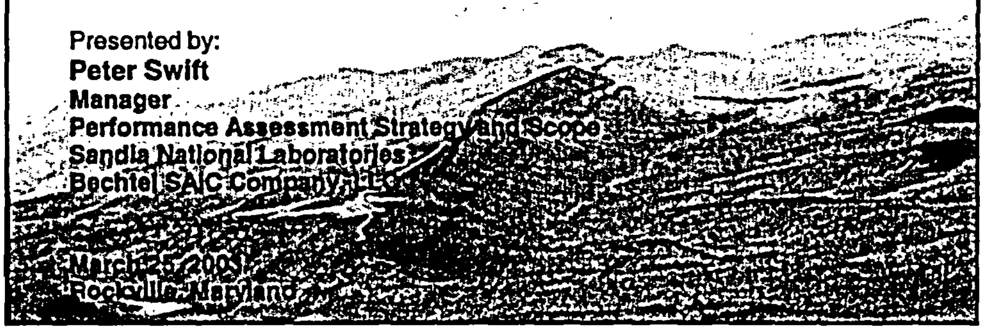
Overview of the U. S. Department of Energy Total System Performance Assessment Model

Presented to:
Advisory Committee on Nuclear Waste

Presented by:
Peter Swift
Manager
Performance Assessment Strategy and Scope
Sandia National Laboratories
Bechtel SAIC Company, LLC

March 25, 2003
Rockville, Maryland



Outline

- **Current Status of the Total System Performance Assessment**
- **Summary of Total System Performance Assessment methodology**
- **Summary of the major model components**
  - **Mapping of workshop topics to DOE Total System Performance Assessment model components**
  - **Process models and abstractions**
    - **Source term discussed separately in later presentation**
  - **Linkage in Total System Performance Assessment model**

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Status of Total System Performance Assessment Analyses

- All DOE Total System Performance Assessment information used at this workshop is from existing Total System Performance Assessment analyses
  - December 2000: Total System Performance Assessment for the Site Recommendation
  - July 2001: FY01 Supplemental Science and Performance Analyses
  - September 2001: Revised Supplemental Total System Performance Assessment to support the Final Environmental Impact Statement and Site Suitability Evaluation
  - Additional analyses completed in 2002
    - "One-off" analyses to support risk-based prioritization
    - "One-on" analyses to provide insight into barrier performance
- Models and analyses that will support the License Application are currently under development

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Total System Performance Assessment Process

- Screen features, events and processes to determine those that must be retained in performance assessment
- Develop models, along with their scientific basis, for each process included in Total System Performance Assessment
- Identify uncertainty in models and parameters
- Construct integrated Total System Performance Assessment model using all retained processes
  - "Nominal" performance model contains all features, events and processes likely to occur
  - "Disruptive event" performance model contains low-probability events (e.g., volcanism)
  - Stylized human intrusion model, as specified by regulation
- Evaluate total-system performance (individual protection, groundwater protection, and human intrusion standard) considering uncertainty through Monte Carlo simulation

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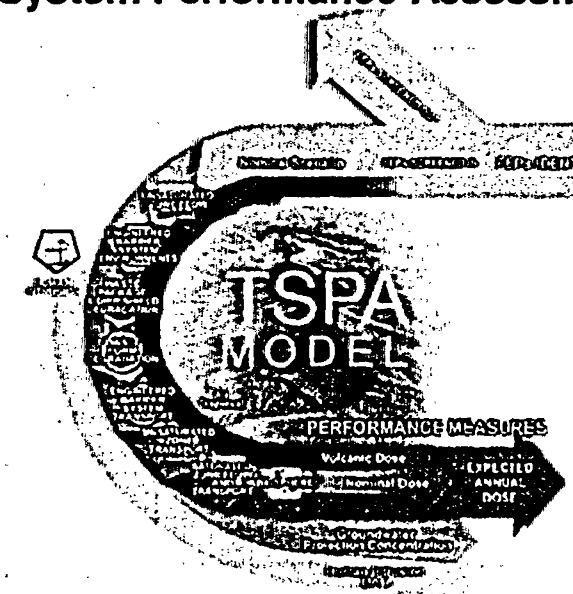
Total System Performance Assessment Process



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Nominal Performance Model Components

Workshop Groupings	DOE Total System Performance Assessment Components
Infiltration/Tunnel Dripping	Climate, Infiltration, Unsaturated Zone Flow, Thermal Effects, Seepage
Source Term	Drip Shield, Waste Package, Cladding, Waste Form
Near Field	Transport in the Engineered Barrier System, including Invert
Unsaturated Zone	Flow and transport in the Unsaturated Zone below the Repository
Saturated Zone	Flow and transport in the Saturated Zone
Biosphere	Biosphere

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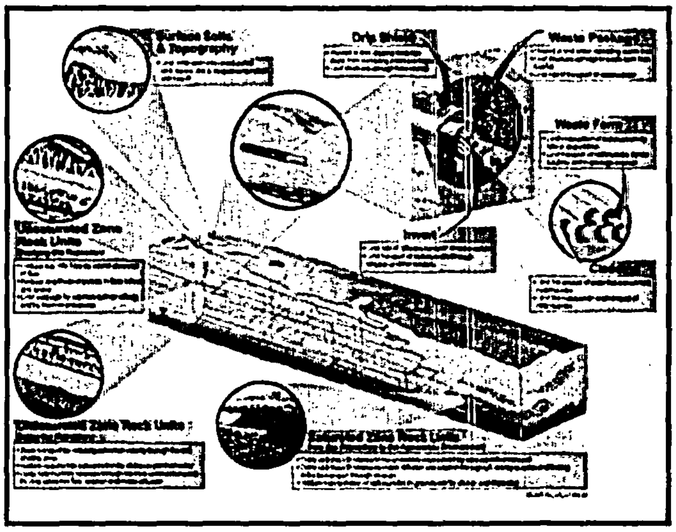
Nominal Performance Model Components Organized by Barriers



- Surface soils and topography (includes climate, infiltration)
- Unsaturated zone above (seepage, drift effects)
- Drip shield
- Waste package
- Cladding
- Waste form
- Invert
- Unsaturated zone below (transport)
- Saturated zone

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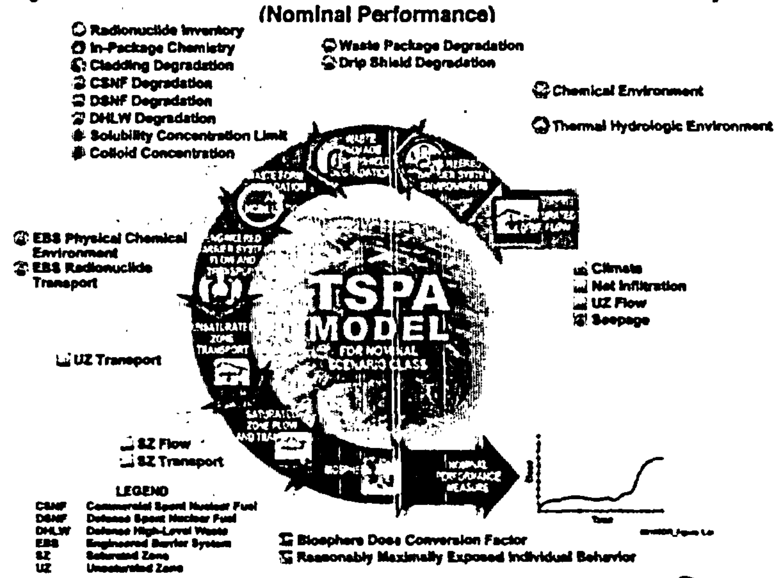
Total System Performance Assessment Model Components

(Nominal Performance)



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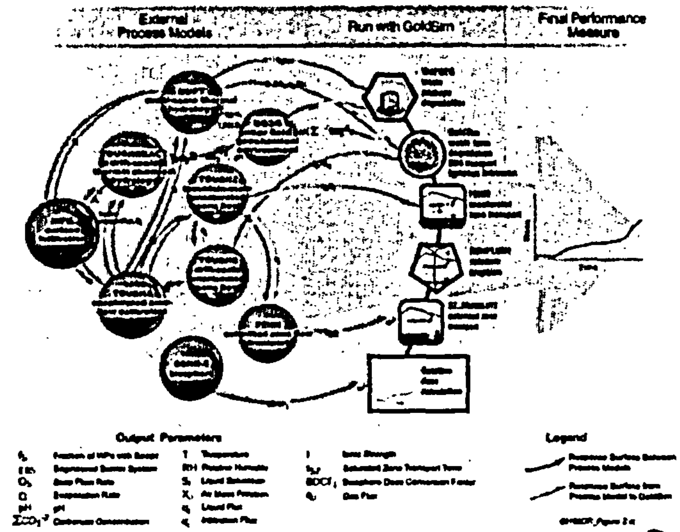
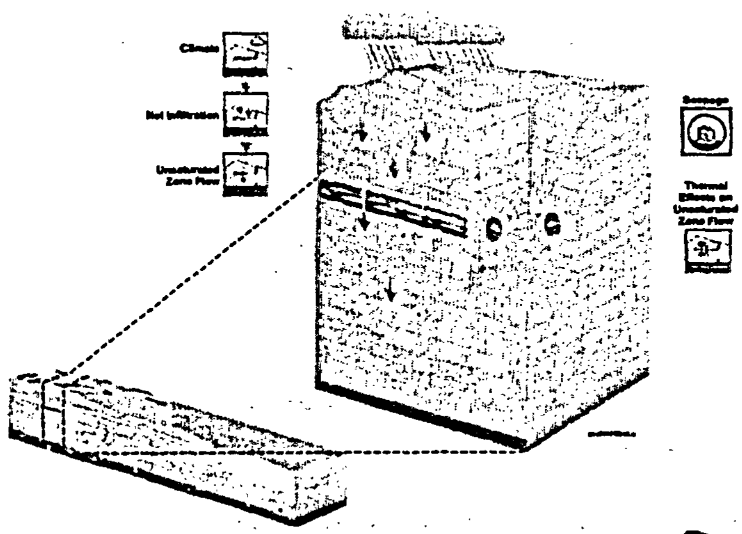
Overview of Model Linkage

(Total System Performance Assessment - Site Recommendation)

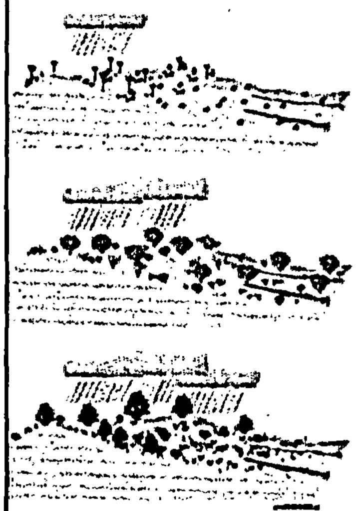


Components Related to Infiltration/Tunnel Dripping



Climate

Total System Performance Assessment Abstraction and Linkage



- Present climate and two future states based on paleoclimate data and modern analogs
  - Timing of climate changes is fixed
  - Uncertainty in magnitude of changes in precipitation and temperature is included through the infiltration model
- Outputs
  - To infiltration model
    - Mean annual temperature and precipitation, timing of changes
  - To unsaturated zone transport model
    - Water table rise with wetter climates shortens transport path
  - To saturated zone flow and transport model
    - Wetter climates increase flow rates, breakthrough curves calculated for present flow field are scaled accordingly

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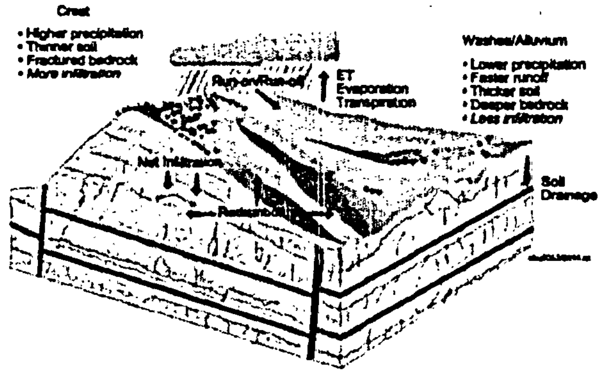
Infiltration

Total System Performance Assessment Abstraction and Linkage



- Inputs from climate model, site and analog data
- Process model includes precipitation, temperature, evapotranspiration, insolation, run-on, run-off, soil storage
- Abstraction implements three detailed net infiltration maps (high, medium, low) calculated for each climate state
- Output
  - Infiltration flux maps to mountain scale flow model and thermal hydrology model
  - Probability of infiltration maps to Total System Performance Assessment for binning waste packages and source term

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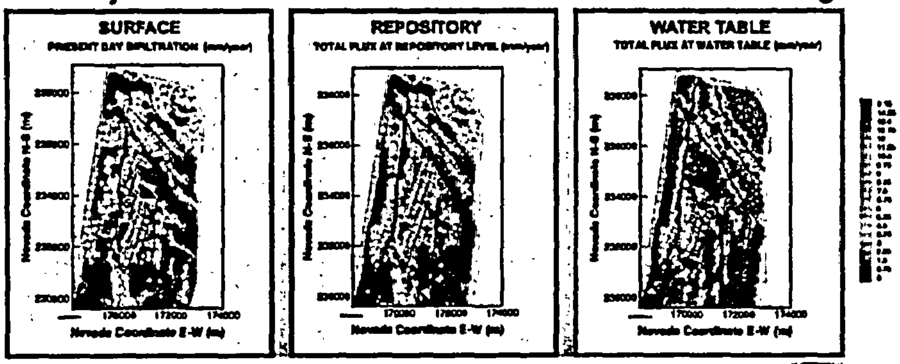
Mountain Scale Unsaturated Zone Flow

Total System Performance Assessment Abstraction and Linkage



- Inputs from infiltration model, site data
- Process model calculates 3-D steady state isothermal flow in an unsaturated dual permeability medium
- Abstraction implements a flow field for each infiltration map
- Outputs
  - Hydrologic properties to thermal hydrology model
  - Flow fields for unsaturated zone transport model

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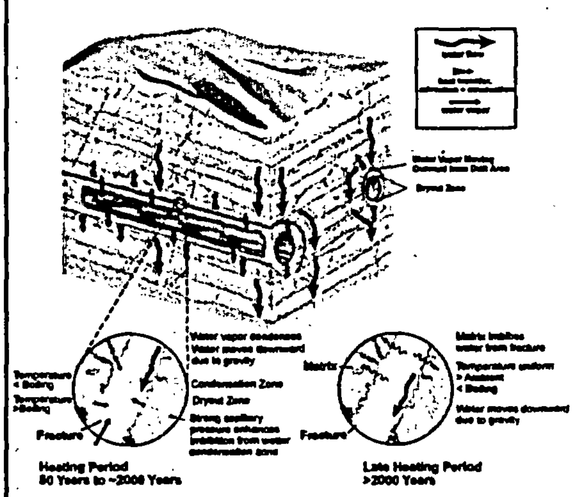
Thermal Hydrologic Environments

Total System Performance Assessment Abstraction and Linkage



- Thermal hydrology model
  - Inputs: drift layout and heat loading from repository design; hydrologic properties from mountain scale flow model; water flux from infiltration model
  - Outputs: percolation flux to seepage model; environmental conditions in drift and adjacent rock
- Thermal hydrologic chemistry model
  - Inputs: initial water chemistry, temperature history from thermal hydrology model
  - Outputs: water chemistry entering drift

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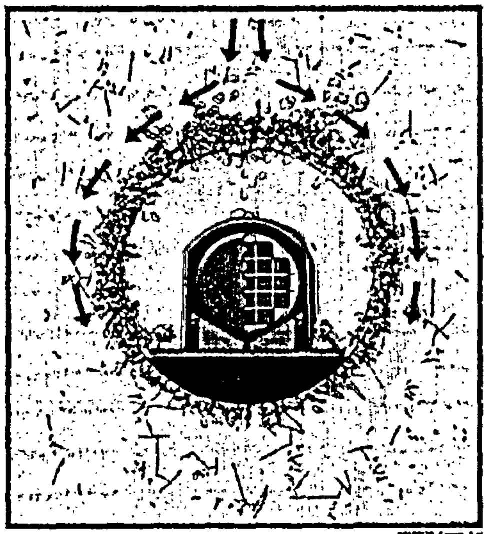
Seepage

Total System Performance Assessment Abstraction and Linkage



- Process model calculates 3-D fracture-only flow, includes flow focusing effects, drift degradation
- Inputs are thermal hydrology flux, drift design, rock properties
- Abstraction uses thermal hydrology flux 5 m above drift as input
- Outputs are seepage fraction (overall 13% for Total System Performance Assessment - Site Recommendation, 48% for Supplemental Science and Performance Analyses and Final Environmental Impact Statement), seep rate (with uncertainty) for different waste package bins (i.e., waste type, infiltration states)

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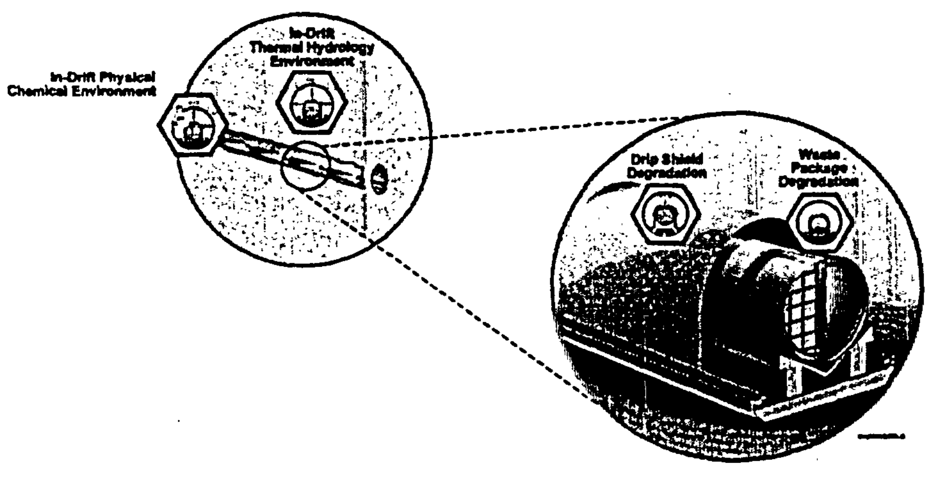
Components Related to the Source Term Waste Package and Drip Shield Degradation



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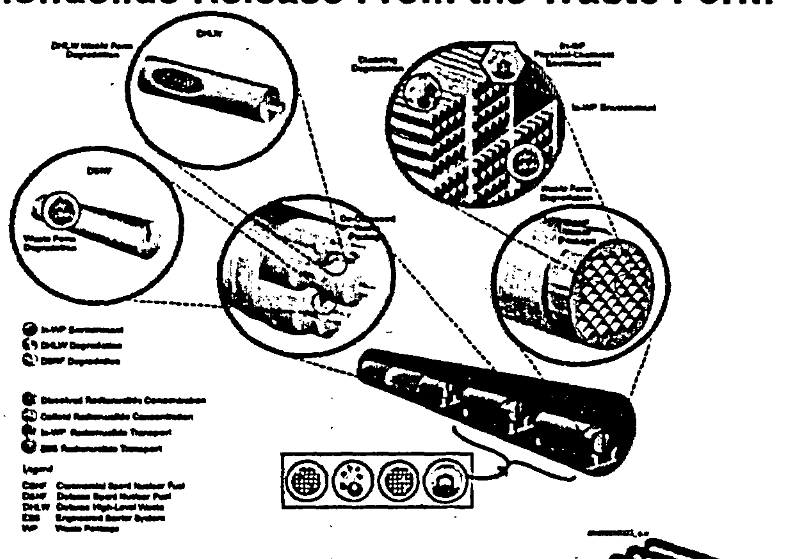
Components Related to the Source Term Radionuclide Release From the Waste Form



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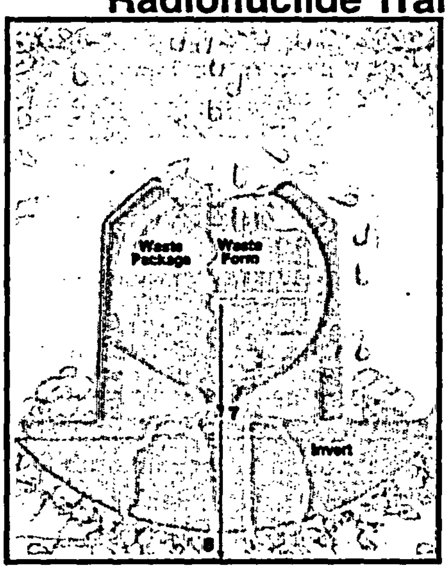
Components Related to the Near Field Radionuclide Transport in the Drift



- Engineered barrier system flow
  - 1-D flow model uses input from thermal hydrology, seepage, waste package (source term)
- Engineered barrier system chemistry
  - Inputs include water chemistry, flux, temperature
  - Outputs: Invert water chemistry to engineered barrier system transport model
- Engineered barrier system transport
  - Advective and diffusive transport
  - Inputs from engineered barriers system flow, waste package
  - Outputs: radionuclide flux to unsaturated zone transport model

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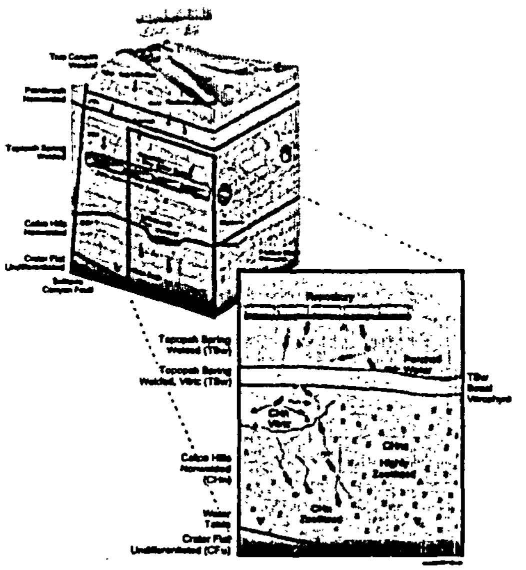
Unsaturated Zone Transport

Total System Performance Assessment Abstraction and Linkage



- 3-D steady-state particle tracker, dual-continuum transport with sorption, reversible and irreversible colloids
- Implemented directly in Total System Performance Assessment
- Inputs:
  - Flow fields from mountain scale flow model
  - Radionuclide fluxes from engineered barrier system transport model
  - Time and magnitude of climatic changes in water table elevation
- Outputs: radionuclide flux to saturated zone transport model

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Saturated Zone Flow and Transport

Total System Performance Assessment Abstraction and Linkage

- Process model calculates site-scale 3-D steady-state flow
  - Inputs include hydrogeologic framework regional model, boundary and recharge fluxes, future flux climate scaling factors
  - Calibration to water table data
- Transport calculated as breakthrough curves for release at initial time
  - Includes sorption, reversible and irreversible colloids
- Total System Performance Assessment abstraction uses convolution integral approach to apply breakthrough curves to releases at all times, scaling for climate effects and accounting for radioactive decay/ingrowth
- Output to biosphere model: radionuclide flux into the withdrawal well

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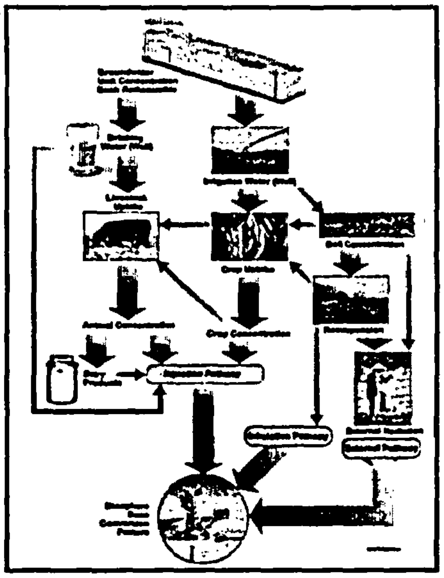
Biosphere

Total System Performance Assessment Abstraction and Linkage



- Exposure pathways include food and water ingestion, dust inhalation, external exposure to contaminated soil
- Human lifestyles and groundwater pumping consistent with regulatory requirements
- Dose methodology based on the International Commission on Radiological Protection 30 standards
- Inputs are radionuclide concentrations in groundwater, human lifestyle data
- Outputs to Total System Performance Assessment are biosphere dose conversion factors

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Summary

- Detailed models characterize water flow, radionuclide transport, and other important processes through the major components of the system
- Total System Performance Assessment links these models, simplified where appropriate and necessary, to provide estimates of system performance
- Total System Performance Assessment and process models can be used to examine behavior of individual components within the system, to be discussed in subsequent presentations

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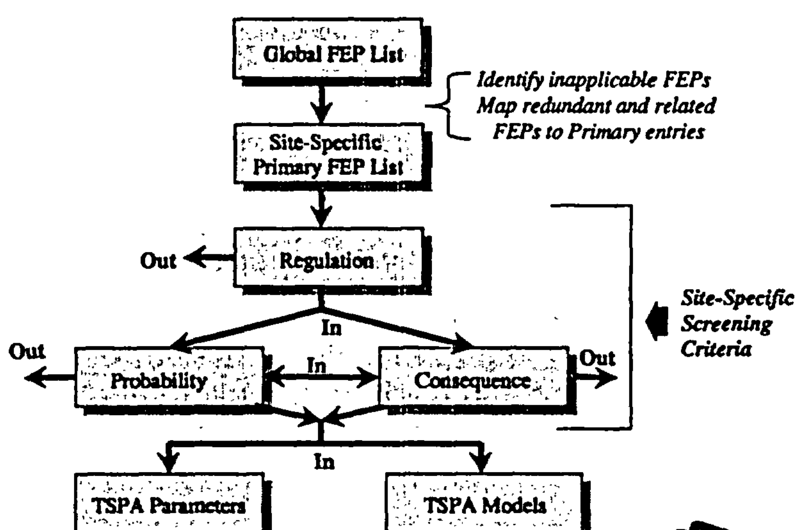
Backup

Screening Features, Events, and Processes



Screening Features, Events, and Processes Screening Criteria

- From 10 CFR 63.114 d,e,f
  - "Any performance assessment used to demonstrate compliance with §63.113 must:
    - ...Consider only events that have at least one chance in 10,000 of occurring over 10,000 years.
    - ...Specific features, events, and processes of the geologic setting must be evaluated in detail if the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission.
    - ...Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting [doses or releases] would be significantly changed by their omission."

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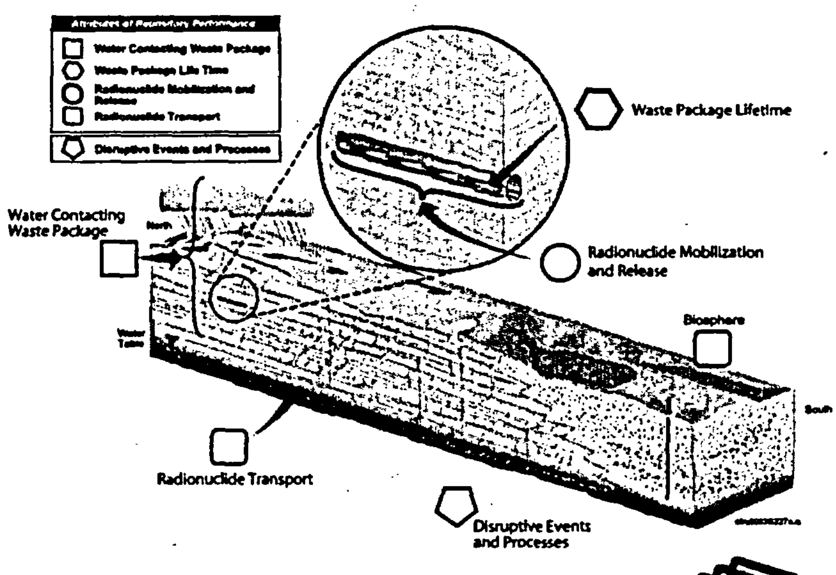
Nominal Performance Scenario Class



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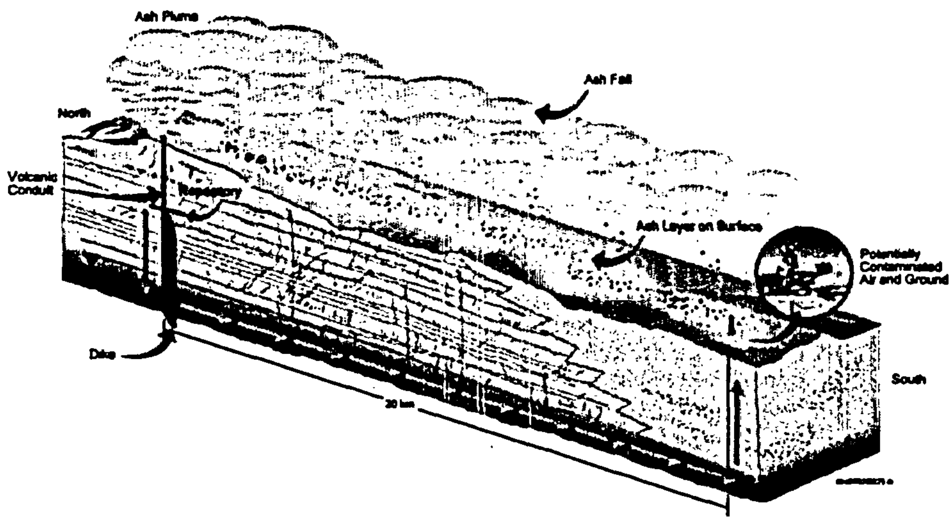
Igneous Disruption Scenario Class



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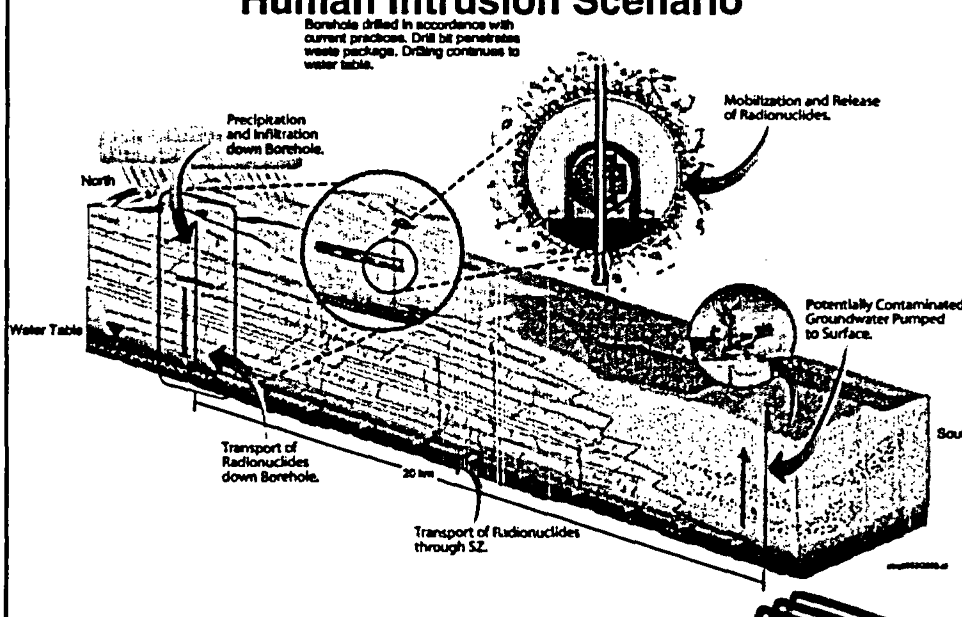
Human Intrusion Scenario



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Left blank intentionally.

M. Morgenstein, Geosciences Management Institute, Inc. (GMII): Why would you use well water data to look at the initial water chemistry, which is in the soil zone? Why not use soil zone chemistry water?

P. Swift, Sandia National Laboratories/Bechtel SAIC Company, LLC (SNL/BSC): We would then be modeling the evolution of the water from here down to there. In fact, we are picking it up most of the way down in modeling this chemical evolution in the thermal environment.

M. Morgenstein, GMII: I don't get this at all.

P. Swift, SNL/BSC: There's an assumption that the real water collected from wells represents the real evolution of water in an undisturbed system from the land surface to the subsurface.

M. Morgenstein, GMII: What gives you the right to make that assumption? What data supports that assumption?

P. Swift, SNL/BSC: I guess I am probably not the person to answer that question.

M. Morgenstein, GMII: Okay. I would suggest this is totally wrong. This is not the direction to go in. There is no reason not to collect initial water chemistry of the soil zone. I cannot believe that the program does not do this.

R. Andrews, Bechtel SAIC Company, LLC (BSC): You're exactly right. Therefore, in the summer of 2001, we did a comparison using so-called J-13 saturated zone water, which Peter is talking about here, and the available data at that time for water chemistry. We evolved both of those chemistries in the drift and compared their results in the supplemental science and performance analyses which were used to support the science and engineering. They were also used to support the site recommendation. Those analyses, which I did not bring but are in the supplemental science analysis report, showed very little difference by the time you evolved them in the drift. You are exactly right. They are different starting water chemistries. But by the time you evolve them and mix them, if you will, with the inert materials, you get very little difference in temporal evolution for the major constituents.

M. Morgenstein, GMII: Is it difficult to actually collect surface water and do a mass balance?

R. Andrews, BSC: These are not surface waters. These are all groundwaters. Taking water chemistry samples from the core is a very difficult process. There are data on those. The U.S. Geological Survey (USGS) has collected those data by extracting water from cores for the last 7 or 8 years. The preliminary sets of those data were used in the site recommendation that I just alluded to, and additional water chemistry data will be used in the license application. In terms of extracting water from the fractures, there is no water right now in the fractures. The fractures are at 5 to 10 percent liquid saturation.

We do have water chemistry data, however, from perched water zones that we have encountered. Those have been used to help constrain the in situ pre-thermal chemistry.

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4.4 Overview of NRC's TPA

Total-System Performance Assessment (TPA)
Approaches and Assumptions for Version 4.1

Christopher J. Grossman
U.S. Nuclear Regulatory Commission

Mr. Christopher Grossman gave an overview of approaches and assumptions for TPA computer code version 4.1. The TPA performs probabilistic dose calculations for given time periods and accounts for (1) essential features of the engineered and natural barriers, (2) chemical and physical processes affecting waste package degradation and release to the biosphere, (3) uncertainties and spatial variability of model parameters and future states, and (4) lifestyle characteristics of the reasonably maximally exposed individual. The TPA analyzes scenarios including a nominal case with climate change and seismic activity, and disruptive cases with faulting and igneous activity. The TPA uses approaches based on fundamental principles and available data.

United States Nuclear Regulatory Commission

Total-system Performance Assessment (TPA):

Approaches and Assumptions for Version 4.1

Christopher J. Grossman

Environmental and Performance Assessment Branch
Contact information: (301) 415-7658, cjg2@nrc.gov

Major Contributors: Sitakanta Mohanty, Richard Codell, Randy Fedors, Jim Winterle, Hans Arlt, Paul Bertetti, John Bradbury, Tae Ahn

Presented to: The Advisory Committee on Nuclear Waste, March 25-26, 2003

United States Nuclear Regulatory Commission

TPA: A Review Tool

- TPA is an **independent** tool used to support review of both pre-licensing activities and a potential license application.
- TPA uses available **data** to construct approaches based on first principles.
- TPA uses approaches based on **fundamental principles** to simulate the repository behavior and allow for **computational efficiency** where warranted.
- TPA uses fundamental approaches to allow **flexibility** in independently evaluating of a license application for the proposed repository and support review capability.

United States Nuclear Regulatory Commission

TPA Approach

- TPA conducts probabilistic dose calculations for specified time periods, accounting for:
  - Essential features of the engineered and natural barriers,
  - Chemical and physical processes affecting degradation and release to the biosphere,
  - Uncertainties and spatial variability of system attributes, model parameters, and future states (scenario classes), and
  - Lifestyle characteristics of the reasonably maximally exposed individual (RMEI).
- Scenario classes include:
  - A nominal case including climate changes and seismic activity,
  - A disruptive case involving faulting, and
  - A disruptive case involving igneous activity.

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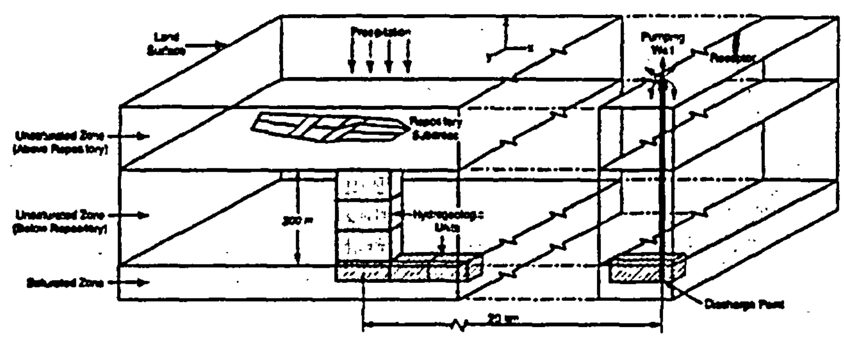
Repository Conceptualization



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Water Movement Through the Repository

- Temperature and precipitation vary with glacial cycles.
- Process-level modeling, which incorporates climate, soil depth, and bedrock permeability, estimates the shallow infiltration flux for bare-soil conditions based on numerical solutions to the Richards equation.
- Deep percolation flux equal to the shallow infiltration flux.
- Water seeping into drifts varies with time during the first few thousand years largely because of coupled heat transfer and fluid flow processes such as vaporization, condensation, and refluxing.
- Large-scale diversion, as well as near- and in-drift diversion or focusing impact the water flux entering the failed waste package.

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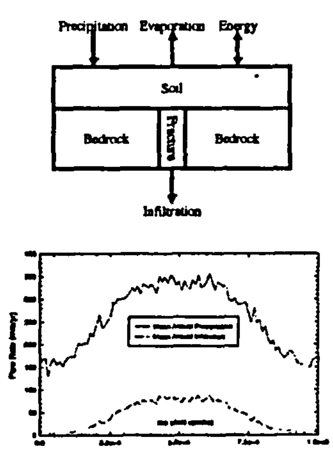
Shallow Infiltration

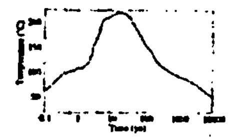


Variation of infiltration with climate change.

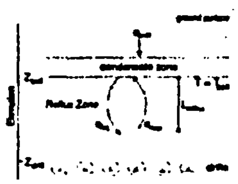
- Evidence suggests precipitation may have been 1.5-2.5 times larger than current climate conditions, while temperature may have been cooler by 5-10 °C at last full glacial maximum.
- Net infiltration for the modern climate is based on 1-D simulation results using a 15-year record of hourly meteorological data from Desert Rock, Nevada.

United States Nuclear Regulatory Commission

Groundwater Reflux



Temperature profile at the drift wall.



Conceptualization of drift-scale thermal hydrologic model.

- Process-level thermohydrologic modeling calculates the thickness of the dry out zone above the repository for TPA.
- Theory suggests water flowing down a fracture will penetrate a distance below the boiling isotherm before completely vaporizing.
- Water reaches the drift when the penetration distance exceeds the thickness of the dry out zone.
- TPA also incorporates two additional alternative conceptualizations to model groundwater reflux.

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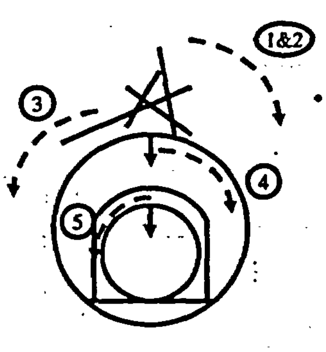
Flow Convergence/Divergence



- TPA utilizes a simple and efficient approach to modify the percolation flux that reaches the waste package.
- Factors account for:
  1. Fraction of waste packages dripped on by flowing fractures,
  2. Focusing/divergence of deep percolation toward/away from drifts,
  3. Divergence due to capillary forces in unsaturated rocks,
  4. Film flow down the surface of the drift walls,
  5. Drips missing holes in the waste package, and the presence of corrosion products in the holes.

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Degradation of the Engineered System

- Process-level modeling based on experimental evidence estimates the time of drip shield failure.
- TPA estimates initial failure of a small number of waste packages due to fabrication defects or emplacement damage.
- TPA simulates uniform or localized corrosion of the waste package depending on conditions (RH, T, [Cl^-], pH) in the near-field environment. TPA assumes the waste package fails with a single penetration of the outer (Alloy-22) and inner (316L SS) overpacks.
- TPA calculates the waste package surface temperature and relative humidity (RH) based on thermal output and the repository horizon temperature.
- Process-level modeling estimates the near-field chemical environment.

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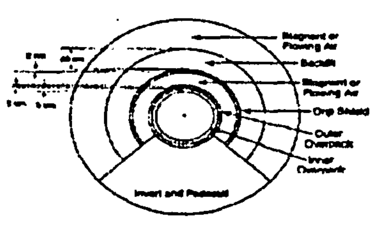
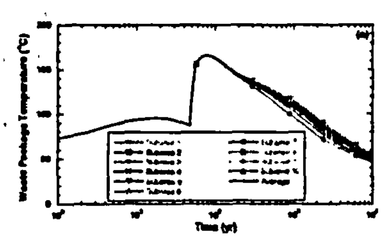
Thermal Modeling



Idealization for thermal calculations.

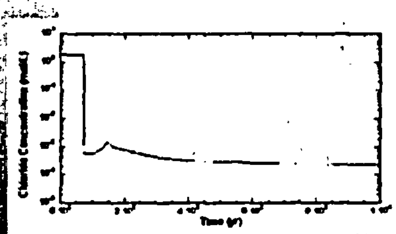


Waste package surface temperatures.

- TPA calculates the temperature of the drift wall using a mountain-scale analytic conduction-only model.
- TPA calculates the waste package surface temperature and maximum temperature of the spent fuel using analytical approximations of multimodal heat transfer.
- TPA calculates RH as a function of drift wall and waste package surface temperatures and moisture present at closure.
- TPA can incorporate an alternative thermal model.

United States Nuclear Regulatory Commission

Near-Field Chemical Environment



ride concentration at the drift wall.

- Currently, process-level modeling simulates the change in chloride concentration due to evaporation.
- TPA adjusts the chloride concentration to account for uncertainties and limitations of the modeling to represent the chemistry on the waste package surface.
- TPA fixes pH at 9 based on process-modeling.
- TPA 5.0 will add a new conceptual model to describe pO_2, pH, CO_3^{2-}, Cl, NO_3^{2-}, F^- evolution thereby improving realism in the corrosion modeling.

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Radionuclide Release

- The quantity of water that enters the failed waste package, composition of water, and solubility of radionuclides impact the transfer of radionuclides from spent fuel into water for transport.
- TPA considers two models, a bathtub and flow-through model, for advective transport of radionuclides from the waste package. TPA 5.0 will add a diffusion transport model.
- Experimental evidence supports the spent fuel dissolution rate model. TPA includes 3 additional alternative dissolution rate models.
- TPA incorporates two spent fuel surface area models, a particle model and a grain model.
- TPA 5.0 will add a high-level waste glass source term model.
- Cladding can reduce the fraction of total spent fuel surface area exposed to water entering the waste package.

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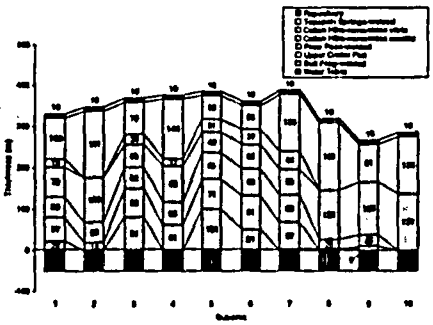
Unsaturated Radionuclide Transport



- TPA utilizes a simple 1-D vertical flow field through hydrostratigraphic layers whose thicknesses were derived from the Geologic Framework Model 3.1.
- UZ flow occurs in fractures when the percolation flux exceeds the matrix hydraulic conductivity for a given tuff layer.
- Due to large uncertainty and long run time, TPA does not include diffusion of radionuclides from fast flowing fractures into near-stagnant matrix pores.
- TPA models retardation in the rock matrix.

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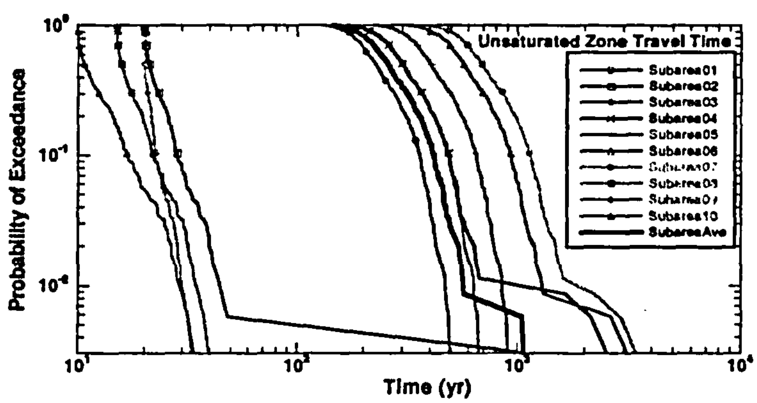
Unsaturated Radionuclide Transport



Unretarded unsaturated zone travel time.

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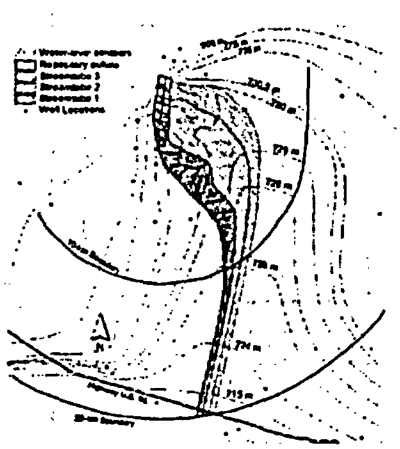
Saturated Radionuclide Transport



- TPA models 3 streamtubes based on a 2-D horizontal flow-net interpretation of hydraulic gradients in the uppermost aquifer.
- Water level data from area wells provides basis for hydraulic gradient and transmissivity.
- TPA samples tuff-alluvium interface.
- TPA models sorption in alluvial aquifer and tuff matrix.
- Radionuclides can diffuse from fractures into matrix in the tuff aquifer.

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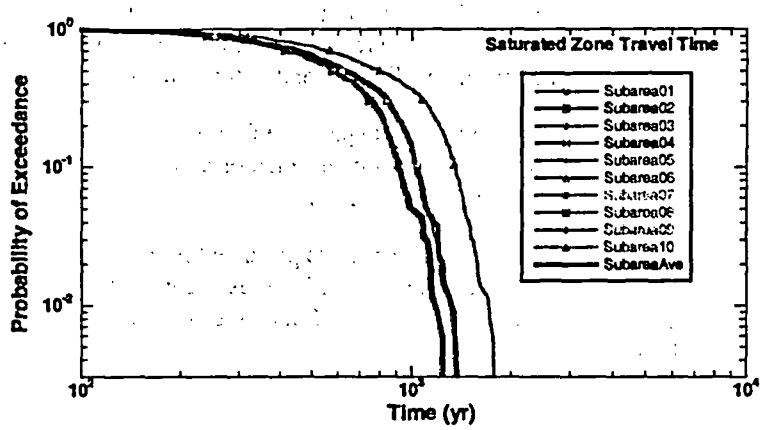
Saturated Radionuclide Transport



Unretarded saturated zone travel time.

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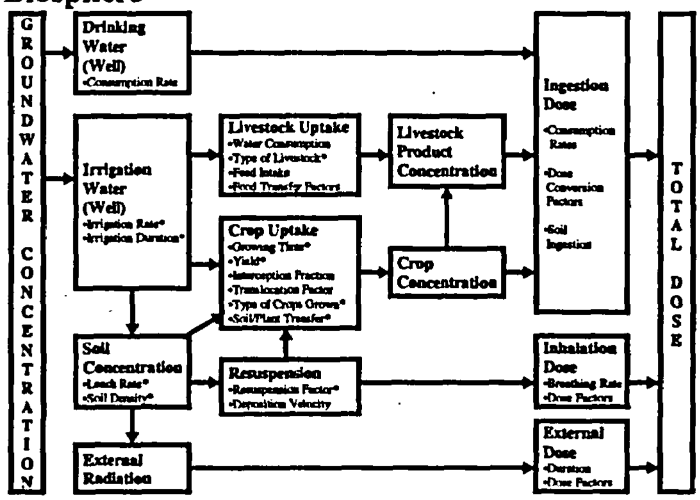
Biosphere



* Examples of Site-Specific Parameters

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Disruptive Events

- TPA predicts the number of waste package failures caused by falling rocks resulting from seismic activity that mechanically load and deform the waste package.
- TPA models waste package failure resulting from movements along undetected or new faults that exceed a displacement threshold.
- TPA accounts for waste package failures caused by both extrusive and intrusive igneous events. TPA models airborne releases of radionuclides for volcanic eruptions.

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Afterword

- TPA provides a **flexible** framework to **independently** review pre-licensing activities and a license application for the proposed repository at Yucca Mountain.
- TPA uses approaches based on **fundamental principles,** where possible, to simulate the repository behavior and allow for some **computational efficiency.**
- Where possible, the approaches are based on available **data.**

J. Payer, Case Western Reserve University (CWRU): Just to follow up on your last comment. What is the overlap, or how consistent are the databases being used by DOE and you folks? Are they the same database?

C. Grossman, NRC Staff: No. In some cases, we rely on information we glean from the prelicensing interactions with the DOE. In other cases, as I mentioned in the beginning, we rely on work that's being conducted at the Center for Nuclear Waste Regulatory Analyses, as well as some of the independent research that they are conducting, such as in the area of corrosion modeling and spent fuel dissolution.

J. Payer, CWRU: If the predictions, or outcomes, are different, is somebody analyzing how much of that difference might be the result of differences in the data that you are using, versus differences in the modeling approaches you are using? Is someone looking at separating that?

C. Grossman, NRC Staff: Yes. We are very interested in where the differences would be. Those highlight potential points where we may challenge the DOE in their models and assumptions.

Currently, we group staff into key technical issues which we believe are areas important for the performance of the repository. The staff involved in those technical issues would then help to evaluate the data and the sufficiency of the data on the Department's part, as well as our own data that goes into the models.

T. McCartin, NRC Staff: I would like to add one real-world example. If I go back 3 to 5 years, the NRC and the DOE were estimating the same release rates from the waste package. However, we had a much lower dissolution rate for the fuel and took no credit for cladding. The DOE had a much higher dissolution rate for the fuel, but took significant credit for the cladding. Even though the end product, that is the release from the waste package, was very similar, it resulted from drastically different assumptions. Those are the kinds of things that we are using this to help assist our thinking, as Chris indicated, and to probe the DOE. But, yes, absolutely we need to understand why the comparison is there. Just the fact that you compare doesn't mean anything.

4.5 Source Term Module Under TSPA

Elements of the U.S. Department of Energy (DOE) Source Term Model for Total System Performance Assessment

Robert W. Andrews
Bechtel SAIC Company, LLC

Dr. Robert Andrews reviewed elements of the DOE's source term model. He described the factors that can potentially affect emplacement drift environments, including coupled thermal-chemical effects on water chemistry, mechanical effects of rock fall, humidity, and groundwater seepage into drifts. Dr. Andrews discussed the degradation models for the drip shield and waste package, including processes of general corrosion and stress-corrosion cracking. The TSPA model includes juvenile failure of waste packages, but the DOE estimates that the expected number of improperly annealed waste packages is only ~0.26 out of ~12,000 waste packages. The first drip shield failures occur at about 20,000 years as a result of general corrosion. The TSPA models bulk chemistry within the waste package under well-mixed, oxidizing conditions. Dr. Andrews also described the possible degradation of fuel cladding via perforation and unzipping.

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

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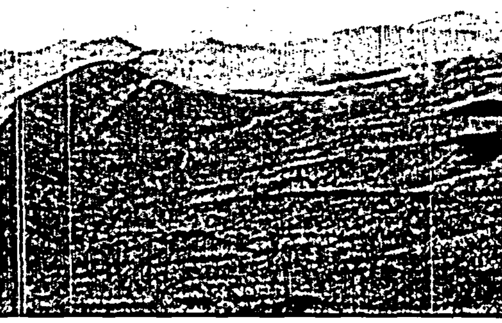
Elements of the U.S. Department of Energy Source Term Model for Total System Performance Assessment

Presented to:
Advisory Committee on Nuclear Waste

Presented by:
Robert W. Andrews
Manager
Performance Assessment Project
Bechtel SAIC Company, LLC



March 25, 2003
Rockville, Maryland

Outline

Factors Potentially Affecting the Total System Performance Assessment Source Term

- **In-Drift Environment**
  - Chemical, mechanical, thermal, hydrologic
- **Drip Shield and Waste Package Degradation**
  - General corrosion
  - Stress corrosion cracking
  - Improper heat treatment
- **In-Package Environment**
- **Waste Form Degradation**
- **Waste Form and Engineered Barrier Radionuclide Release**
- **Summary and Conclusion**

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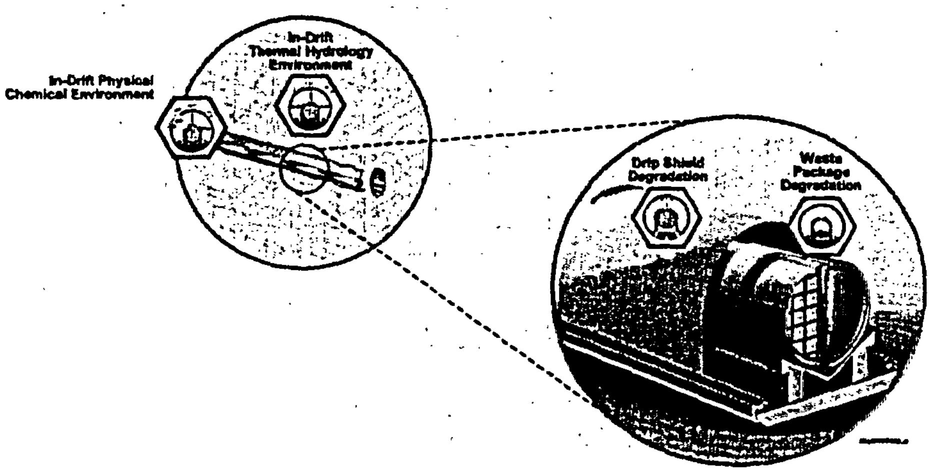
Components Related to the Source Term, Waste Package, and Drip Shield Degradation



Coupled Thermal Chemical Effects on Water Composition

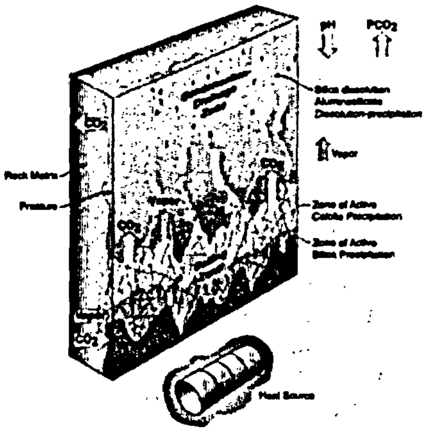
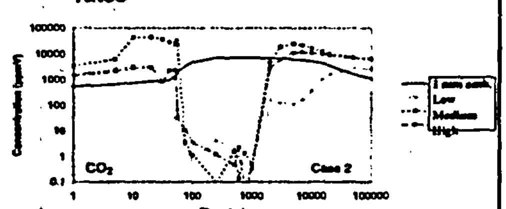


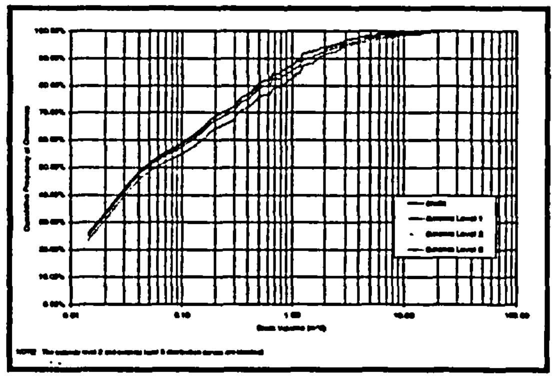
Diagram Showing THC Processes

- Incoming water and gas composition derived from coupled thermal-hydro-chemical model for a range of infiltration rates
- Model validated based on drift-scale heater test results
- Aqueous chemical constituents include CO_3^{2-}, pH, HCO_3^-, F^-, and Cl^-
- Gas composition considers CO_2 evolution over a range of infiltration rates



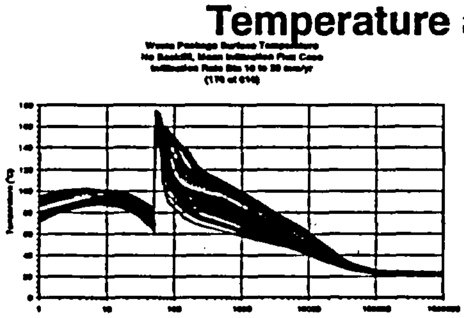
In-Drift Physical Environment
Mechanical Degradation by Rock Fall

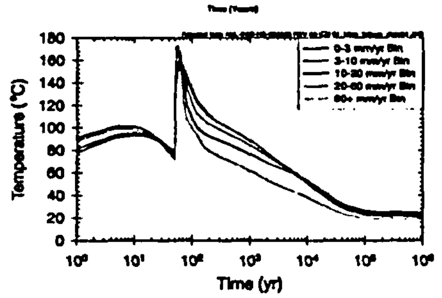
- Key-block analysis defines rock-fall size and frequency, which are a function of
  - Lithology
  - Joint strength
  - Drift orientation
  - Seismic level
    - 1 (1,000 yr recurrence)
    - 2 (5,000 yr recurrence)
    - 3 (10,000 yr recurrence)



- Rock falls induce mechanical stress on drip shield but are insufficient to induce stress corrosion cracking of drip shield
- Rock fall assumed to occur after design life of drift support system
- Rock-fall model compared to analog information

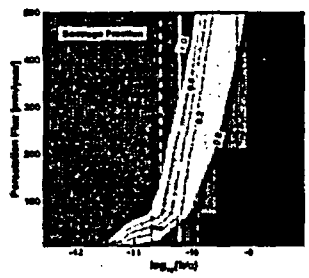
In-Drift Physical Environment
Temperature and Humidity

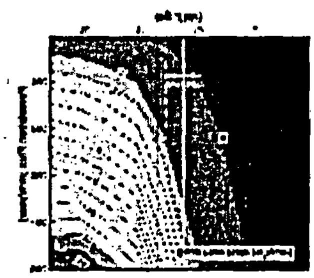




- Temperature and relative humidity on drip shield and waste package determined by repository design
  - Thermal load (areal and line)
  - Ventilation (rate and duration)
- Initiation of corrosion is a function of water composition, critical relative humidity, and deliquescent salts
- Model compared with drift scale test results

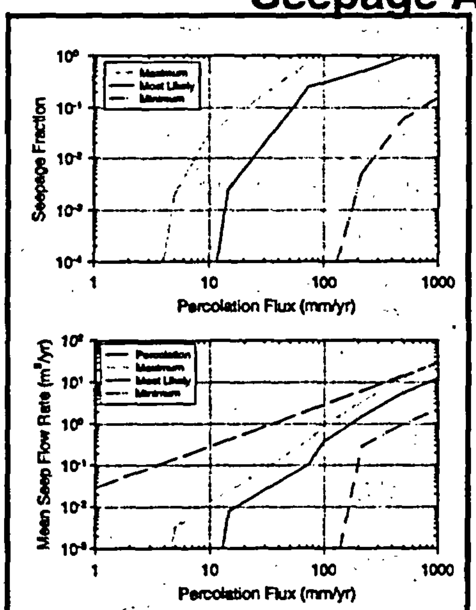
Seepage into Emplacement Drifts





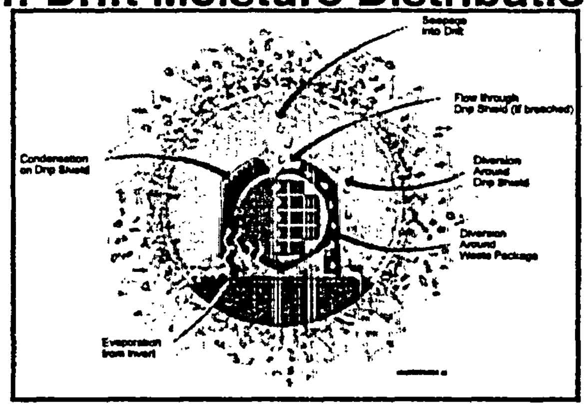
- Seepage model applied over range of fracture characteristics, drift shapes, flow focusing, and episodicity
- Seepage model validated using niche experiments in Exploratory Studies Facility
- Fracture characteristics (especially permeability (k) and capillarity ($^1/_\alpha$)) are uncertain and variable based on Exploratory Studies Facility tests
- Percolation flux from thermo-hydrologic model modified to account for flow focusing and episodicity

Seepage Abstraction



- Seepage fraction and seep flow rate are sampled from triangular distributions
- Seepage is calculated for 610 spatial locations and then averaged over five discrete infiltration bins
- Seepage fraction and seepage flow rate vary with climate state, which affects percolation flux

In-Drift Moisture Distribution



- All seepage flux into drift assumed to contact drip shield
- Seepage flux through drip shield depends on area of drip shield degraded
- No credit taken for thermal gradient between commercial spent nuclear fuel, waste package and drip shield

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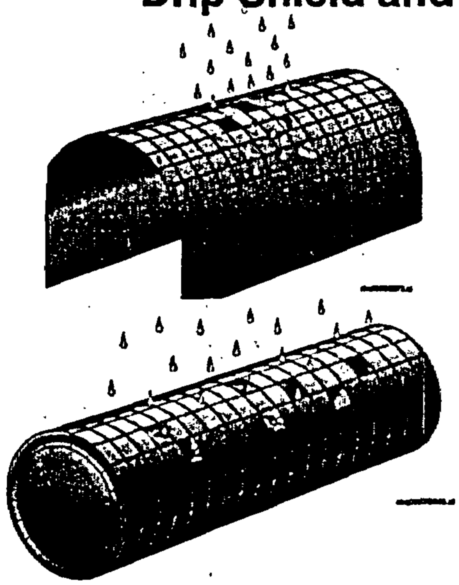
Implementation of Degradation Models for the Drip Shield and Waste Package



- Divide drip shield and waste package surface into patches
- General corrosion occurs dependent on relative humidity of deliquescent $NaHCO_3$
- Local corrosion model included but never invoked because critical potential > corrosion potential for expected environments based on cyclic polarization tests
- Stress corrosion cracking model dependent on stress state following stress mitigation at welds and failure criterion (% of yield)
- Early failures considered derived from possible improper heat treatment

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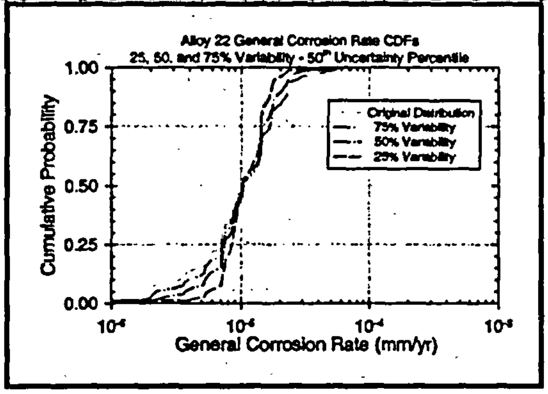
General Corrosion of Waste Package



- Uncertainty and variability in rates considered based on 2-year data from long-term corrosion test facility
- Corrosion rates increased by up to 2x for microbiologically influenced corrosion effects and up to 2.5x for aging effects based on data from laboratory tests

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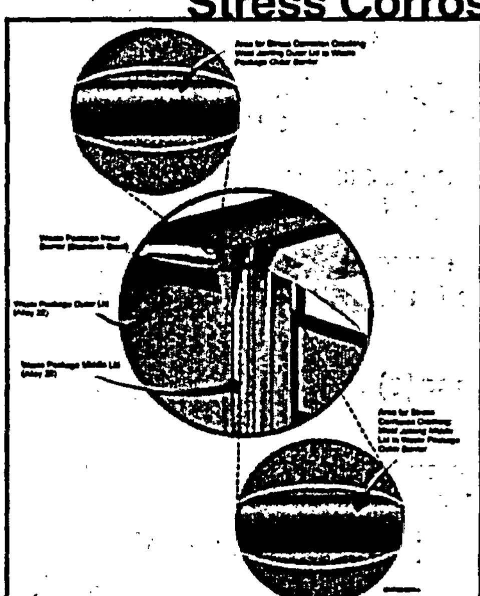
Stress Corrosion Cracking



- Occurs only in weld-region patches for outer and middle closure lids
- Stress corrosion cracking modeled using slip dissolution model
  - Rate of crack growth a function of
    - Stress intensity factor
    - Crack growth rate parameter
- Stress corrosion cracking requires stress at crack tip to be greater than stress threshold
  - Uncertainty in stress state (following stress mitigation) and yield stress evaluated
- Stress mitigation method was solution annealing for outer lid and laser peening for middle closure lid

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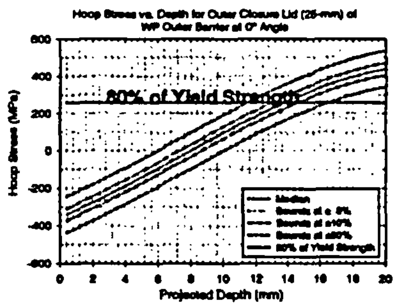
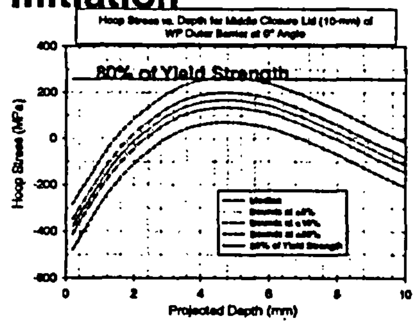
Uncertainties Affecting Stress Corrosion Cracking Initiation





- Total System Performance Assessment - Final Environmental Impact Statement model used stress value of 80% of yield as point where stress corrosion cracking could initiate based on laboratory testing
- Total System Performance Assessment - Final Environmental Impact Statement model included very small probability of stress corrosion cracking initiation of the inner closure-lid weld region
- Total System Performance Assessment - Site Recommendation used 20 to 30% of yield strength as the stress threshold (therefore stress corrosion cracking was initiated earlier in the Total System Performance Assessment - Site Recommendation model)

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Early Waste Package Failure Representation in Total System Performance Assessment - Final Environmental Impact Statement – Improper Heat Treatment

- Probability of undetected improper heat treatment (solution annealing) estimated to be ~ 2×10^{-5}
- For ~ 12,000 waste packages, expected number of improperly heat treated waste packages is ~ 0.26
- 20 out of 100 realizations have at least one waste package failed early, and 3 realizations have two waste packages failed early
- Assume affected waste package(s) fail immediately when corrosion initiates
  - Assume conservatively weld regions of both the outer and inner closure-lids of the outer barrier fail immediately
- Current approach will use laser peening instead of solution annealing

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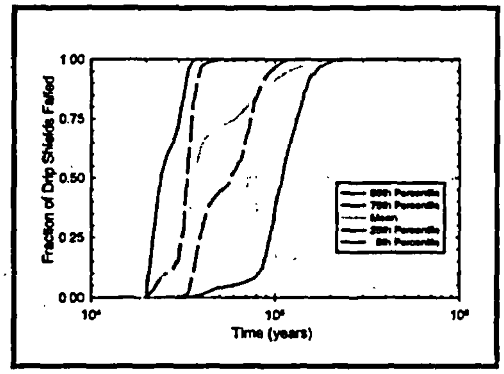
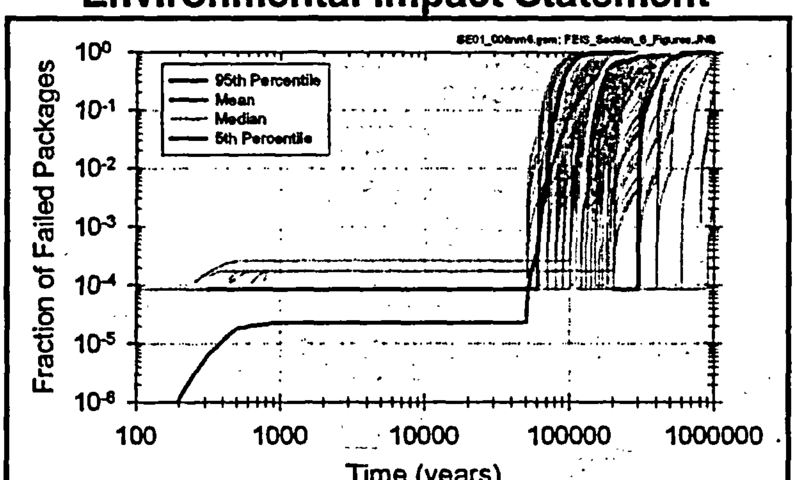
Calculated Cumulative Drip-Shield Failures

- The first drip-shield failures occur at about 20,000 years
- General corrosion only
- On average, most of the drip shields fail within 40,000 years and almost all fail within 100,000 years
- At the 95% probability level, almost all drip shields fail within 30,000 years

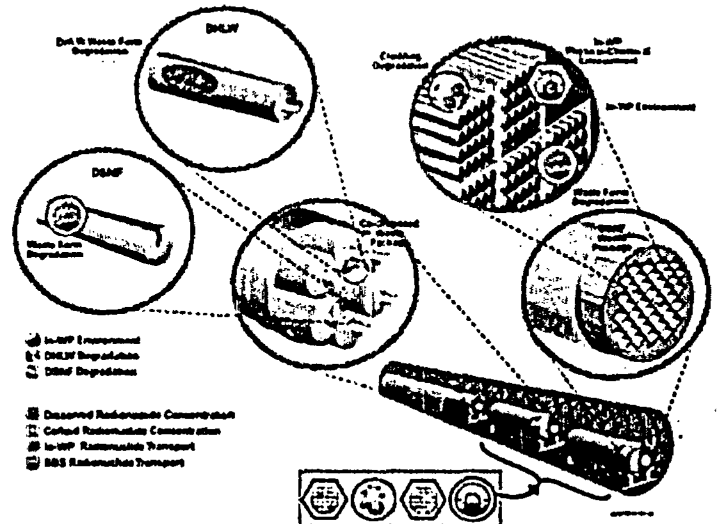


Total System Performance Assessment - Site Recommendation Nominal Performance

Fraction of Failed Waste Package for the Total System Performance Assessment - Final Environmental Impact Statement



Components Related to the Source Term Radionuclide Release from the Waste Form



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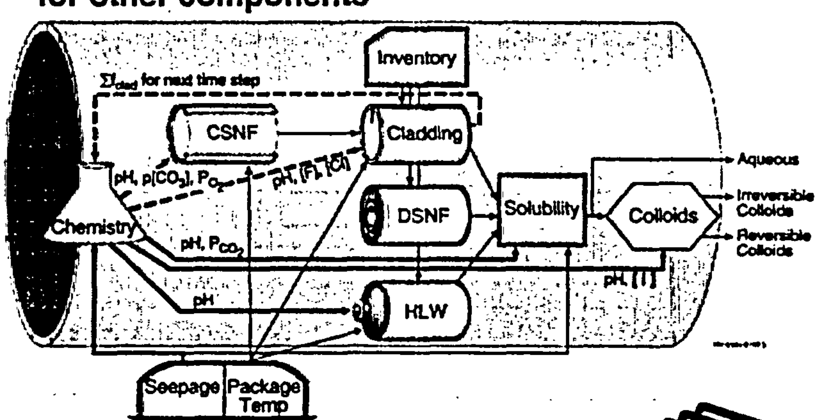
Waste Form Degradation Model in Total System Performance Assessment-Site Recommendation Consists of Eight Components

Chemistry component coordinates conditions for other components



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Technical Bases of In-Package Chemistry Component

- Cladding, high-level waste, and basket (e.g., stainless steel) degradation rates, and fixed gas pressures (CO_2 and O_2) control bulk chemistry (pH, $[CO_3^{-2}]_T$, [I], [Cl⁻], and [F⁻])
  - Degradation rates of basket and high-level waste evaluated in uncertainty
- Bulk chemistry approximated by well mixed, oxidizing conditions
  - Localized chemistry effects on cladding degradation (including the effects of radiolysis) not included, except for F⁻ flux
- Chemical condition in waste package dominates effect of incoming chemistry
  - Influence of evaporation evaluated
  - Influence of cement evaluated in features, events, and processes analysis

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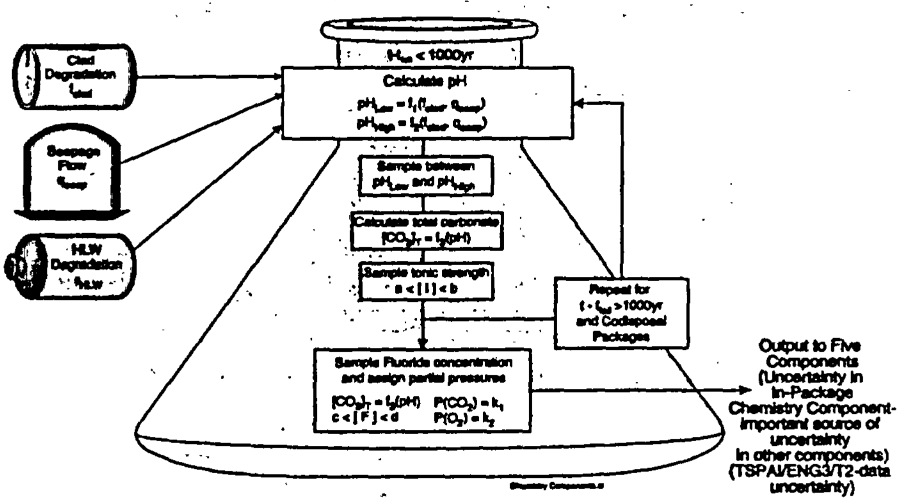
In-Package Chemistry Component Estimates pH, Calculates $[CO_3^{-2}]_T$, and Samples [I] and [F⁻]



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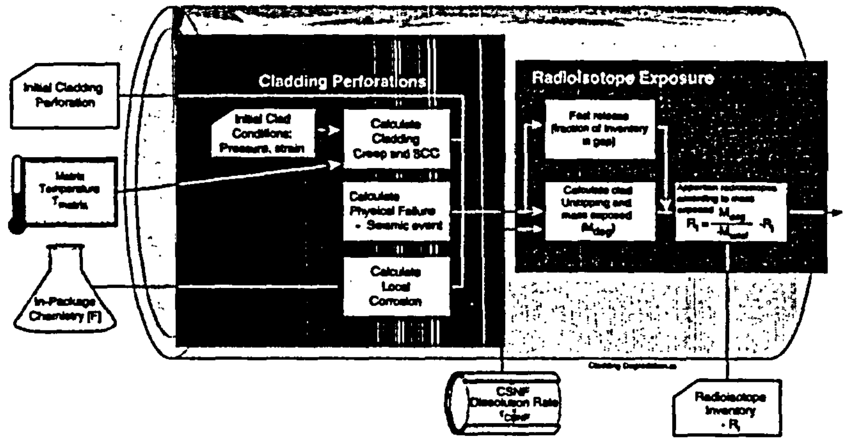
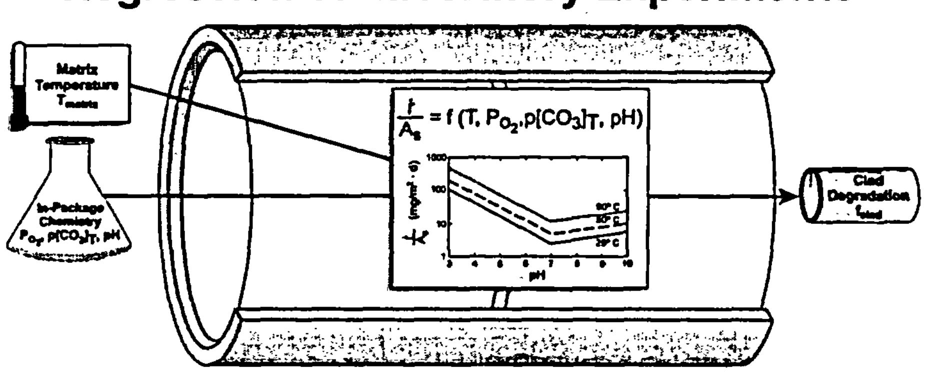
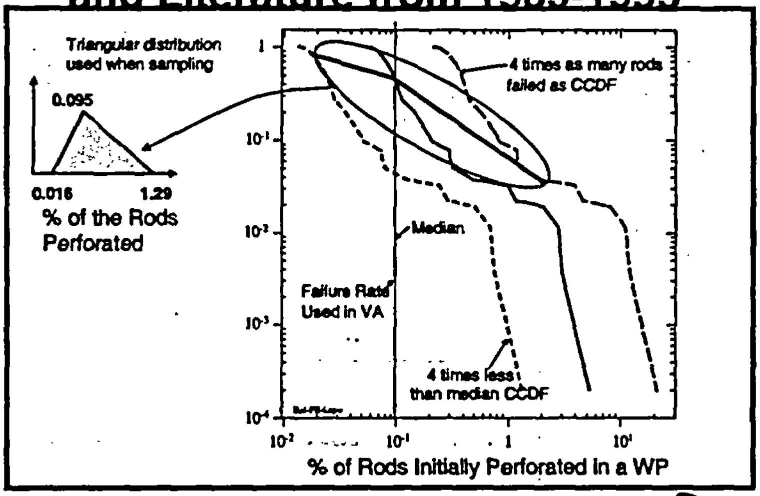
Cladding Degradation Consists of Two Steps Perforation and Unzipping



Commercial Spent Nuclear Fuel Matrix Degradation Component Based on Regression of Laboratory Experiments



Cladding Perforations before Receipt based on NRC Contractor Report (1969-1985) and Literature from 1985-1995



Radionuclide Inventory

Nominal Performance

^{14}C, ^{99}Tc, ^{129}I, ^{227}Ac, ^{229}Th, ^{230}Th, ^{231}Pa, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{241}Am, ^{243}Am, ^{210}Pb, ^{226}Ra

Direct Release (volcanic eruption)

Above, plus ^{90}Sr, ^{137}Cs, ^{232}U

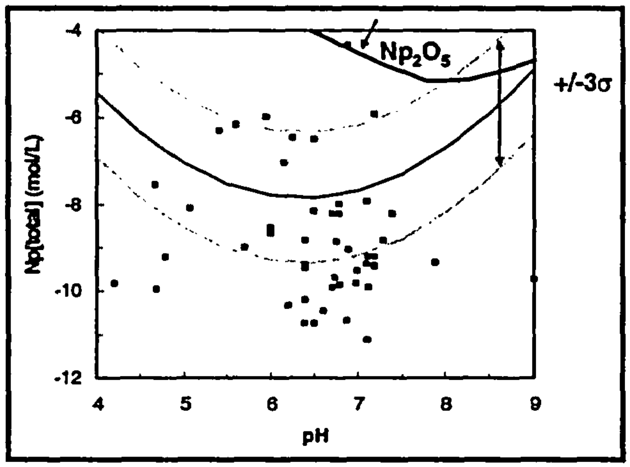
Human Intrusion

Above, plus ^{90}Sr, ^{137}Cs

- **Radionuclide suite depends on scenario**
  - **Parents and intermediate daughters of chains are included**
  - **Human intrusion and volcanic eruption scenarios require additional nuclides be included**
- **Radionuclide suite also depends on performance measure**
  - **Ground-water protection requires some additional nuclides, e.g., ^{228}Ra and ^{232}Th**

Np Dissolved Concentrations

- Distribution based on laboratory data
- Conservatively selected pure phases to control solubility
- Conservatively fixed gas pressures CO_2, O_2 at atmospheric conditions
- Conservatively neglect sorption or coprecipitation of radionuclides



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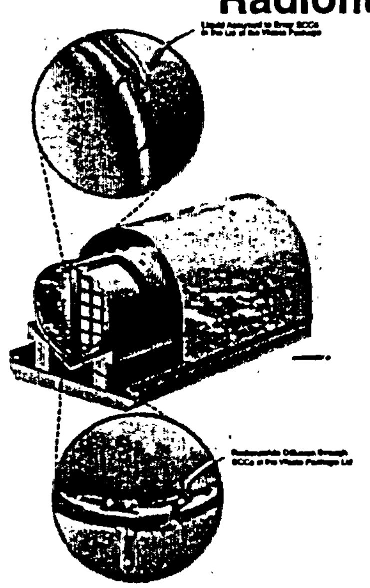
Engineered Barrier System Radionuclide Transport



- Releases for most locations will occur by diffusion only, if
  - Little or no water seeps into drift
  - Little or no water seeps through drip shield
  - Little or no water condenses under drip shield
  - Only small cracks (stress corrosion cracking) in waste package
- Advective releases require flux to seep into drift, through degraded drip shield and degraded waste package
- Possible in-package evaporation of seepage into waste package for commercial spent nuclear fuel waste packages conservatively ignored

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Summary of Potential Differences Between the DOE and NRC Source Term Models

- In-Drift Environment
  - Fraction of repository with seeps
- Drip Shield and Waste Package Degradation
  - Fraction of degraded drip shields and waste packages due to improper placement, rock fall, seismic events
  - Degradation rate of Titanium and Alloy 22
  - Treatment of uncertainty and variability in degradation rates
  - Treatment of conditions potentially initiating localized corrosion of drip shield (F^-) and Alloy 22

Summary of Potential Differences Between the DOE and NRC Source Term Models
(Continued)

- In-Package Environment
  - Cladding degradation rates
  - Fraction of exposed waste that is contacted by moisture (available for diffusive transport) versus contacted by seepage flux (available for advective transport)
  - Chemical environment
- Waste Form and Engineered Barrier System Mobilization and Transport
  - Alteration rate of various waste forms
  - Solubility of radionuclides
  - Advective versus diffusive transport

Backup

Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

YUCCA MOUNTAIN PROJECT

Backup - Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Engineered Barrier System Environments

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Waste Package Lifetime	In-Drift Physical and Chemical Environments In-Drift Thermal-Hydrologic Environment	• Rock volume and mass distribution • Temperature and RH on the drip shield and waste package surface – f (time, location, waste type, time, [illegible]) • Fugacity of CO_2 • pH – f (region, time) • Chloride – f (region, time) • Mass of microbes • Seepage flux through the drip shield • Fraction of drip shield and waste package surface that is wet

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Backup - Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Drip Shield and Waste Package Degradation

Key Attributes of Performance	Process Model Factor	TSPA-SR Input Parameters
Waste Package Lifetime	Drip Shield Degradation and Performance	• Probability of material and manufacturing defect flaws in drip shield • Size of material and manufacturing defect flaws in drip shield • Probability and size of rockfall induced by seismic activity • Threshold for general corrosion initiation • General corrosion rate under drip and no-drip conditions • Crevice corrosion initiation threshold • *Probability (or area) of crevice formation on drip shield* • Stress and stress intensity factor profile in drip shield • SCC initiation threshold • SCC crack growth rate • Effect of material and manufacturing defects on SCC initiation and crack growth rate • Effect of rockfall damage on SCC initiation and crack growth rate • Hydrogen concentration profile in drip shield • HIC initiation threshold • Penetration opening size by general corrosion, localized corrosion and SC
	Waste Package Degradation and Performance	• Probability of material and manufacturing defect flaws in waste package • Size of material and manufacturing defect flaws in waste package • Threshold RH for general corrosion initiation under drip and no-drip conditions • General corrosion rate under drip and no-drip conditions • Crevice corrosion initiation threshold of WP outer barrier • *Penetration opening size by general corrosion, localized corrosion and SCC* • Stress and stress intensity factor profile at closure welds • SCC initiation threshold • SCC crack growth rate • Effect of material and manufacturing defect on SCC initial and crack growth rate • MIC factor on corrosion rate • Kinetics phase instability processes in base metal and weld • Aging factor on corrosion rate

NOTE: HIC - Hydrogen-Induced Cracking
MIC - Microbiologically Influenced Corrosion
SCC - Stress Corrosion Cracking
SC - Stress Corrosion
WP - Waste Package

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Backup - Summary of Total System Performance Assessment Model Input Parameters Related to the Source Term

Radionuclide Release From the Engineered Barriers

Key Attributes of System	Process Model Factor	TSPA-SR Input Parameters
Radionuclide Mobilization and Release from the Engineered Barrier System	*In Package Environments*	• pH – f (region, time) • Total dissolved carbonate (CO_3^{2-}) – f (region, time) • Oxygen fugacity – f (region, time) • Ionic strength – f (region, time) • Fluoride – f(region, time) • CO_2 fugacity • Volume of water in the waste package/waste form cell
	Cladding Degradation and Performance	• Fraction of surface area of Zircaloy-clad CSNF exposed as a function of time
	CSNF Degradation and Performance	• CSNF intrinsic dissolution rate
	DSNF Degradation and Performance	• DSNF intrinsic dissolution rate
	HLW Degradation and Performance	• HLW intrinsic dissolution rate • Specific surface area
	Dissolved Radionuclide Concentration	• Concentration limits (solubilities) for all isotopes
	Colloid-Associated Radionuclide Concentrations	• Types of waste form colloids • Concentration of colloids • K_d and/or K_c for various colloid types • Fraction of inventory that travels as irreversibly attached onto colloids
	In-Package Radionuclide Transport	• *Porosity of corrosion products – f (time)* • Saturation of corrosion products – f (time) • Evaporation – f (temperature, relative humidity, composition)
	EBS (Invert) Degradation and Performance	• Thermally perturbed saturation in the invert – f (waste type, region, time, climate) • Porosity of the invert • *Diffusion coefficient* • Volumetric flux through the invert – f (climate, time) • Saturation in the invert after thermal pulse – f (time)

NOTE:
CSNF - Commercial Spent Nuclear Fuel
DSNF - Defense Spent Nuclear Fuel
EBS - Engineered Barrier System
HLW - High Level Waste

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G. Hornberger, ACNW Chairman: Bob, I just want to make sure I understand your response to Rod's question [regarding chemistry inside the waste packages] and whether you have the geochemical modeling right to get the right phases. Even if you do not have the right phases, do you have any phases?

R. Andrews (BSC): Yes.

G. Hornberger, ACNW Chairman: Are you taking into account secondary mineral precipitation?

R. Andrews (BSC): Yes, secondary phases are in there.

G. Hornberger, ACNW Chairman: This morning, Joe Payer, I believe, had a question as to how radionuclides get incorporated into these crystal structures?

R. Andrews (BSC): Argonne has some data from their degradation tests of the different phases and phase evolutions of the spent fuels. We have compared those phases with the phases that we have incorporated in the EQ-36-type thermodynamic model. I think Rod's point is well taken. The actual thermodynamic data for some of those phases is scarce.

R. Ewing, Univ. of Michigan: Good experimental data do exist for two of the phases. Also, there are calculational methods that are turning out to be very accurate.

4.6 Source Term Module Under the TPA

Source-Term Modeling and Support

David W. Esh
U. S. Nuclear Regulatory Commission

Dr. David Esh provided a review of the NRC's source-term modeling. This included conceptualizations of how groundwater could enter repository drifts and come into contact with drip shields and waste packages. The amounts of water that could actually enter corroded waste packages in the future appears to be affected by diversion around drifts caused by capillary barriers and by the tendency for water to run down walls rather than drip into openings. Two conceptual models for water contact are the "bathtub" and the "flow through" models. Dr. Esh reviewed processes of drip shield corrosion, uniform and localized corrosion of waste packages, and waste package stress-corrosion cracking. Dr. Esh then reviewed various models for dissolution of spent nuclear fuel within the waste form. The current TPA code version simulates advective transport of radionuclides out of waste packages. The TPA version 5.0 will include transport by diffusion in films of water inside and outside of waste packages. Dr. Esh concluded that the NRC models are primarily data based, use simple concepts, and provide the NRC staff with the flexibility to evaluate data and model uncertainties for the proposed Yucca Mountain site.

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Source-Term Modeling and Support

David W. Esh, Ph.D.

Environmental and Performance Assessment Branch
Contact info: (301) 415-6705, dwe@nrc.gov

Main Contributors: **Tae Ahn, Gustavo Cragnolino, Vijay Jain, Richard Codell, Osvaldo Pensado, Roberto Pabalan, Sitakanta Mohanty**

Presented to: **The Advisory Committee on Nuclear Waste, March 25-26, 2003**

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Overview- NRC Source-Term Modeling

- **"Data"-based** (as much realism as practical)
- Based on **simple** concepts
- **Flexible** - to enable review considering uncertainty
- Development **independent** of DOE
- Computationally **efficient**
- **Alternatives** represented (conceptual models)

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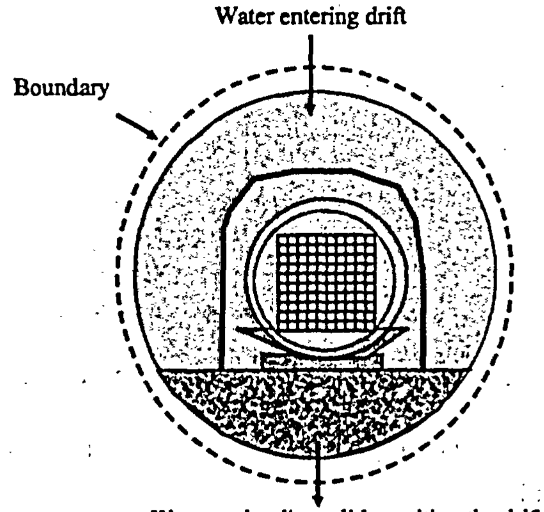

- Seepage and water contacting waste
- Drip shield corrosion
- Waste package corrosion
- Spent fuel degradation
- Glass degradation
- Cladding failure
- Radionuclide release

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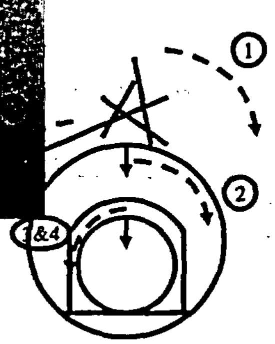
Seepage and water contacting waste

<u>POTENTIAL DRIPPING TO ENGINEERED BARRIERS:</u>

- Account for variability in dripping water
- Spatial variability in both infiltration and hydraulic conductivity
- Variability in the fraction of engineered barriers getting wet and the amount of flow
- Many parameters correlated to prevent unphysical results



<u>FRACTION OF DRIPPING ENTERING WASTE PACKAGE (F_{mult}):</u>

- Assumes thru-going holes in WP
- Multipliers for diversion of water by:
  (1) diversion around drift by capillarity
  (2) water running down walls
  (3) water not impacting holes
  (4) diversion from holes because of corrosion products

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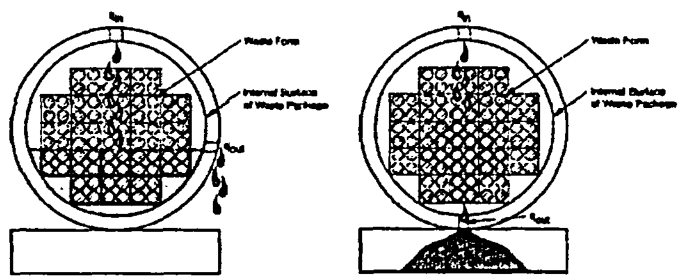
Conceptual Models for Water Contact



- Bathtub and flow-through conceptual models for water contacting the waste.
- Bathtub modeled as a stirred-tank and solubility limits are applied.

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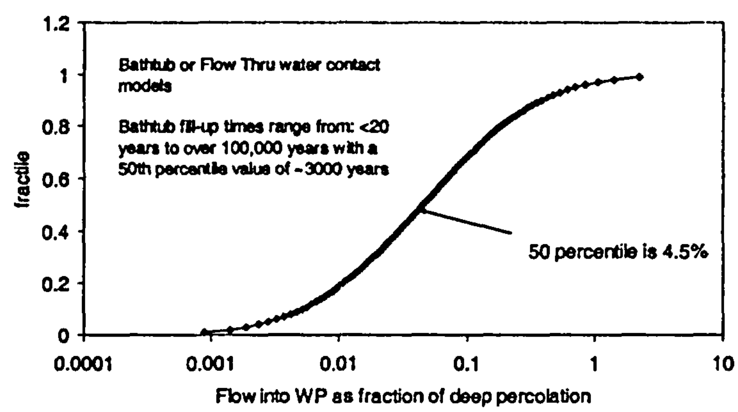
Seepage and water contacting waste



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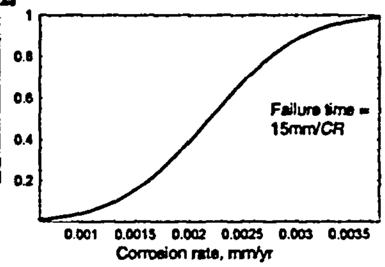
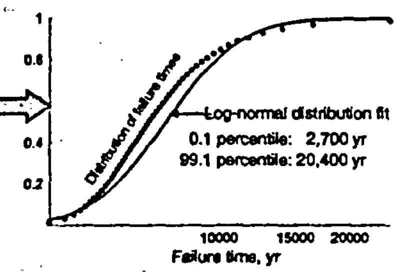
Drip shield corrosion

- Ti Grade 7 current densities in the range 10^{-8} to 5×10^{-7} A/cm^2 (pH range 2.1 to 10.7, [Cl] range 0.1 to 1M, 95°C)
- Corrosion rates ranging from 8.7×10^{-5} to 4.3×10^{-3} mm/yr (assumed 0.1 and 99.9 percent quantile values of a normal distribution)
- Assumptions: general corrosion occurs from only one side of the drip shield, general corrosion is the only degradation mechanism





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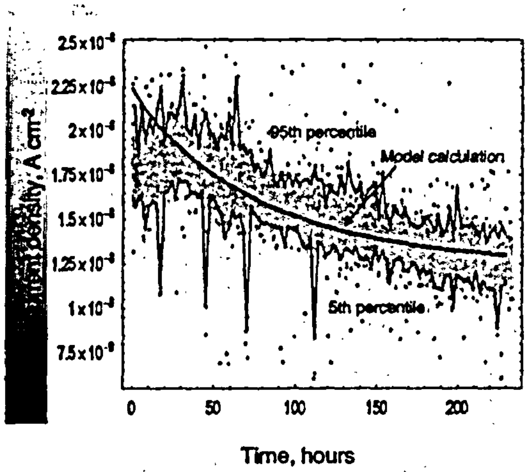
Waste package – uniform corrosion



- Extension of Point Defect Model to ternary alloy system based on Cr_2O_3-rich passive film with Ni, Cr, and Mo (interstitial cations) as predominant charge carriers
- Vacancies created by alloy dissolution and accumulated at the metal-film interface lead to a passive current density (i_{pass}) decrease until steady state is reached
- Breakdown of passivity or enhanced dissolution for extended periods is unlikely

Measured in 0.028M Chloride solution at 95 °C

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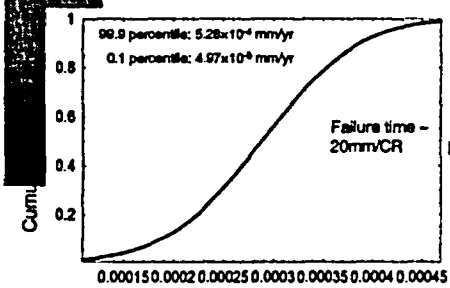
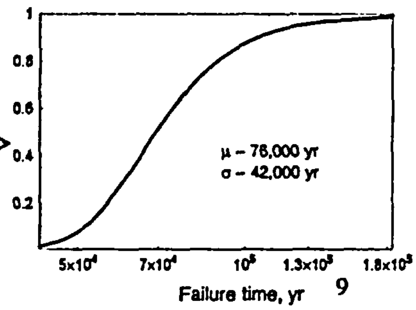
Waste package – uniform corrosion

- Passive current densities in the range 5×10^{-9} A/cm^2 to 5.4×10^{-8} A/cm^2 (pH range 2.7 to 8, [Cl] range 0.028 to 4 M, 95°C)
- The corrosion rate in the code is computed using Faraday's law.
- Corrosion rates ranging from 4.97×10^{-5} to 5.28×10^{-4} mm/yr (assumed 0.1 and 99.9 percentiles of a normal distribution)
- Assumptions: breach defined to occur as complete penetration of the waste package wall thickness by the corrosion front





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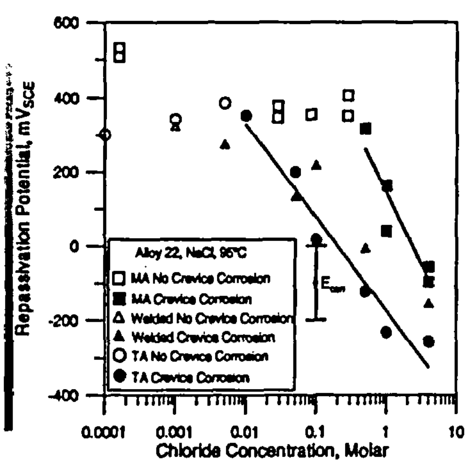
Waste package – localized corrosion



MA – Mill Annealed
TA – MA + Aged 5 minutes at 870 °C
Welded – MA + Welded

- Localized (crevice) corrosion occurs when the corrosion potential (E_{corr}) is higher than the crevice corrosion repassivation potential (E_{rcrev})

$$E_{rcrev} = E^{o}_{rcrev}(T) + B(T)\log[Cl^{-}]$$

where $E^{o}_{rcrev}(T)$ and $B(T)$ are linear functions of temperature

- As a result of welding and post-welding processes, E_{rcrev} may become lower than E_{corr}, facilitating the occurrence of localized corrosion at Cl^{-} concentrations lower than those required for the MA alloy
- These effects, as well as the inhibiting effect of NO_3^{-}, can be introduced in the code through changes in the E_{rcrev} expression

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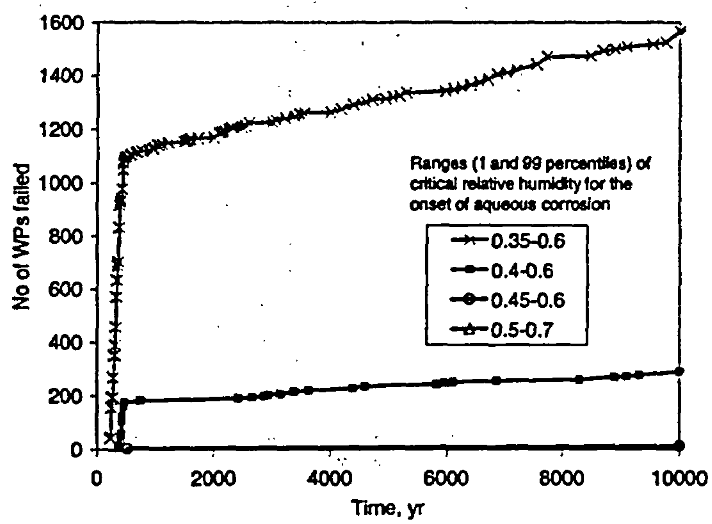
Waste package – localized corrosion



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Waste package – stress corrosion cracking (SCC)

Test conditions and results for the testing of Alloy 22 precracked double cantileverbeam (DCB) specimens

Specimen ID (Orientation)	Test Solution and Temperature	Potential (mVSCE)	Duration (hr)	Results
22-1 (T-L)	0.9 molal Cl^- (5% NaCl), pH 2.7 90 °C, N_2 deaerated	-330 to -310 (OC)	9,264 (386 days)	No crack growth
22-2 (T-L)	14.0 molal Cl^- (40% $MgCl_2$), 110 °C	-280 to -260 (OC)	9,264 (386 days)	No crack growth Grain boundary attack
22-7 (S-L)	14.0 molal Cl^- (40% $MgCl_2$), 110 °C	-270 to -250 (OC)	9,264 (386 days)	No crack growth Minor secondary cracking

T-L – Transverse-Longitudinal; S-L – Short tranverse-Longitudinal; OC – Open Circuit

- For the conditions evaluated and types of tests performed, stress corrosion cracking has not been observed.
- It appears that $E_{corr} < E_{SCC}$ and/or $K_I < K_{Iscc}$, which seems to be high for Alloy 22

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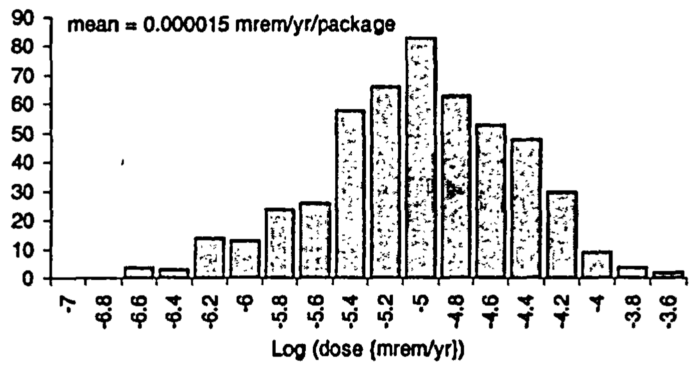
Waste package – SCC

- The TPA 4.1 code does not have an SCC abstraction.
  - experimental observations
  - additional analyses for risk impacts



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Wasteform - spent nuclear fuel (SNF)

Select Representative Spent Fuel Dissolution Rates

Dissolution Rate (mg/m2-day)	Sample	Solution (pH)	Test Method	Reference
0.2 - 1.0 – 1/140 for partially clad fuel	Spent fuel	J-13 (8.4)	Immersion	Wilson, 1990
3 x (10^{-3} - 1)	UO_2	$NaHCO_3$ + $CaCl_2$ +Silicic Acid (8.4)	Flow Through	Gray and Wilson, 1995
(0.8 - 2.5) x 10^{-3}	UO_2	Silicate Solution (Near Neutral)	Flow Through	Tait, 1997
0.07 36 (initial, will decrease)	Spent fuel	Allard Synthetic Groundwater (8.1) (2.0)	Immersion	Forsyth, 1997
2.7	Spent fuel	J-13 (8.4, down to 3.2)	Drip	ANL, Finch et al., 1999
10 (Factor 1/30 at pH 3 wrt pH 8)	UO_2	HCO_3 (3) Reducing	Flow Through	Bruno et al., 1991

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Wasteform - spent nuclear fuel (SNF)

- The NRC has 4 different models in TPA for SNF dissolution.
- Models based on experimental data for different conditions (model 1 and model 2), natural analogs (model 3), and secondary mineral formation [schoepite] (model 4).
- Base case is Model 2 (T=25 to 85 °C, J-13 and carbonate solutions)
- Temperature dependence from spent fuel tests under immersion and flow through conditions at 25 and 85 °C (Wilson 1990; Gray et al. 1992)
- Two models for SNF surface area: particle and grain.

$$r = r_o \exp[-E_a/RT]$$

E_a=activation energy [kJ/mol]
r_o=preexponential coefficient [mg/m^2-d]
R=universal gas constant [kJ/mol-K]
T= WP temperature [K]

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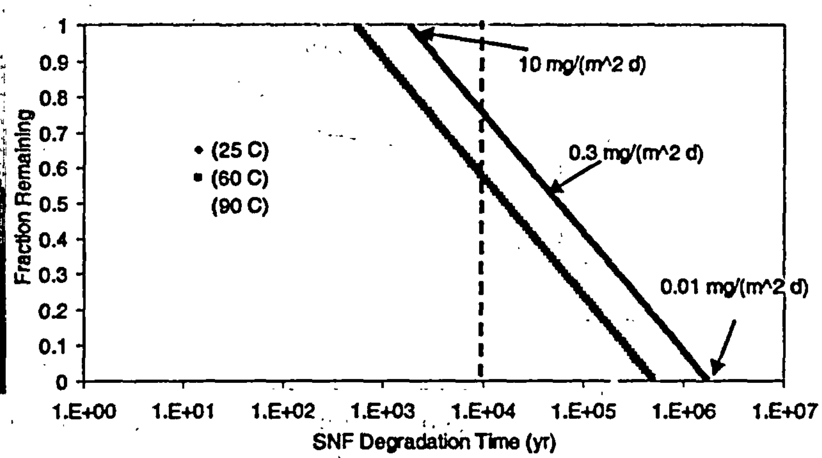
Wasteform - spent nuclear fuel (SNF)



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Wasteform – high-level waste glass*

- Estimated glass dissolution rates can be dependent on many variables (e.g., glass formulation, testing methods, test conditions)
- MANY experiments completed to determine dissolution rates
- Typical rate expression:

$$\text{Rate} = S\{\, k\,[1-(Q/K)]\}$$

$$k = k_0\, 10^{\eta\, pH} \exp(-E_a/RT)$$

S - surface area of glass immersed in solution
k - forward dissolution rate
Q - concentration of dissolved silica in the solution
K - a quasi-thermodynamic fitting parameter equal to the apparent silica saturation value for the glass

k_0 - intrinsic dissolution rate in g/m²-day
η - pH dependence coefficient
E_a - activation energy in kJ/mol
R - gas constant (8.314 kJ/mol-K)
T - temperature in Kelvin

* New for TPA 5.0

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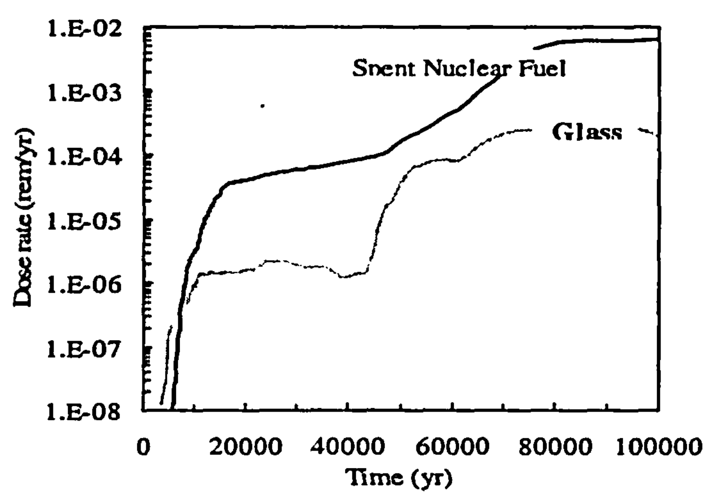
Wasteform – high-level waste glass



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Wasteform – cladding

- The failure mechanisms of cladding include (i) mechanical failure by external forces, (ii) localized corrosion, (iii) creep, (iv) hydrogen-induced failure, (v) splitting by matrix volume expansion, (vi) uniform corrosion, (vii) creep, and (viii) stress corrosion cracking.
- TPA4.1j has a factor (CladdingCorrectionFactor) to represent the fraction of the spent fuel surface area protected by cladding.
- CladdingCorrectionFactor is set by the code user for complete to no protection (can be time dependent in TPA 5.0).
- Approach allows flexibility and ease of use.

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Wasteform – cladding

- To assess the performance of spent fuel cladding as a metallic barrier to radionuclide release is as complicated as assessing the performance of the waste packages without the flexibility offered by improvements in design
- Complications arise largely from uncertainties associated with in-package chemistry. To assess the incidence of localized corrosion and external stress corrosion cracking, better estimates of concentrations of chloride, ferric ion, and radiolysis products, as well as pH, are needed
- To assess the possibility of hydride embrittlement and creep, better estimates of hoop stresses and temperatures profiles are required for upper range of fuel burn-ups

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Release and transport out of the package

Advective Transport

- Requires flow out of WPs carrying dissolved radionuclides.

Diffusive Transport (for TPA 5.0)

- Transport out of WP by diffusion in films of water inside and outside of WP.
- User defines lengths and thickness of films.
- Zero concentration boundary at outer surface of WP, and solubility limit at terminus of film inside WP.

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Release and transport out of the package

- Two models for aqueous release of radionuclides are available for selection by the user: bathtub and flow-through.
- Bathtub can have variable height, modeled as well-stirred tank with solubility limits applied.
- Flow-through model is the same, but doesn't allow buildup of fluid. The fraction of fuel wetted is independent:

$$M_{out}[i]=Q \cdot C[i]$$

where Q is the water flow rate and C[i] is the concentration of radionuclide i in solution determined by solubility limits.

- Solubility limits abstraction is based on (i) the likely solid phase precipitated or coprecipitated and (ii) the chemistry of the fluid that reacts with the solid phase.

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Release and transport out of the package

- For a number of radioelements (C, Cs, Cl, I, Se, Tc) solubility limits are set to 1.0 M because no solubility-limiting solids are estimated to form.
- The range and probability distributions of solubility limits for many other elements in TPA are based on and elicitation of experts conducted by DOE in 1993 (Wilson et al., 1994, CWRMS M&O, 1998).
- The assumptions behind the expert panel's distributions are:
  - the UZ water composition is bounded by that of J-13 well water and well UE-25p#1.
  - the solubility limits are determined by far-field groundwater environment.
  - the environment is oxidizing.
- TPA has a model for transport through the invert (simple advection/retardation/diffusion model) and a factor to bypass transport through the invert.

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Conclusions

- To extent practical, NRC models are <u>"data"-based</u>
- Based on <u>simple</u> concepts
- TPA provides NRC reviewer's the <u>flexibility</u> to complete review considering uncertainty

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Backup Slides

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Waste package – uniform corrosion (TPA 5.0)

- Range of corrosion rates will be redefined in TPA 5.0 (mean close to ~4×10^{-8} A/cm^2 (3.9×10^{-4} mm/yr) at 95°C).
- The definition for failure will be reconsidered in TPA 5.0:
  - Mechanical damage of partially corroded engineered barriers (need to consider the Type 316L inner container).
  - There is stochastic variability in the corrosion rates that could produce an irregular corrosion front. More flexibility in the consideration of distributed failures.
- Refinements in TPA 5.0 are not anticipated to change the conclusion indicating that waste packages will not breach in 10,000 years solely due to general corrosion.

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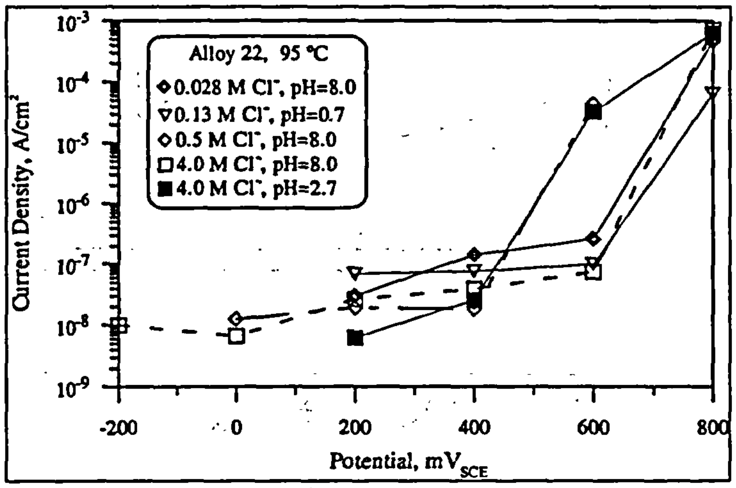
Waste package – uniform corrosion



Anodic current density of Alloy 22 measured under potentiostatic conditions for a period of 48 hours.

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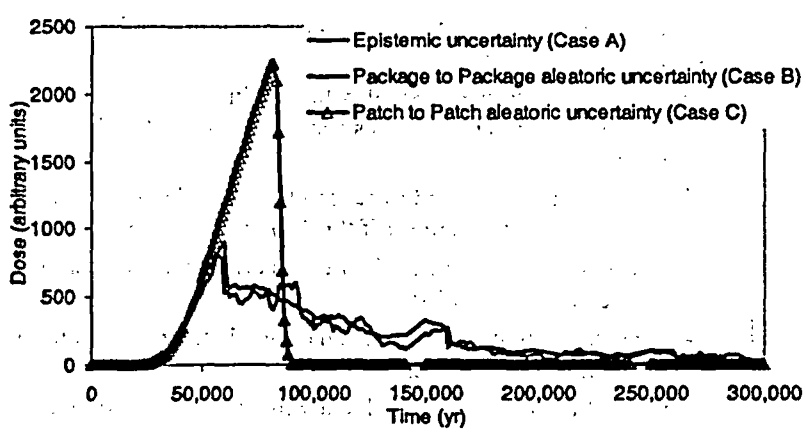
Waste Package Distributed Failure



Analysis by Codell et al. (2001 SRA) investigated the impacts on risk of the conceptual model to represent distributed waste package failure.

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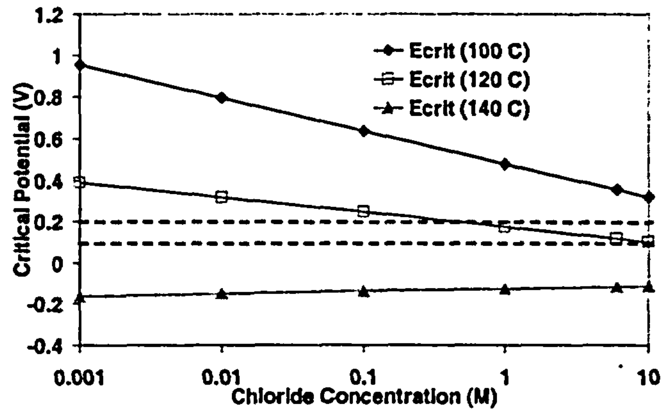
Waste package – localized corrosion



Corrosion potential range shown by dashed lines, localized corrosion only predicted by the model for temperatures at or above boiling and concentrated solutions.

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Drip shield corrosion (TPA 5.0)

- Influence of fluoride on corrosion rate disregarded in TPA Code Version 4.1j, because:
  - Amount of fluoride is possibly limited in Yucca Mountain system (fluoride forms Ti complexes and it is consumed in the corrosion reactions).
  - A mechanism is needed to accumulate fluoride on the drip shield surface (water tends runs off the drip shield surface).
- Nonetheless, the influence of fluoride on drip shield corrosion rate will be included in TPA 5.0
  - A multiplication factor, function of the fluoride concentration, will affect the corrosion rate.
- Mechanical failure of the drip shield will also be incorporated into TPA 5.0.

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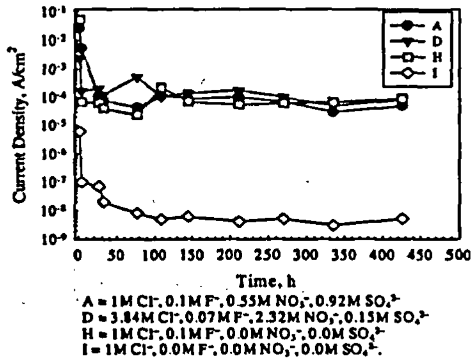
Drip shield – flouride effects



Effects of fluoride under passive current density of Ti Grade 7 in various deaerated solutions containing chloride, nitrate, and sulfate at 95 C and an applied potential of of 0 V_{SCE}.

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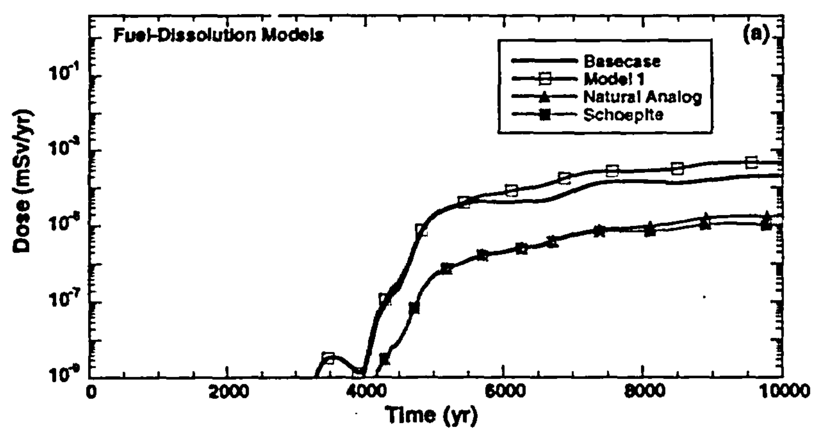
Spent Fuel Dissolution Model Sensitivity Analysis



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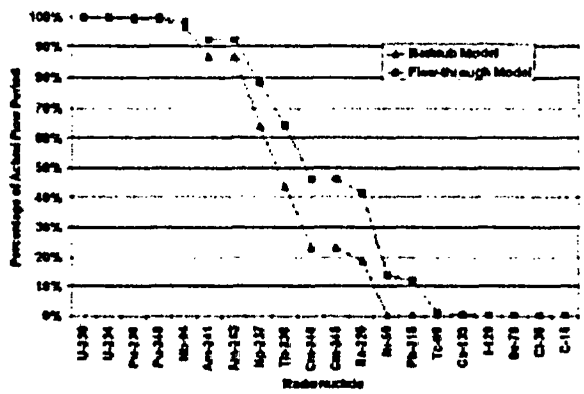
Solubility Limits Sensitivity Analysis



From Mohanty, Adams, Pabalan (MRS Fall 2002 Meeting), '*The Role of Solubility as a Barrier to Radionuclide Release*'

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R. Latanision, MIT: The data in these [corrosion] studies are at 95°C. If the project goes forward with a high temperature operating mode, then a considerable period of the lifetime of these packages and drip shields will be at higher temperatures.

D. Esh, NRC Staff: Sure.

R. Latanision, MIT: Intuitively I think the conclusion is right, that uniform corrosion probably is not an issue. But I guess I would feel more comfortable if I saw temperature dependent corrosion rates that would allow that sort of careful analysis. Is there project data that show the temperature dependence?

R. Andrews (BSC): Yes, there is some limited general data and temperature dependence [for uniform corrosion]. Those were also documented in the Supplemental Science Performance Analysis.

R. Latanision, MIT: Up to what range of temperature?

R. Andrews (BSC): That is a good question. The temperature range probably only went up to about 95°C.

J. Payer, CWRU: I think there's polarization data both at the center, perhaps Gustavo [Cragnolino] could mention.

R. Latanision, MIT: I know that.

J. Payer, CWRU: I believe passive current density data are up to 120° and 130°C.

D. Esh, NRC Staff: Your point is right on. If you believe you have a window of susceptibility, possibly at a higher temperature, because that is what the fundamental science says, then you would want to have some information on which to hang your hat. It is completely reasonable.

R. Latanision, MIT: My point is very simple. I think intuitively your conclusion is correct. But I would also be much more certain or comfortable with that if I could see some temperature-dependent data.

D. Esh, NRC Staff: What we find for the general corrosion information, both at the Center and this, I believe, would hold for the DOE weight loss data. They are very noisy or uncertain, whatever you want to call it. Experimental uncertainty. If you try to do a regression on the change in the general corrosion rate based on the environmental influences, you cannot come up with anything. You do not see that it is sensitive to pH, you don't see it is sensitive to chloride. You don't see it being sensitive to temperature. You just see it is an uncertain set of data. So you have to go to other types of measurements than those measurements that are confounded by silica precipitation in the DOE's case. Also, I think inherent measurement uncertainty exists in some of the measurements we get.

R. Latanision, MIT: I'm sorry, but I don't buy that. That is just not good enough. I mean, if you look at a couple of different temperatures with the same solutions, that is what I'm looking for. You have a reasonable environment here. And if you look at 90°or 120° and get corrosion rates, then I'm not sure that would be all that noisy.

D. Esh, NRC Staff: I did a regression with the data I had at 25°, 60° and 90°.

R. Latanision, MIT: We have to go into your lab and look at this.

D. Esh, NRC Staff: You basically get R squares that are statistically not significant. There is a lot of additional uncertainty in that data.

R. Latanision, MIT: So classical rate theory doesn't apply to corrosion rates in this case?

D. Esh, NRC Staff: I would expect that it but you can't elucidate that from the data.

R. Latanision, MIT: Yes

G. Cragnolino, Center for Nuclear Waste Regulatory Analyses (CNWRA): Let me clarify this point. I think I would have to combine the range of temperatures of all the boiling points of water solutions and diluted solutions. We did experiments in the range of room temperature to 95°C. It is true that, as was mentioned, there is a lot of uncertainty in the data, and we cannot come out with a very worthy value for the activation of energy and for the preintervention value. But we are confident that at least the temperature is right. Now we are using temperatures of about 100°C, but in order to do this, we have to work with the concentrated solution of cells. I asked to do experiments on the liquid cells without using a natural system that could create particular complications. This is what we have done, and are trying to do now, to see if the values that we are getting in the temperature range that we know (i.e., 25°to 95°C) can be extended out to 120°or 130°C.

R. Latanision, MIT: Right.

G. Cragnolino, CNWRA: This is the current situation. There is good reason to believe that the continuity of this physical process is going to have to work with the final concentrated solution, and we have a few weeks. I think the DOE is sensitive to doing the same thing, but they are confronting the same problem that we are.

4.7 Simplified Models of Key Contributors to Dose Traced Through Various Modules (DOE)

Component Performance and Key Contributors to Nominal Scenario Class Dose in the U. S. Department of Energy Total System Performance Assessment

Peter Swift
Sandia National Laboratories/Bechtel SAIC Company, LLC

Dr. Peter Swift reviewed the overall results for nominal repository performance, including the TSPA total dose, major contributors to dose over time, and the chronology of major events in nominal performance. Dr. Swift showed changes in radionuclide inventories over time. He showed estimates for major chronological events, such as stages in climate change, timing for peak waste package surface temperatures, first drip shield failures, waste package failures due to defects and general corrosion, and relative transport times in the natural system. He traced Np-237 and Tc-99 through the system, component by component (i.e., waste form, waste package, invert, and unsaturated and saturated zones). Dr. Swift noted that the TSPA models and analyses for the license application are currently under development.

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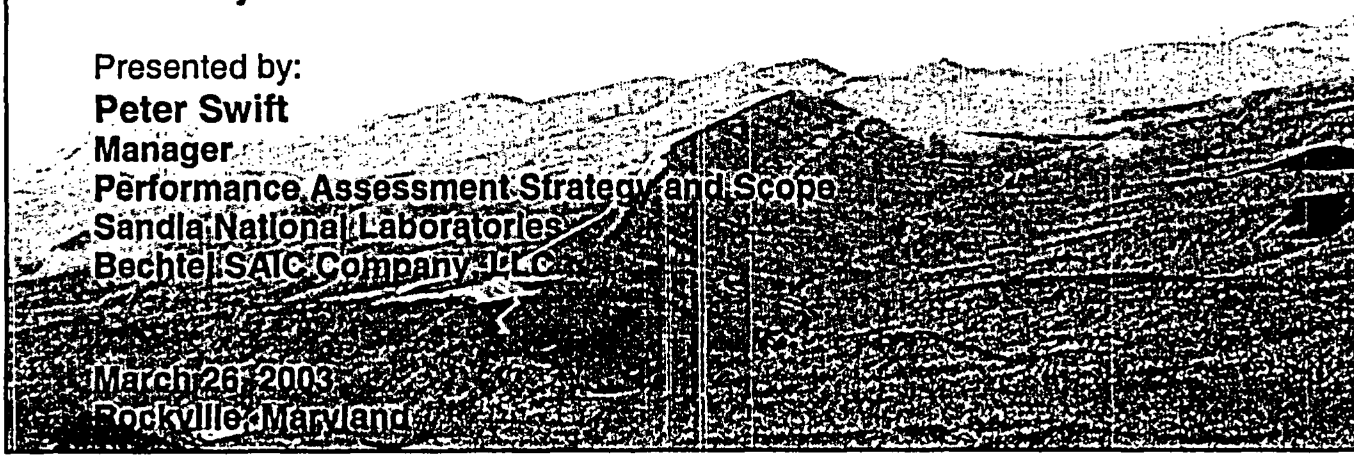
U.S. Department of Energy
Office of Civilian Radioactive Waste Management

Component Performance and Key Contributors to Nominal Scenario Class Dose in the U.S. Department of Energy Total System Performance Assessment

Presented to:
Advisory Committee on Nuclear Waste

Presented by:
Peter Swift
Manager
Performance Assessment Strategy and Scope
Sandia National Laboratories
Bechtel SAIC Company, LLC

March 26, 2003
Rockville, Maryland

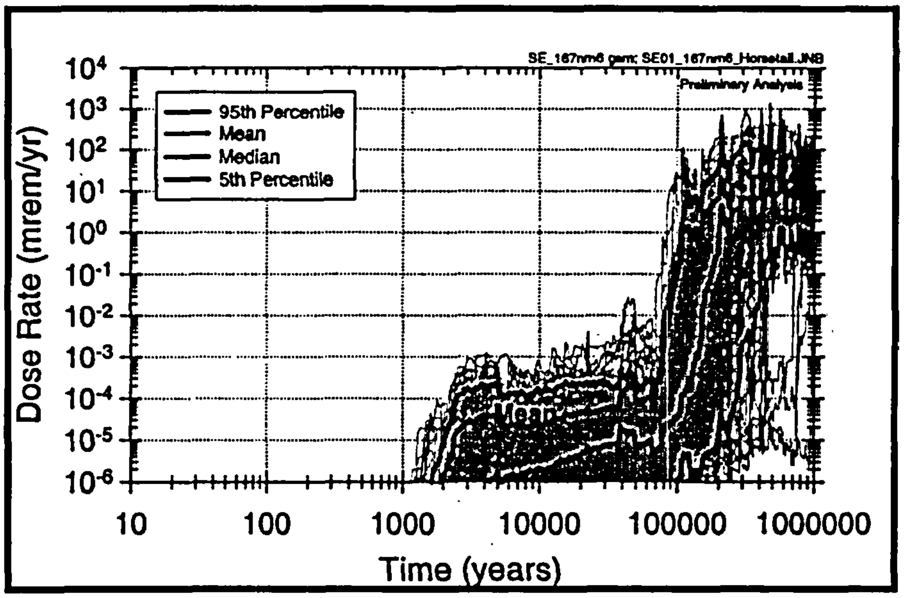


Outline

- Nominal performance scenario class overall results
  - Total System Performance Assessment total dose
  - Major contributors through time
  - Chronology of major events in nominal performance
- Component performance
  - Np-237 and Tc-99 traced through the system component by component
  - Additional results for water flux and radionuclide flux, as appropriate, available from one-on and one-off analyses, in backup material
- All results are draft examples, extracted from existing analyses, and shown as mean values
  - FY01 Supplemental Science and Performance Analyses
  - Final Environmental Impact Statement Analyses
  - "One - Off Analyses" performed with the Total System Performance Assessment - Final Environmental Impact Statement model
  - "One - On Analysis" performed with the Total System Performance Assessment - Final Environmental Impact Statement model
- Total System Performance Assessment Models and Analyses for the License Application are under development

Overall Performance Nominal Scenario Class

- Total System Performance Assessment - Final Environmental Impact Statement model, modified to include Sr-90 and Cs-137 transport, updated long-term climate states, one early waste package failure per realization, and regulatory specification for 3,000 acre-ft annual groundwater usage
- Results from ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12)



Mean annual dose based on 300 realizations of high-temperature operating mode nominal performance. Models and input values are preliminary. Results are for information only, and are not suitable for comparison to regulatory standards.

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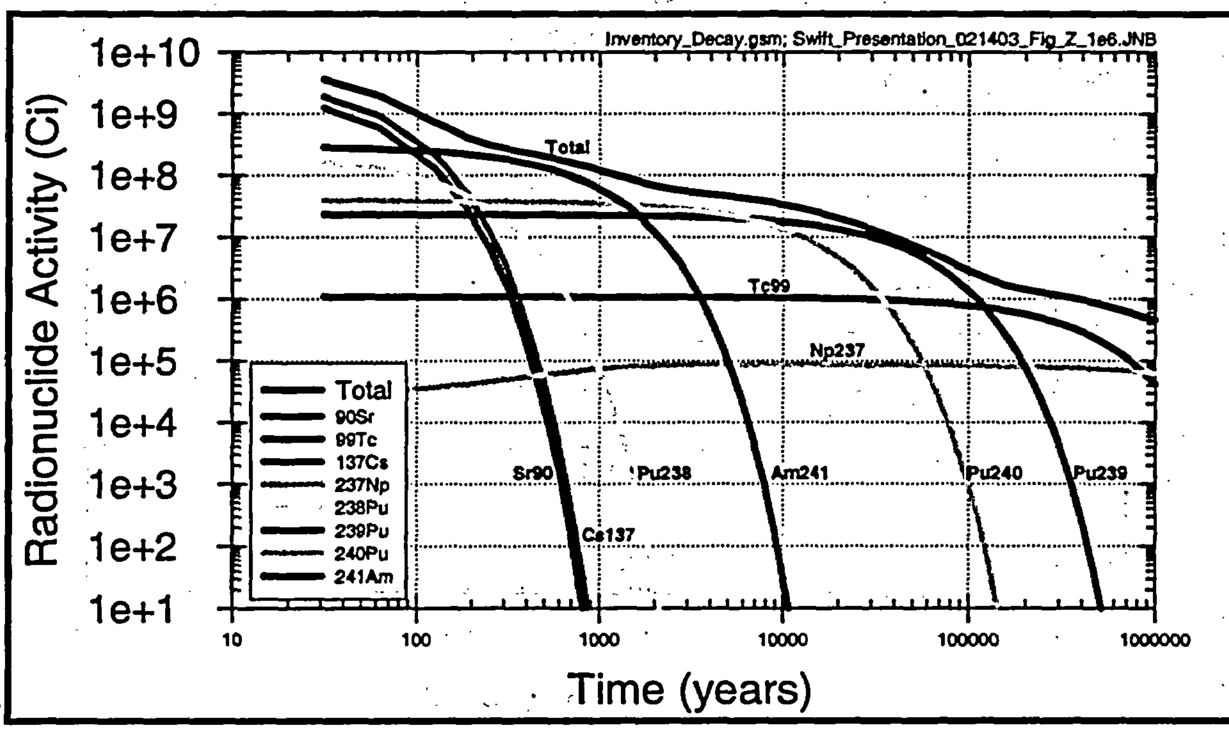
Yucca Mountain Radionuclide Inventory
(page 1 of 3)



Initial inventory from Total System Performance Assessment - Site Recommendation, adjusted for radioactive decay and ingrowth.

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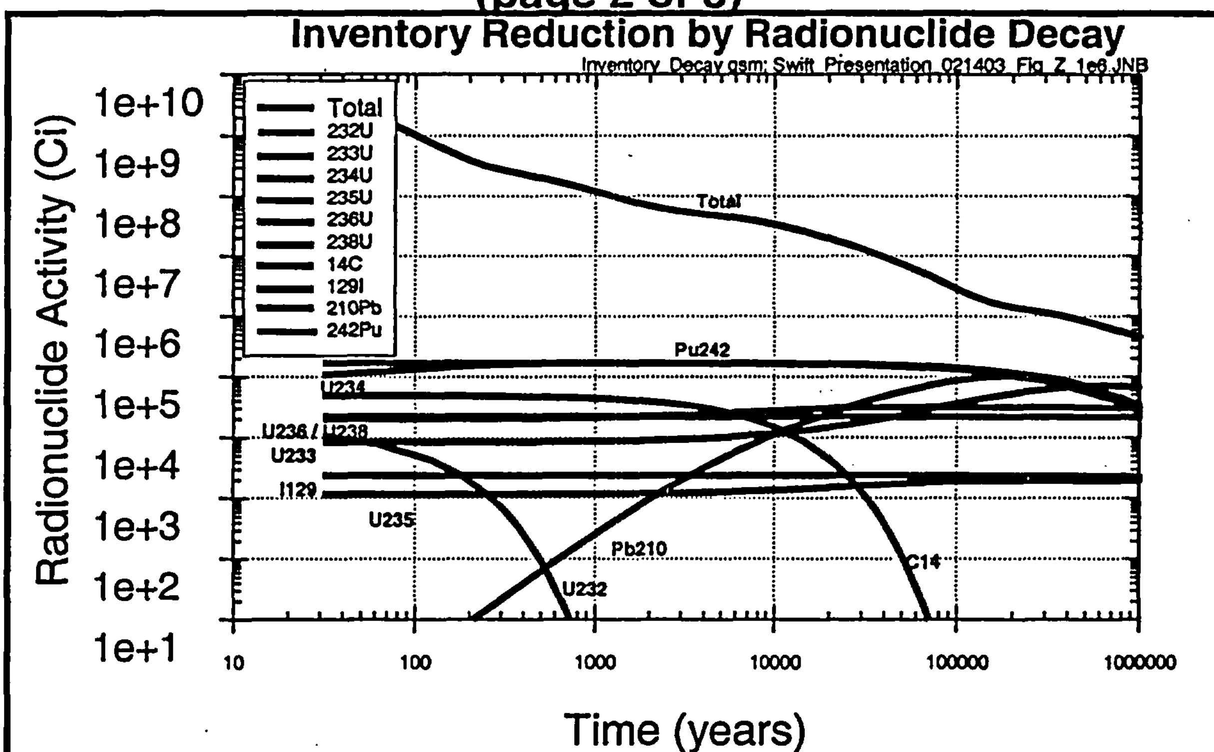
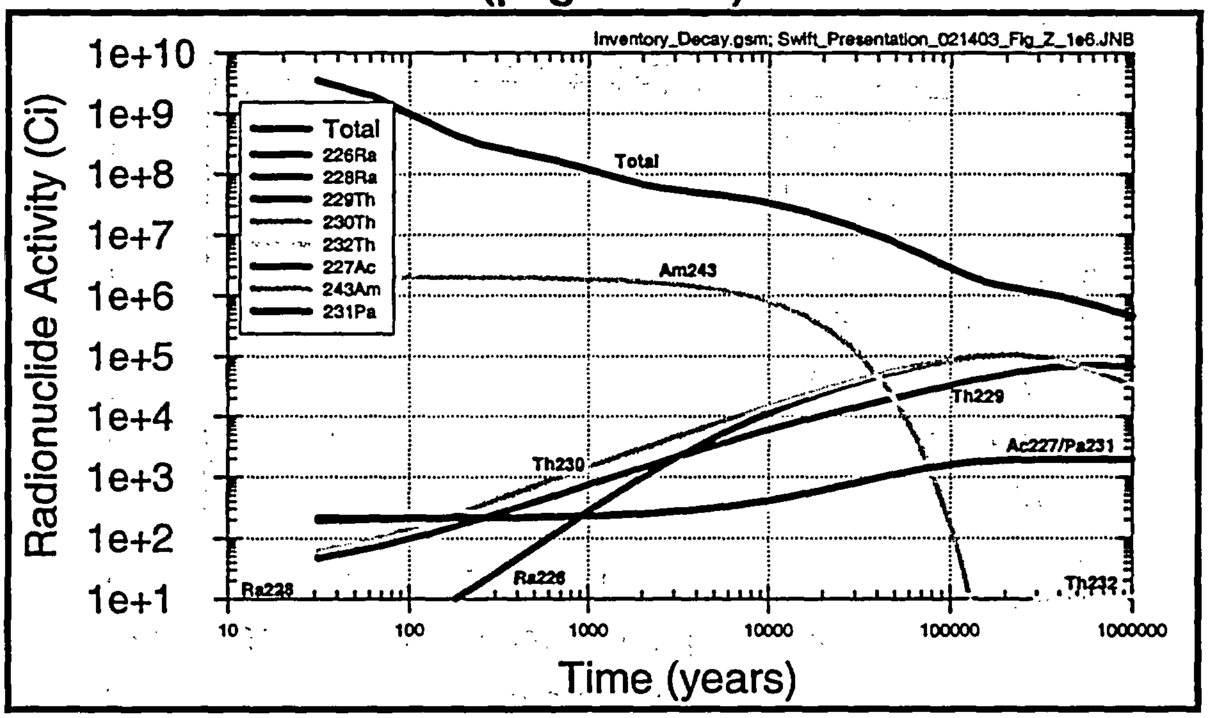
Yucca Mountain Radionuclide Inventory

(page 2 of 3)



Initial inventory from Total System Performance Assessment - Site Recommendation, adjusted for radioactive decay and ingrowth.

Yucca Mountain Radionuclide Inventory
(page 3 of 3)



Initial inventory from Total System Performance Assessment - Site Recommendation, adjusted for radioactive decay and ingrowth.

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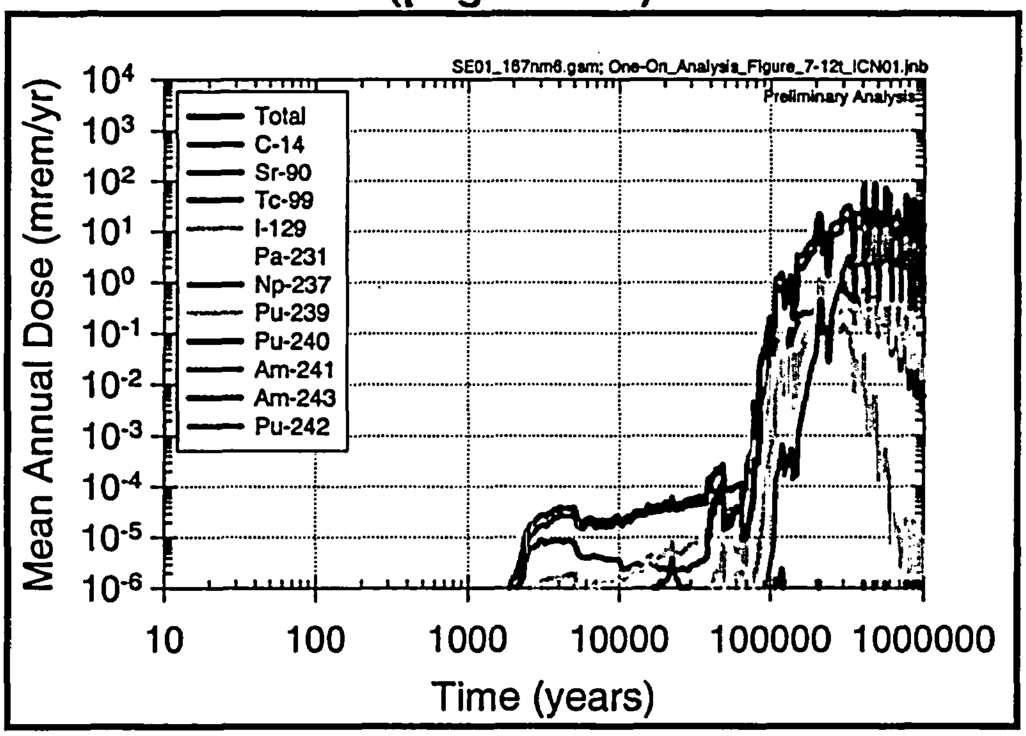
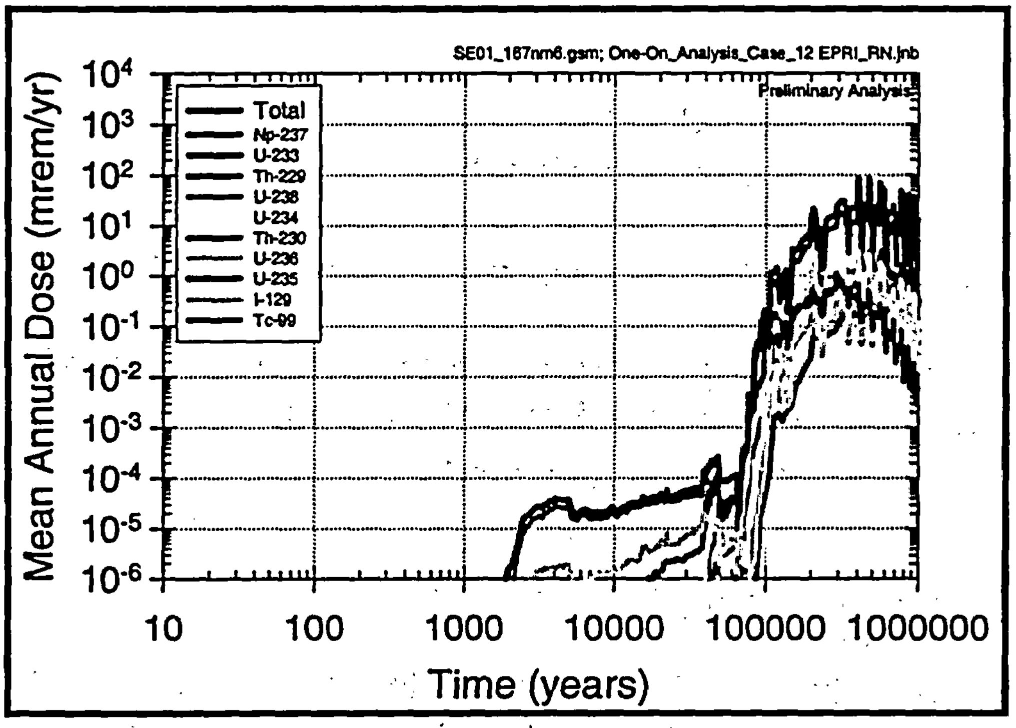
Contributors to Nominal Performance Dose
(page 1 of 2)



Results from ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12).

Contributors to Nominal Performance Dose
(page 2 of 2)



Results from ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12).

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Selected Chronology Information - Nominal Performance

(Total System Performance Assessment - Supplemental Science and Performance Analyses)

- Climate changes
  - 0-600 yr: present climate
  - 600-2000 yr: monsoonal climate
  - 2000-38,000 yr: glacial transition climate
  - 38,000 yr: first full glacial climate (recurs at 106 kyr, 200 kyr, etc.)
- Peak waste package surface temperature (repository average) for commercial spent nuclear fuel
  - High temperature operating mode: ~ 160 C, ~ 70 yr
  - Low temperature operating mode : ~ 84 C, ~ 350 yr
- Average high temperature operating mode temperatures fall below boiling at
  - Waste package surface (commercial spent nuclear fuel): ~ 700 yr
  - Drift wall (commercial spent nuclear fuel): ~ 600 yr

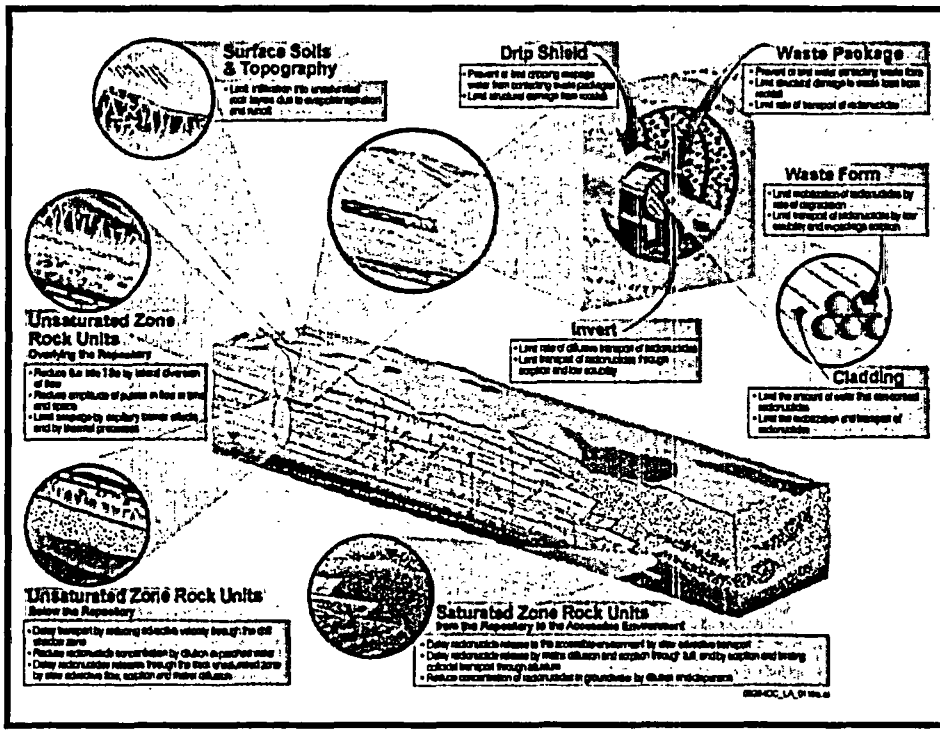
Selected Chronology Information - Nominal Performance

(Total System Performance Assessment - Supplemental Science and Performance Analyses)

(Continued)

- **Drip shield failures**
  - First failures by corrosion ~ 28 kyr, half of realizations show failure by ~ 100 kyr
- **Waste package failures due to weld defects**
  - Supplemental Science and Performance Analyses and Final Environmental Impact Statement: 1-2 packages per realization, probability ~ 0.23
  - Subsequent modeling: assumption of 1 package per realization, probability 1
- **Waste package general corrosion failures**
  - Supplemental Science and Performance Analyses high temperature operating mode: ~ first failures ~ 110 kyr, mean ~ 40% of waste packages intact at 1 Myr
  - Supplemental Science and Performance Analyses low temperature operating mode: ~ first failures ~ 170 kyr, mean ~ 40% of waste packages intact at 1 Myr
  - Final Environmental Impact Statement model without temperature-dependent corrosion: most packages fail between ~ 50 kyr and 200 kyr
- **Transport times in the natural system**
  - Described later in the presentation in the context of radioactivity flux

Major Nominal Performance Model Components Organized by Barriers



Surface soils and topography (includes climate, infiltration)

Unsaturated zone above (seepage, drift effects)

Drip shield

Waste package

Cladding

Waste form

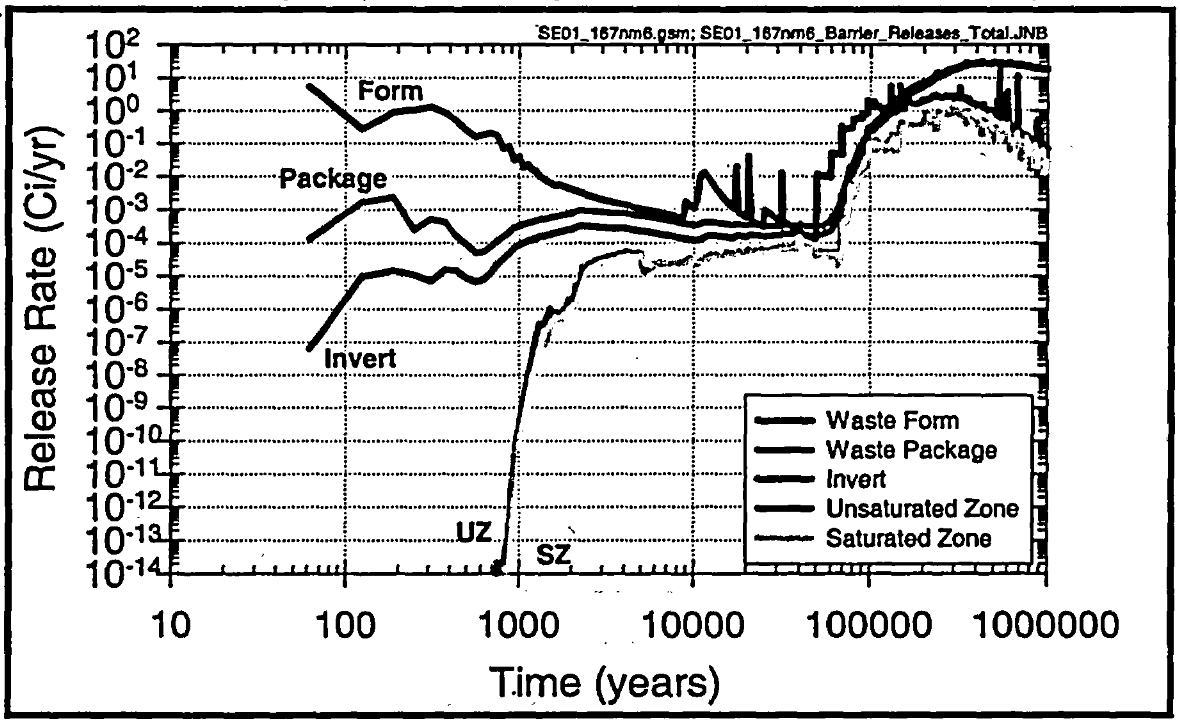
Invert

Unsaturated zone below (transport)

Saturated zone

Radionuclide Transport

Activity Flux (All Species) Leaving Each Component



Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12).

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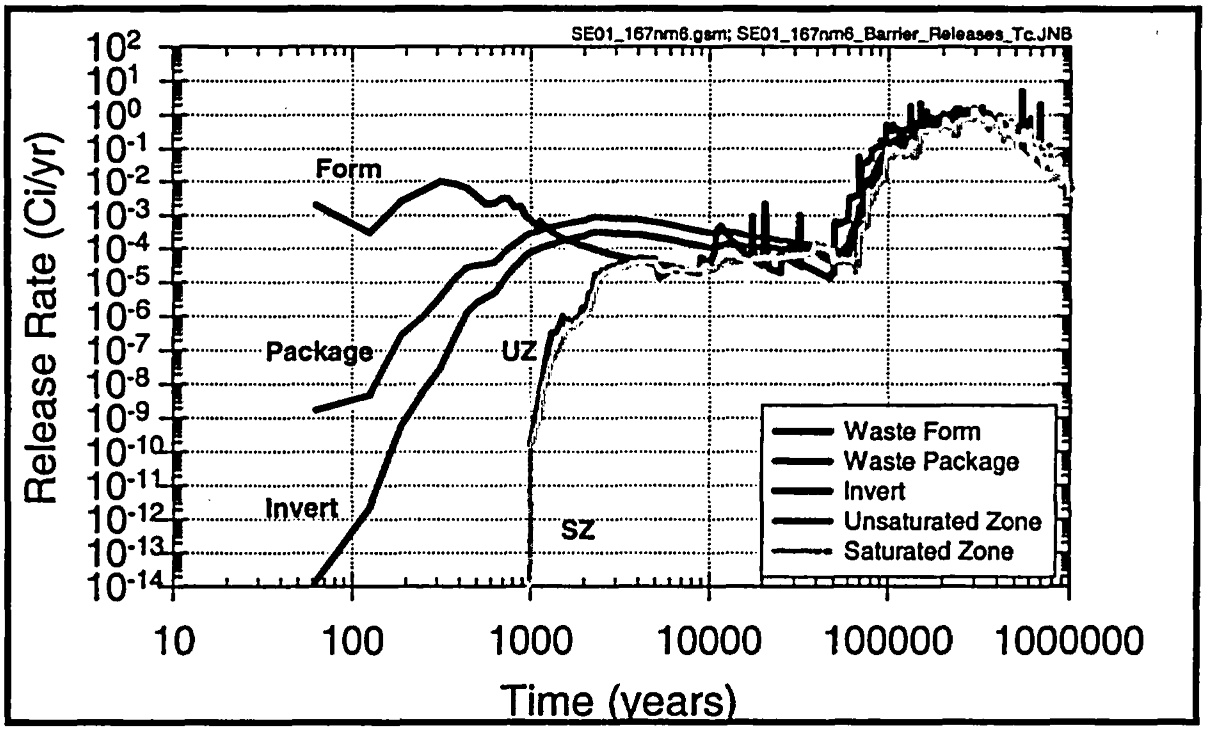
Technetium-99 Transport

Activity Flux Leaving Each Component



Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12).

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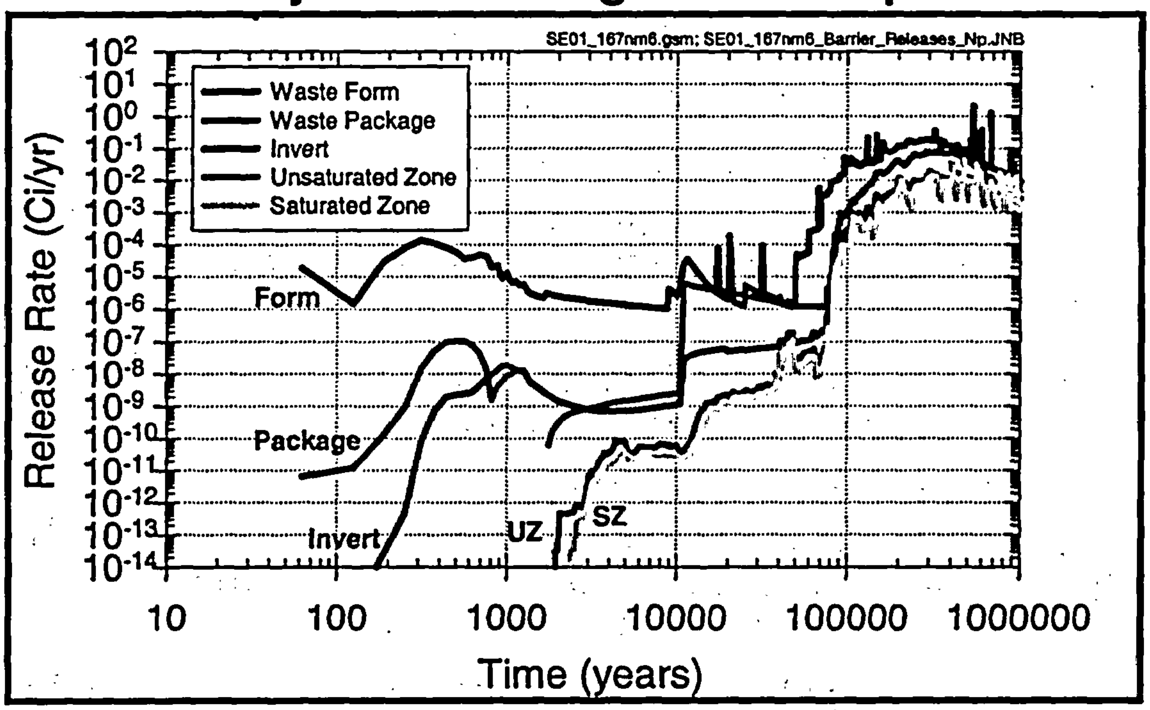
Neptunium-237 Transport

Activity Flux Leaving Each Component



Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12).

Nominal Performance Scenario Class: Summary from Current Total System Performance Assessment Analyses

- Total dose before ~ 40 kyr essentially equivalent to Tc-99 dose
  - Prior to drip shield failure, diffusion is dominant release mechanism
- At later time, drip shield failures allow advective transport from the waste package, and Np-237 becomes an important contributor
- Total dose after large-scale waste package failure (> 100 kyr) essentially equivalent to Np-237 dose
- Contributions to dose from the radionuclides that dominate radioactivity in the initial inventory Sr-90, Cs-137, Am-241, and Pu-238 are not significant because retardation in the natural system prevents release while inventory is high
- Contributions from long-lived Pu species do not dominate total dose because of effective retardation in the natural system

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References

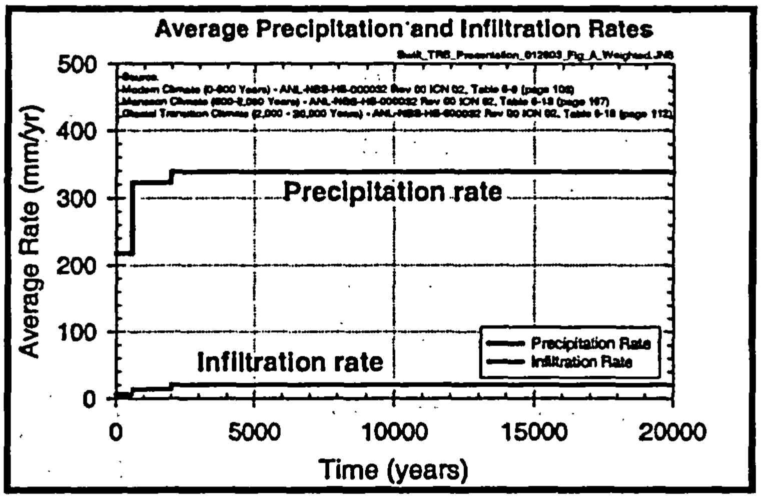
- "Total System Performance Assessment - Site Recommendation"
  - CRWMS M&O 2000. *Total System Performance Assessment for the Site Recommendation.* TDR-WIS-PA-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001220.0045
- "Total System Performance Assessment - Supplemental Science and Performance Analysis"
  - BSC (Bechtel SAIC Company) 2001. *FY01 Supplemental Science and Performance Analyses, Volume 2: Performance Analyses.* TDR-MGR-PA-000001 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010724.0110
- "Total System Performance Assessment - Final Environmental Impact Statement"
  - Williams, N.H. 2001. "Contract No. DE-AC08-01RW12101 – Total System Performance Assessment – Analyses for Disposal of Commercial and DOE Waste Inventories at Yucca Mountain – Input to Final Environmental Impact Statement and Site Suitability Evaluation REV 00 ICN 02." Letter from N.H. Williams (BSC) to J.R. Summerson (DOE/YMSCO), December 11, 2001, RWA:cs-1204010670, with enclosure. ACC: MOL.20011213.0056 (SL986M3, Rev. 00)
- "One-Off Analyses"
  - BSC (Bechtel SAIC Company) 2002. *Risk Information to Support Prioritization of Performance Assessment Models,* TDR-WIS-PA-000009 Rev. 01 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20021017.0045
- "One-On Analysis"
  - Saulnier, G. J., 2002. *Use of One-on Analysis to Evaluate Total System Performance.* Las Vegas, NV: Bechtel SAIC Company. ANL-WIS-PA-000004 Rev. 00 ICN 00

Backup

Surficial Soils and Topography

Example Barrier Capability Description

- Capability: reduce the rate of movement of water
- Comparison of precipitation and infiltration
  - Precipitation and infiltration are shown as spatial averages for 38.7 km^2 domain
  - Curves are weighted averages for low, medium, and high infiltration conditions corresponding to uncertainty in climate states
  - Steps in time history correspond to climate changes
- Surficial soils and topography reduce spatially-averaged water movement at 10,000 years approximately 16x

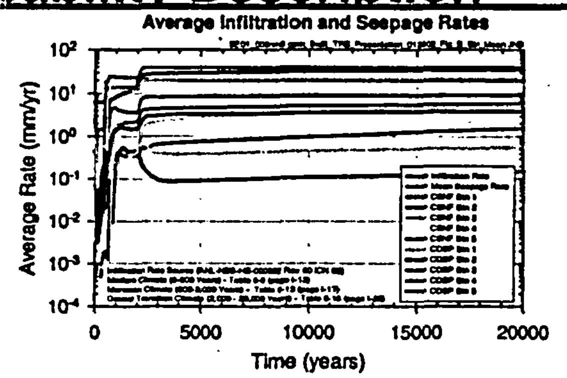


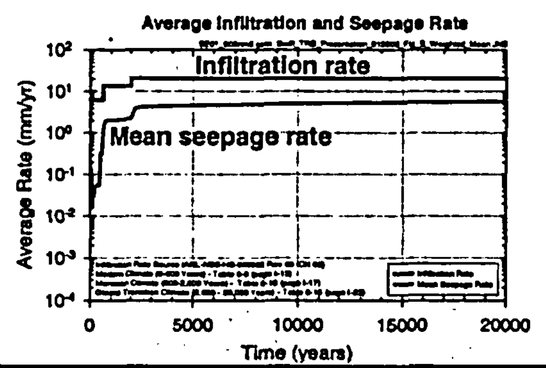
Extracted precipitation and infiltration based on spatially-averaged results from ANL-NBS-HS-000032 Rev. 00 ICN 02 [*Final Environmental Impact Statement/Supplemental Science and Performance Analyses Infiltration Model analysis model report*) for three infiltration maps, weighted by the relative frequency of occurrence of these maps in Total System Performance Assessment - *Final Environmental Impact Statement*.

Unsaturated Zone above the Repository

Example Barrier Capability Description

- **Capability: reduce the rate of movement of water**
- **Comparison of mean seepage flux for seeping environments to average infiltration flux**
  - Mean seepage shown for 10 waste package bins (upper plot) and for overall mean weighted by bin frequency in 300 realizations (lower plot)
  - Infiltration shown as spatial average for 38.7 km ^{2} model domain (see previous page)
- **Unsaturated zone flow and drift effects reduce total water flux onto drip shields at 10,000 years ~ 4x relative to infiltration**





Extracted seepage results show mean performance from 300 realizations.
Source: calculations performed for SL986M3 Rev. 00, figure 6-5 (Total System Performance Assessment - Final Environmental Impact Statement).

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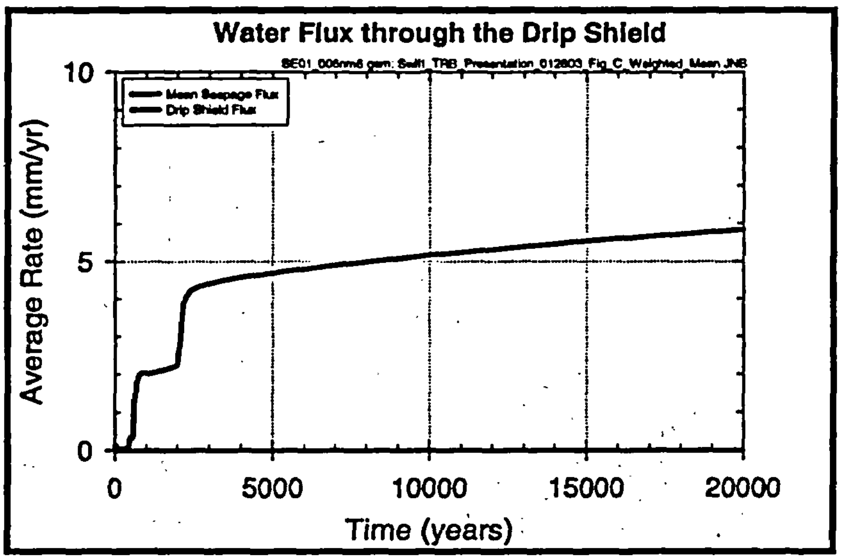
Drip Shield

Example Barrier Capability Description

- **Capability: reduce the rate of movement of water**
- **Comparison of spatially-averaged mean seepage flux to mean water flux reaching waste package**
- **Drip shields reduce water flux at 10,000 years to zero (no drip shield failures during first 20,000 years)**

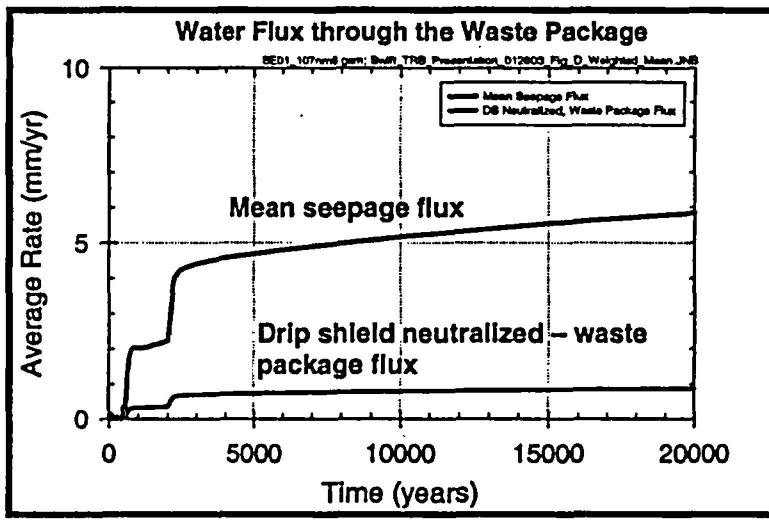


Extracted results show mean performance from 300 realizations. Note linear scale rather than logarithmic scale shown for same information on figure 9. Source: calculations performed for SL986M3 Rev. 00, figure 6-5 (Total System Performance Assessment - Final Environmental Impact Statement).

Waste Package

Example Barrier Capability Description

- Capability: reduce the rate of movement of water
- Comparison of spatially-averaged mean seepage flux to mean water flux through waste packages with early failures and without a drip shield
- Waste packages alone (independent of drip shields) can reduce water flux to less than 1 mm/yr for packages with early failures and to zero for all other packages



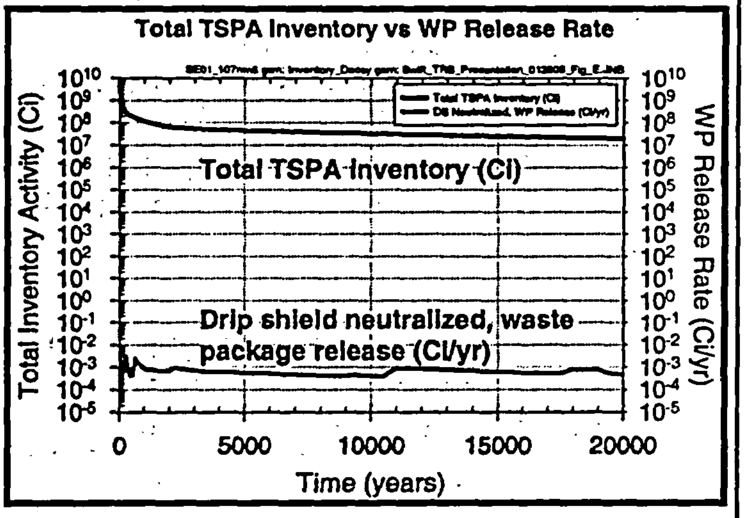
Extracted results show mean performance from 300 realizations. Source: Extracted mean seepage calculations prepared for figure 9 of this presentation, scaled by area fraction of early package failure opening.

Waste Package

Example Barrier Capability Description

(Continued)

- Capability: reduce the rate of radionuclide movement
- Comparison of total activity leaving waste package to total activity in Total System Performance Assessment inventory shows capability of barrier to limit radionuclide movement
  - Drip shield removed
  - Releases result from one early waste package failure in each realization
- Waste packages alone limit annual releases to less than one ten-billionth of the total inventory

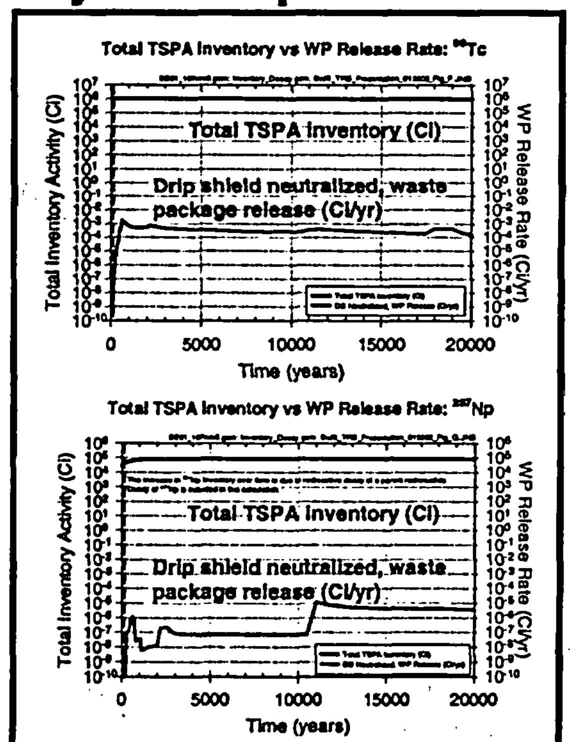


Extracted results show mean performance from 300 realizations.
Source: calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01, figure 10.

Waste Package

Example Barrier Capability Description

(Continued)



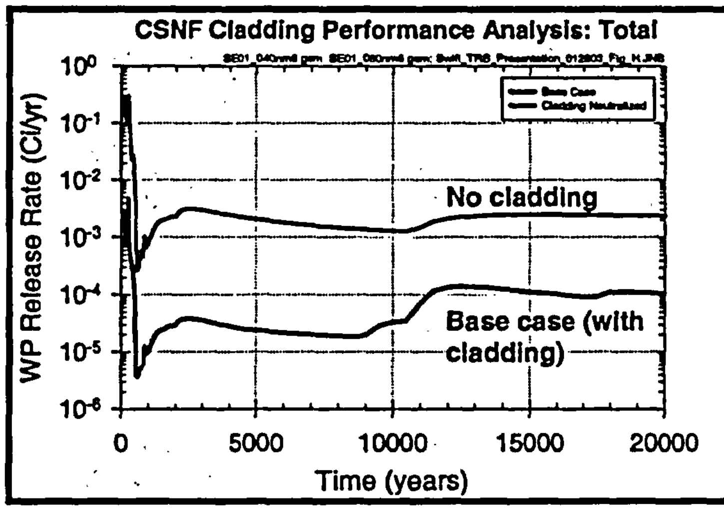
- Capability: reduce the rate of radionuclide movement
- Comparisons of Tc-99 and Np-237 leaving waste package to total activity of these species in Total System Performance Assessment inventory movement
  - Drip shield removed
  - Releases result from one early waste package failure in each realization
- Waste packages successfully contain both highly soluble species (e.g., Tc-99, upper plot) and moderately soluble species (e.g., Np-237, lower plot)

Extracted results show mean performance from 300 realizations.
Source: calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01, figure10.

Cladding

Example Barrier Capability Description

- Capability: reduce the rate of radionuclide movement
- Comparison of total activity leaving waste package with and without cladding present on commercial spent nuclear fuel
  - Other barriers (e.g., drip shield and waste package) perform as expected
- Cladding has the potential to reduce total activity flux leaving the commercial spent nuclear fuel waste packages at 10,000 years ~ 40x



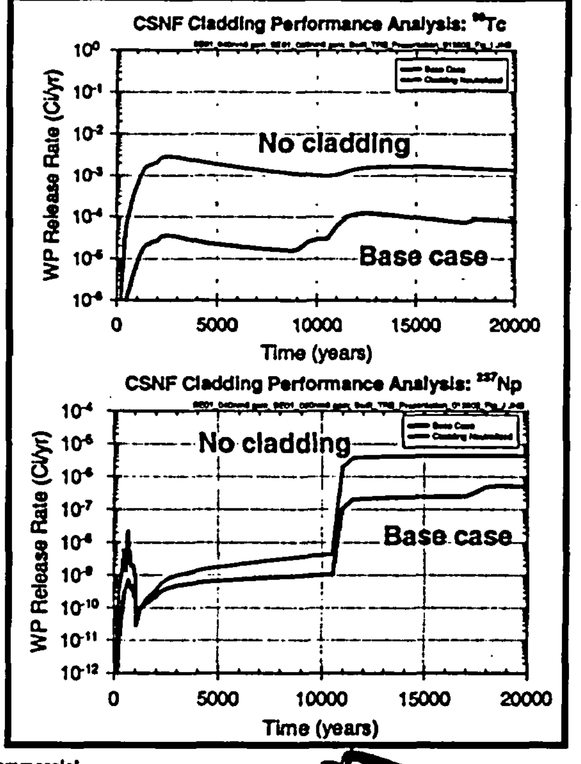
Extracted results show mean performance from 201 realizations, which represent the commercial spent nuclear fuel fraction early waste package failures in the the total of 300 realizations. Source: calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01, figure 19.

Cladding

Example Barrier Capability Description

(Continued)

- Capability: reduce the rate of radionuclide movement
- Comparison of activity leaving waste package with and without cladding for two radionuclides
  - Tc-99: highly soluble, rapid diffusive transport (upper plot)
  - Np-237: solubility-limited concentrations, slow diffusive transport (lower plot)



Extracted results show mean performance from 201 realizations, which represent the commercial spent nuclear fuel fraction early waste package failures in the the total of 300 realizations.
Source: calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01, figure 19.

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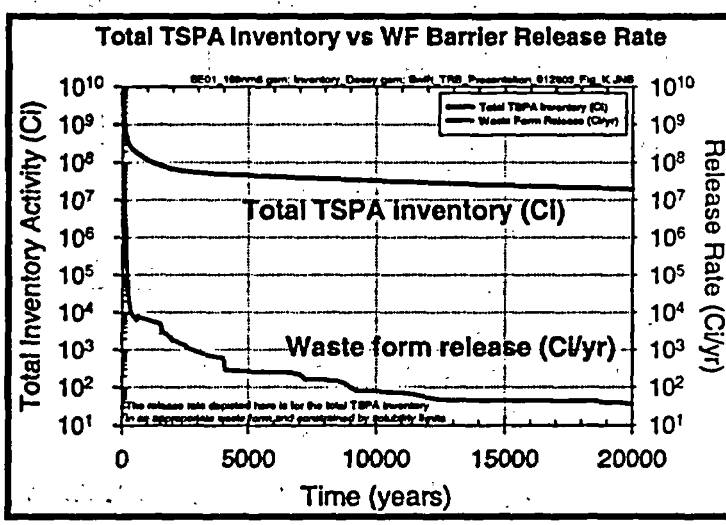
Waste Form Degradation and Dissolution

Example Barrier Capability Description

- Capability: reduce the rate of radionuclide release from waste
- Comparison of total activity in Total System Performance Assessment inventory and total activity mobilized from waste form exposed to precipitation flux
  - Drip shield, Waste Package, and Cladding removed
- At 10,000 years, waste form alone has the potential to reduce annual radionuclide mobilization to approximately 1/400,000 of total inventory



Extracted results show mean performance from 300 realizations. Source: calculations performed for ANL-WIS-PA-000004 Rev. 00 ICN 00, figure 7-3 (one-on analysis case 3).

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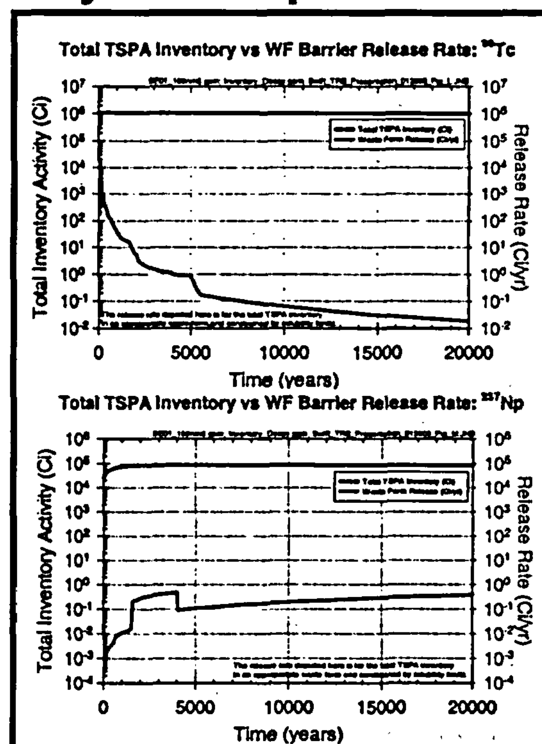
Waste Form Degradation and Dissolution

Example Barrier Capability Description

(Continued)

- **Capability: reduce the rate of radionuclide movement**
- **Comparisons of Tc-99 and Np-237 activity in Total System Performance Assessment inventory and activities mobilized from waste form exposed to precipitation flux**
  - **Drip shield, waste package, and cladding removed**



Extracted results show mean performance from 300 realizations. Source: calculations performed for ANL-WIS-PA-000004 Rev. 00 ICN 00 figure 7-7 (one-on analysis case 3).

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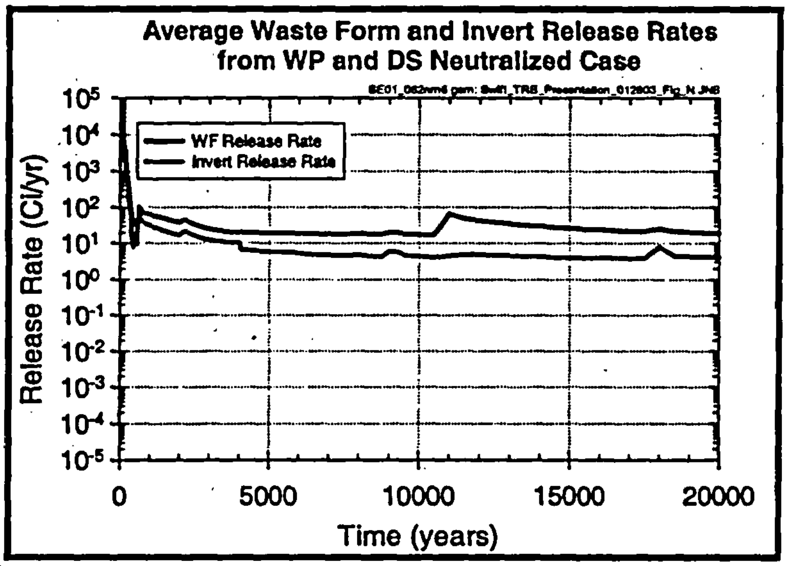
Invert
Example Barrier Capability Description

- Capability: reduce the rate of radionuclide movement
- Comparison of total activity entering and exiting the invert
  - Waste package and drip shield removed
- At 10,000 years, invert has the potential to reduce total activity in groundwater approximately 4x

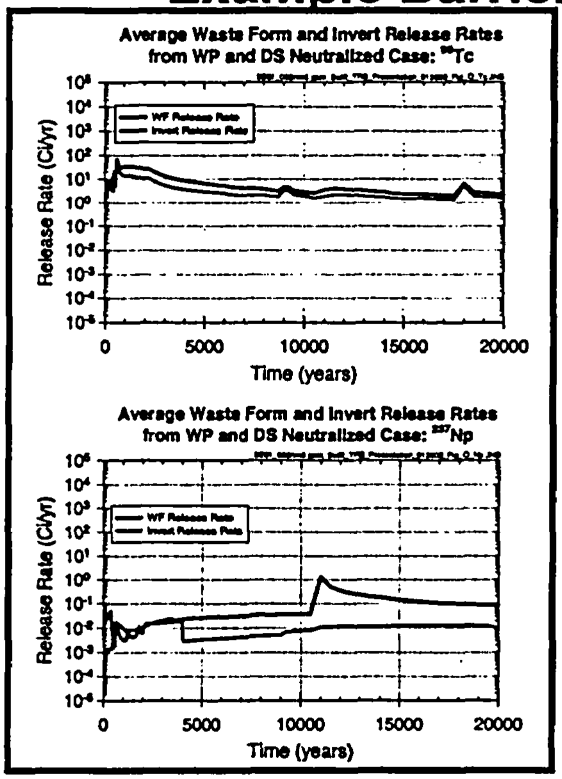


Extracted results show mean performance from 300 realizations.
***Source:* unpublished calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01.**

Invert

Example Barrier Capability Description

(Continued)



- Capability: reduce the rate of radionuclide movement
- Comparisons of Tc-99 and Np-237 activity in Total System Performance Assessment entering and exiting the invert
  - Waste package and drip shield removed

Extracted results show mean performance from 300 realizations.
Source: unpublished calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01.

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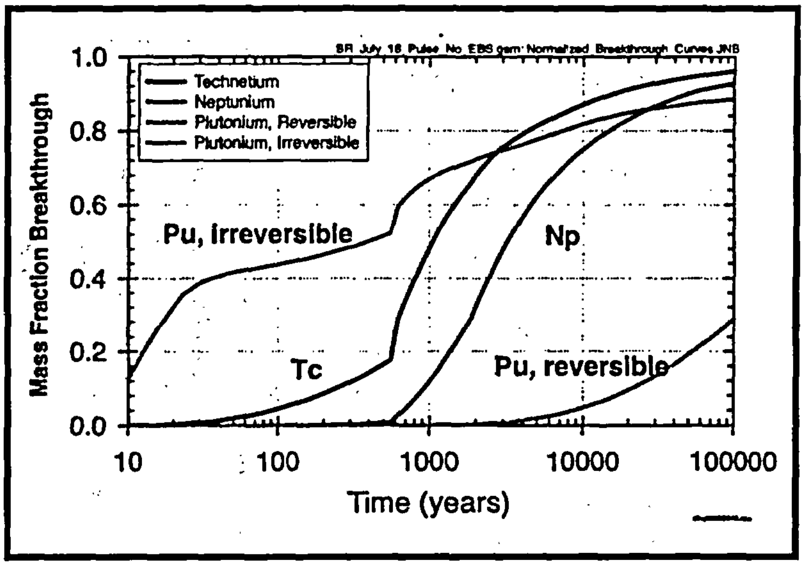
Unsaturated Zone below the Repository

Example Barrier Capability Description

- Capability: reduce the rate of radionuclide movement
- Breakthrough curves for Tc, Np, Pu
  - Breakthrough based on unit release into unsaturated zone at time zero, effectively removes all engineered barriers
  - No radioactive decay
- Median unsaturated zone transport times for mean breakthroughs vary for different species
  - Tc-99: ~ 1000 yr
  - Np-237: ~ 3000 yr
  - Pu (dissolved and reversible colloids): > 100,00 yr
  - Irreversible Pu colloids: ~ 300 yr



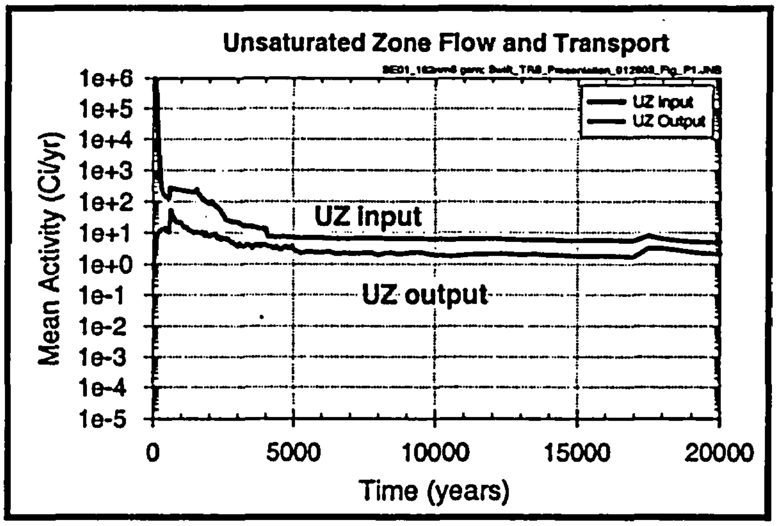
Total System Performance Assessment - Site Recommendation Rev. 00 ICN 01 figure 3.7-12.

Unsaturated Zone below the Repository

Example Barrier Capability Description

(Continued)

- Capability: reduce the rate of radionuclide movement
- Comparison of total activity entering and exiting the unsaturated zone
  - Results shown with seepage effects, drip shield, waste package, and invert removed
- Potential activity reduction at 1000 years is > 10x, due to strong retardation of Am-241, Cs-137, Sr-90



Extracted results show mean performance from 300 realizations. Source: calculations performed for ANL-WIS-PA-000004 Rev. 00 ICN 00, figure 7-6 (one-on analysis case 6).

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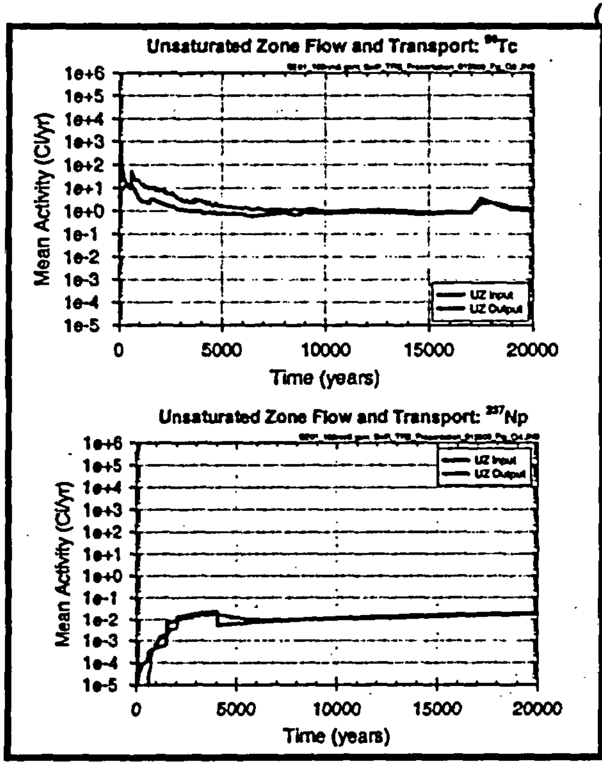
Unsaturated Zone below the Repository

Example Barrier Capability Description

(Continued)



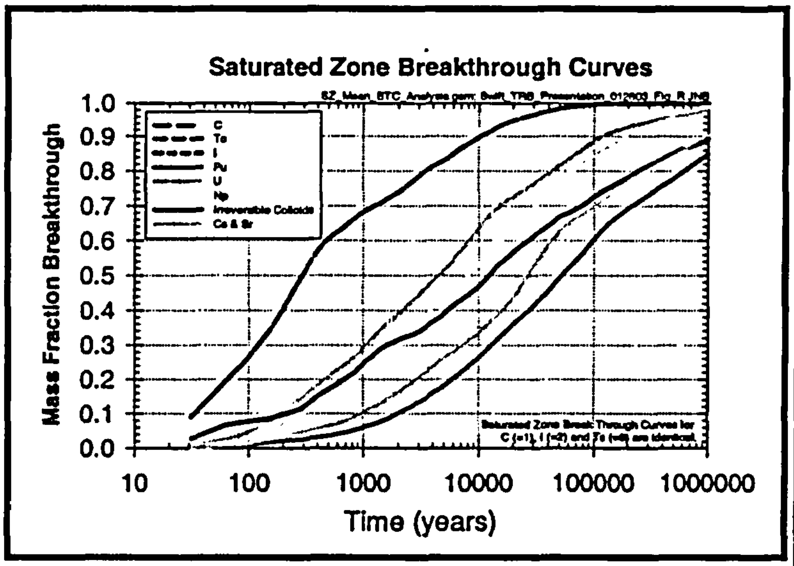
- Capability: reduce the rate of radionuclide movement
- Comparisons of Tc-99 (upper plot) and Np-237 (lower plot) activity entering and exiting the unsaturated zone
  - Results shown with seepage effects, drip shield, waste package, invert removed

Extracted results show mean performance from 300 realizations. Source: calculations performed for ANL-WIS-PA-000004 Rev. 00 ICN 00, figure 7-6 (one-on analysis case 6).

Saturated Zone

Example Barrier Capability Description

- Capability: reduce the rate of radionuclide movement
- Mean breakthrough curves for saturated zone
  - Breakthrough based on unit release into saturated zone at time zero, effectively removes all engineered barriers
  - Present climate, scaled for wetter conditions
  - No radioactive decay
- Median saturated zone transport times for mean breakthroughs vary for different species
  - Tc-99: ~ 300 yr
  - Np-237: ~ 8,000 yr
  - Pu (dissolved and reversible colloids): ~ 53,000 yr
  - Cs-137, Sr-90: ~ 27,000 yr
  - Irreversible colloid species ~ 12,500 yr



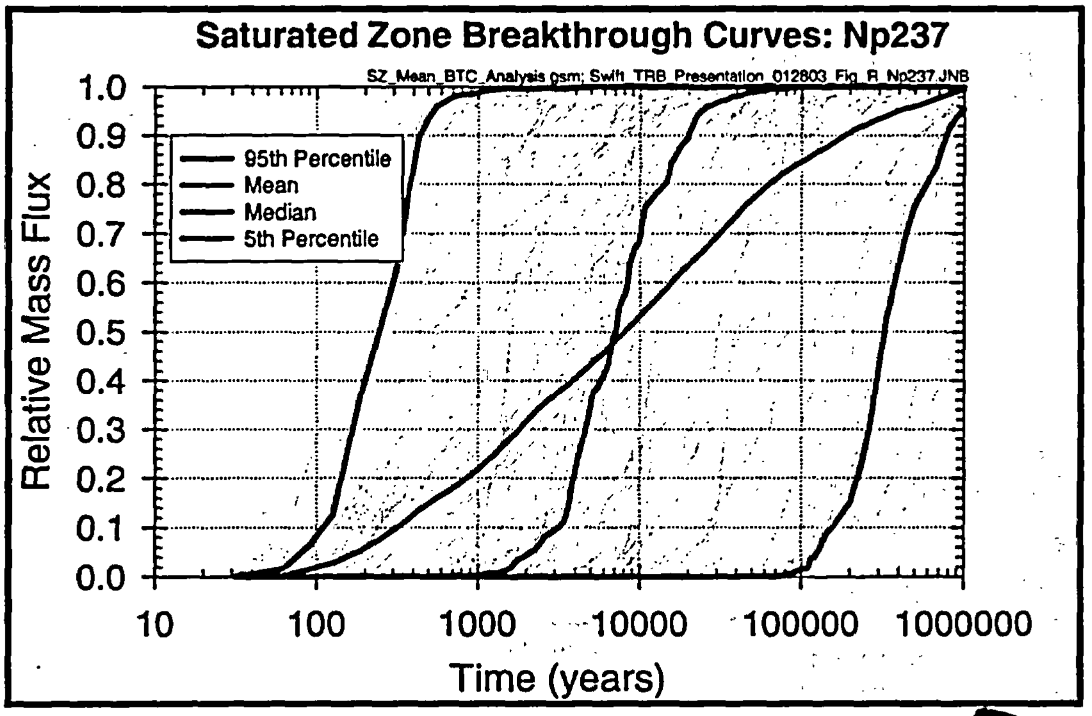
Extracted results show mean performance from 100 realizations. Source: calculations performed for this presentation using models developed for SL986M3 Rev. 00, figure 6-5 (Total System Performance Assessment - Final Environmental Impact Statement).

YUCCA MOUNTAIN PROJECT

Saturated Zone

Example Barrier Capability Description

(Continued)

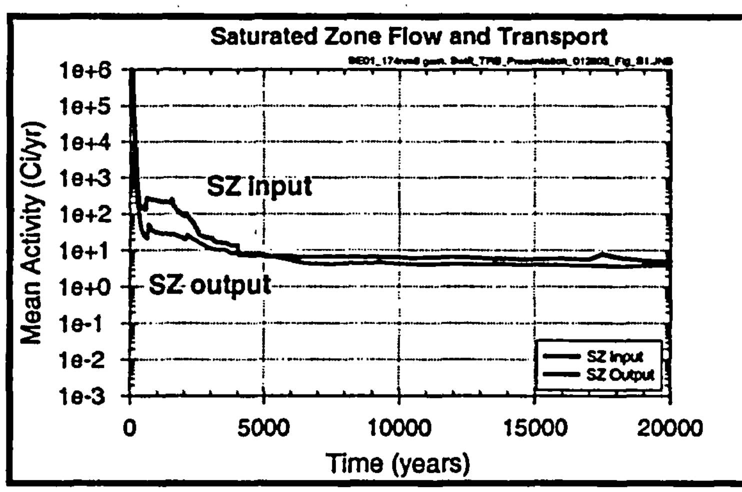


Saturated Zone

Example Barrier Capability Description

(Continued)

- Capability: reduce the rate of radionuclide movement
- Comparison of activity entering and exiting the saturated zone
  - Results shown with the unsaturated zone removed
  - For comparison with unsaturated zone results in previous example, seepage effects, drip shield, waste package, and invert also removed
- Potential activity reduction at 1000 years ~ 7x, due to strong retardation of Am-241, Cs-137, Sr-90

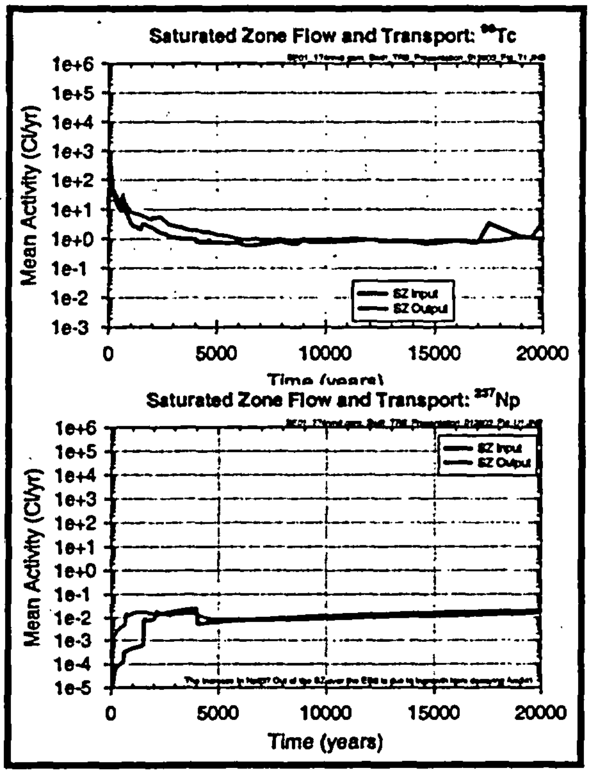


Extracted results show mean performance from 300 realizations. Source: calculations performed for ANL-WIS-PA-000004 Rev. 00 ICN 00, figure 7-13 (one-on analysis case 13).

Saturated Zone

Example Barrier Capability Description

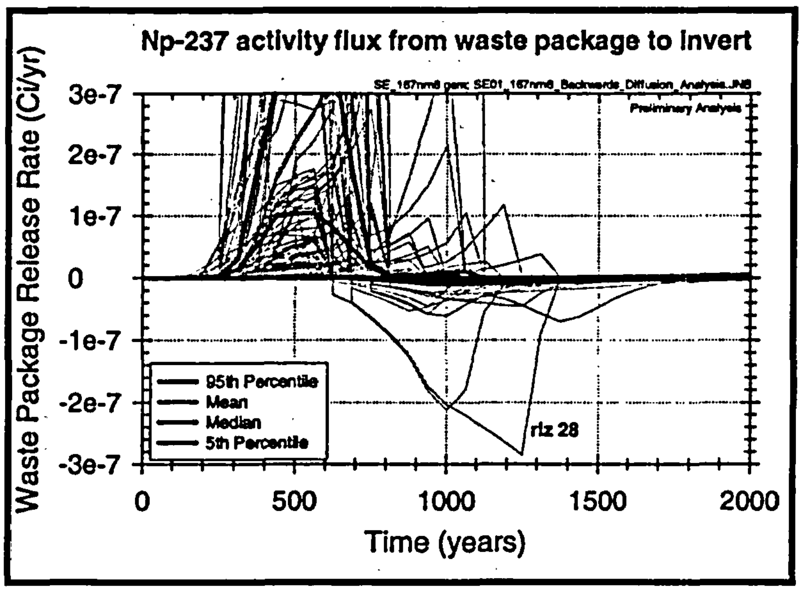
(Continued)



- Capability: reduce the rate of radionuclide movement
- Comparisons of Tc-99 (upper plot) and Np-237 (lower plot) activity entering and exiting the saturated zone
  - Results shown with the unsaturated zone removed
  - For comparison with unsaturated zone results in previous example, seepage effects, drip shield, waste package, and invert also removed
  - Increase in Np-237 due to Am-241 decay, ingrowth

Extracted results show mean performance from 300 realizations. Source: calculations performed for ANL-WIS-PA-000004 Rev. 00 ICN 00, figure 7-13 (one-on analysis case 13).

Explanation of Np-237 flux from Waste Package to Invert at ~ 1000-2000 yr



Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12).
Detail showing 300 realizations of Np-237 activity flux from waste package to invert.

- All transport in this time period is by diffusion along concentration gradients
- Several realizations show small negative flux (movement from invert to waste package)
  - Realization 28 examined in more detail in subsequent pages
- Mean flux (also shown on slide 14 at a different scale) is negative from 1100 years to 1750 years

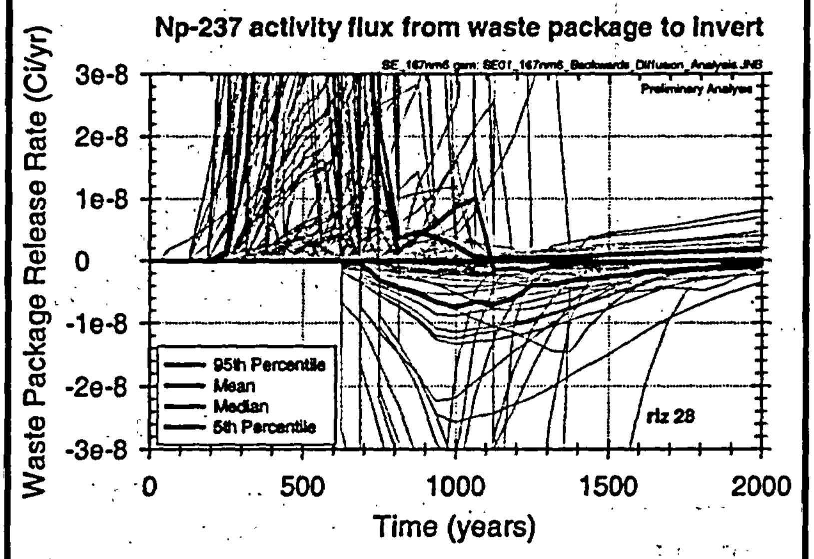
YUCCA MOUNTAIN PROJECT

BSC Presentations_ACNW_YMSwift_03/26/03 37

Explanation of Np-237 flux from Waste Package to Invert at ~ 1000-2000 yr

(Continued)

Enlargement of previous figure



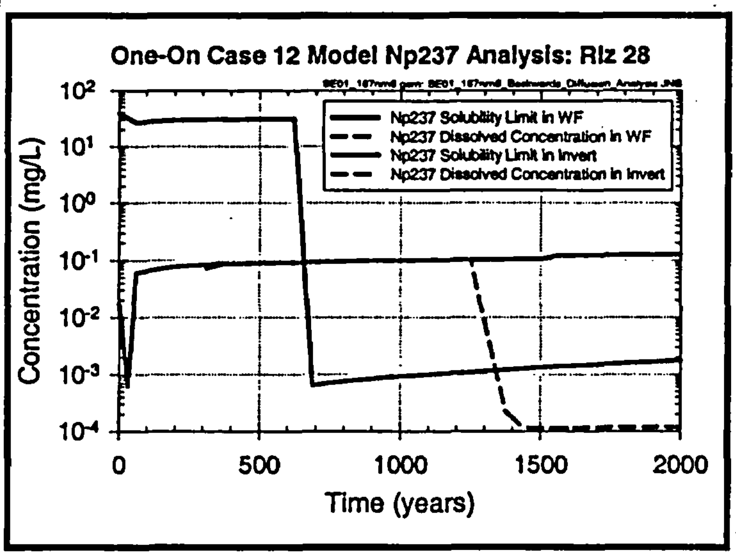
As shown in following pages, the behavior observed in realization 28 is controlled by the dependency of Np solubility limits on pH, and changes in the calculated pH in waste package and invert.

Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12). Detail showing 300 realizations of Np-237 activity flux from waste package to invert.

YUCCA MOUNTAIN PROJECT

Explanation of Np-237 flux from Waste Package to Invert at ~ 1000-2000 yr

(Continued)

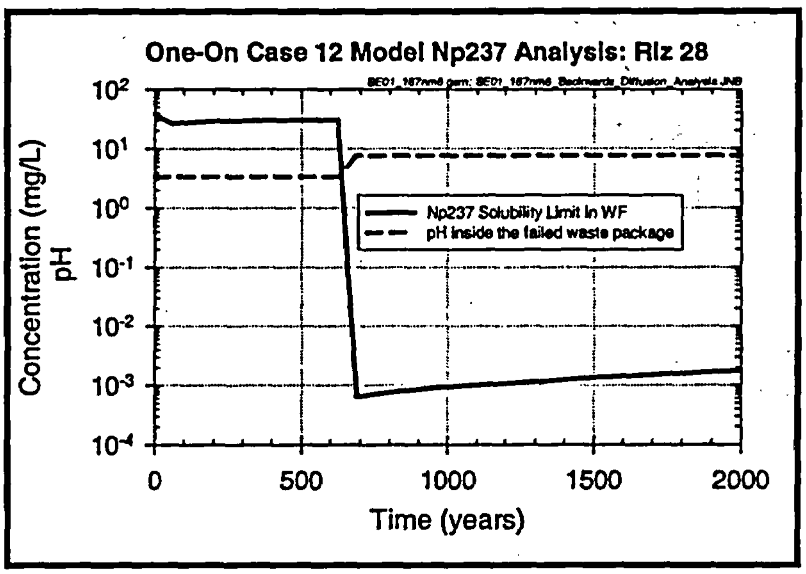


Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12). Detail showing realization 28 Np-237 calculated solubility limits and concentrations in waste form / waste package and invert.

- Np concentrations in the waste package are at the waste form solubility limit throughout the time of interest
- Np solubility limits in the waste form drop precipitously at 625 years, coincident with a rise in pH (see next slide) caused by the depletion of free iron in the waste form
- Np solubility limits in invert are unaffected, and invert concentrations remain high until diffusive transport in both directions causes them to drop

Explanation of Np-237 flux from Waste Package to Invert at ~ 1000-2000 yr

(Continued)



- pH in the waste package increases from 3.38 to 7.70 at 625 years
- Np solubility limits drop more than four orders of magnitude

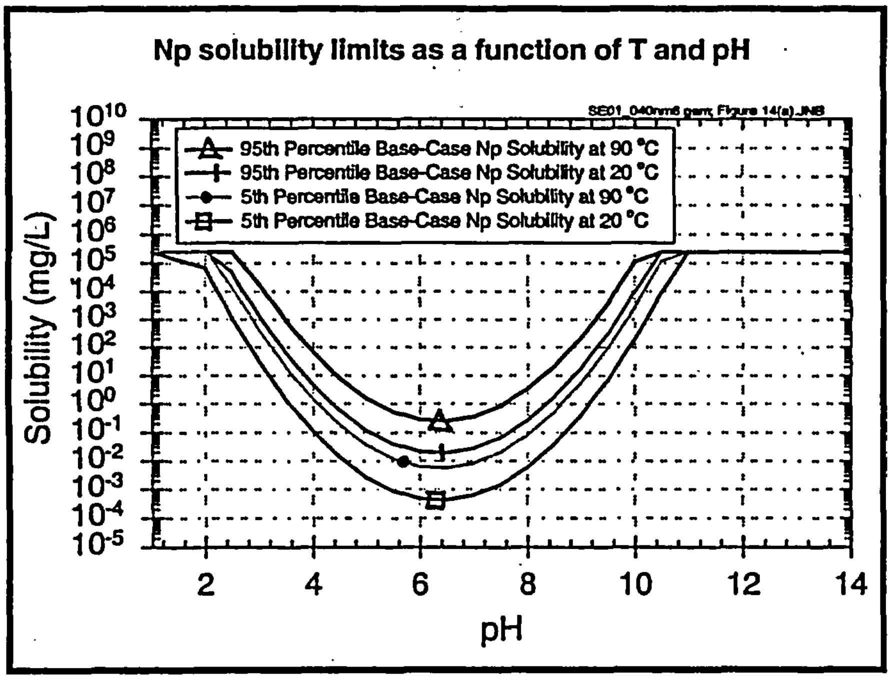
Based on results of ANL-WIS-PA-000004 Rev. 00 ICN 00 ("one-on analysis" Case 12). Detail showing realization 28 Np-237 solubility limit in waste form and pH inside the waste package.

YUCCA MOUNTAIN PROJECT

BSC Presentations_ACNW_YMSwift_03/26/03 40

Explanation of Np-237 flux from Waste Package to Invert at ~ 1000-2000 yr

(Continued)



- **Np solubility limits are strongly influenced by pH, varying many orders of magnitude**
- **Temperature effects are secondary**

Draft results show summary performance from 300 realizations. Source: calculations performed for TDR-WIS-PA-000009 Rev. 01 ICN 01, figure 16.

D. Bullen, Iowa State University: My interpretation was that there wasn't an extrapolation of those rates beyond 95°. If it was above 95°, it didn't corrode at all. Bob, do you want to comment on that one?

R. Andrews (BSC): Yes, the initiation of aqueous corrosion was assumed to occur at the point where the most deliquescent salt was on packaged surface. I am not sure which salt was assumed, but that was generally at a relative humidity of about 40 percent. I would have to verify that, to be honest with you.

Once you hit the relative humidity of 40 percent, you would have to compute the temperature where that occurs. Then it was assumed that humid air/aqueous corrosion processes could begin and their rates would be those rates sampled over the entire distribution of possible rates over a range of different chemistries. The initiation criterion was humidity, not temperature.

D. Bullen, Iowa State University: Were there no localized corrosion models in that? It was all general corrosion?

R. Andrews (BSC): No, as I said yesterday, the localized corrosion model is in the general degradation model for the waste package and the drip shield. However, the chemical environments on the package and the drip shield were such, and the temperature was such, that it was never initiated.

D. Bullen, Iowa State University: Okay.

R. Andrews (BSC): There is a localized corrosion model. It was just never initiated.

P. Swift, SNL/BSC: It was not an assumption that there was no localized corrosion. It was a model result that there was no localized corrosion.

D. Esh, NRC Staff: And it was sodium nitrate salt at 120°C, I believe.

J. Payer, CWRU: I will make the observation that when we say general corrosion in the way that it is being handled here, it is the material in the passive state. There have been a couple of approaches to determining the corrosion rate of this material. One approach is looking at the current density on electrochemical polarization measurements and turning that into a penetration rate. Another approach is weight loss, and other spectroscopies, trying to measure very small penetration rates with microscopy and so forth, out of longer term weight loss type specimens. So that is, I think, the basis for this. It is really the passive corrosion rate, yet passivity remains stable.

R. Latanision, MIT: I agree with that, John. My concern is that if we are working above the boiling point, then the question becomes What sorts of solutions are we using as their representative environment. Obviously, they would have to be concentrated because we are not pressuring the system. I do not think there are measurements of passive current densities under those circumstances. Unless I'm really unaware of data that exist. I think those experiments have not been done.

J. Payer, CWRU: My understanding is that there are some crevice corrosion results.

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4.8 Simplified Models of Key Contributors to Dose Traced Through Various Modules (NRC)

Understanding Performance Assessment Results

Mr. Tim McCartin
U. S. Nuclear Regulatory Commission

Mr. Tim McCartin gave a talk about the NRC's performance assessment results to date. He noted that estimated doses within 10,000 years are influenced by the very mobile nuclides, I-129 and Tc-99. Estimated doses beyond 10,000 years are strongly influenced by Np-237, which is somewhat mobile. He described how performance assessment results are complex and reflect nuclide-specific behavior, temperature dependence, and the "masking" effects of redundant barriers.

The NRC staff is currently studying sensitivities within and relationships between various attributes (e.g., waste package, water flow into waste packages, waste forms, and unsaturated and saturated zone transport). The results of these studies will provide the perspective to understand and interpret performance assessment results. Waste package performance is easy to explain and understand (breached vs. not breached), despite complexities in technical basis. Mr. McCartin described the performance sensitivities for waste forms and for water flow into waste packages. He discussed dissolution rates of spent fuel, solubility limits used for radionuclides of interest (within waste packages), rates of deep groundwater percolation, and the relative degrees of flow diversion or enhancement.

Mr. McCartin also discussed the sensitivity of retardation in the Calico Hills nonwelded vitric unit, which is below the repository and covers about 50 percent of the repository "footprint." Poorly mobile radionuclides, like Am-241 and Pu-240, are strongly retarded by the Calico Hills vitric unit. Neptunium-237 is also retarded by this unit. All three radionuclides can also be strongly retarded in saturated valley fill alluvium. In his summary, Mr. McCartin observed that a large number of waste package failures are needed for I-129 and Tc-99 to be important due to their limited inventory. Neptunium-237 is sensitive to solubility limit and water flow, and to the presence of the Calico Hills nonwelded vitric unit. In the saturated zone, Np-237 is sensitive to variations in retardation, has limited sensitivity to matrix diffusion, and limited sensitivity to the extent of alluvium (assuming a minimum of 1 kilometer of alluvium in the flowpath).

Understanding Performance Assessment Results

140th Meeting of
Advisory Committee on Nuclear Waste
March 26, 2003

Tim McCartin 301-415-7285 tim3@nrc.gov
Division of Waste Management
U.S. Nuclear Regulatory Commission

Main Contributors: Sitakanta Mohanty and Gordon Wittmeyer (CNWRA)
Hans Arlt, Richard Codell and Dave Esh (NRC)

OUTLINE

- Current Results
- Performance Attributes and Analyses
- Summary

2

Current Performance Assessments (nominal performance)

- Dose within 10,000 years influenced by very mobile nuclides (i.e., I-129, Tc-99)
- Dose beyond 10,000 years influenced by Np-237 (somewhat mobile)
- What about the rest of the waste inventory?

3

Inventory Perspective (based on inventory at 1,000 years)

Nuclide	Half-Life (years)	Inventory at 1000 yrs (by Curies)	Dose Conv. Factor (rem/yr per Ci/m^3)
Tc 99	2.1×10^5	0.7%	1.2×10^3
I 129	1.6×10^7	0.002%	2.3×10^5
Np 237	2.1×10^6	0.06%	3.7×10^6
Am 241	430	54%	3.1×10^6
Pu 240	6,500	25%	3.0×10^6

4

Understanding Repository Performance

- What "does" and "does not" cause potential exposures and why
- Performance assessment results are complex
  - nuclide specific behavior
  - temperature dependence (causing temporal sensitivity)
  - "masking" effects

5

Current Approach

- Probe specific attributes of repository system
  - sensitivities within each attribute
  - relationships between different attributes
- Identify potential performance indicators
- Provide perspective to understand and interpret performance assessment results

6

Attributes of Repository System

- Waste Package
- Water Flow into Waste Package
- Waste Form
- Unsaturated Zone Transport
- Saturated Zone Transport

7

Performance Indicators

- Waste Package Lifetime
- Water Flow into Waste Package and Waste Form
  - number of waste packages needed to release 15 mrem/yr at drift wall (assumes no geologic delay)
- Unsaturated and Saturated Zone Transport
  - time for initial release into a zone to exit

8

Waste Package

- Initial Component (no releases until the waste package is breached)
- Waste package performance is straightforward to explain and understand (e.g., breached or not breached) despite complexities in technical basis

9

Water Flow into Waste Package
Performance Sensitivities

- Solubility Limits
  - Tc 99 (99 kg/m^3)
  - I 129 (129 kg/m^3)
  - Np 237 (1.2×10^{-3} to 2.4×10^{-1} kg/m^3)
  - Am 241 (2.4×10^{-8} to 2.4×10^{-4} kg/m^3)
  - Pu 240 (2.4×10^{-6} to 2.4×10^{-4} kg/m^3)
- Deep Percolation (initial rate of 4 to 13 mm/year)
- Flow Diversion or Enhancement (2.4×10^{-4} to 8)

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Water Flow into Waste Package

Solubility Limit Sensitivity

[packages needed to release 15 mrem/yr at drift wall - no geologic delay]

Nuclide	WP breach at 5,000 yrs Low Sol.	WP breach at 5,000 yrs High Sol.	WP breach at 1,000 yrs Low Sol.	WP breach at 1,000 yrs High Sol.
Tc 99	>7,000	>7,000	4,150	4,150
I 129	>7,000	>7,000	>7,000	>7,000
Np 237	3,200	260	3,000	110
Am 241	>7,000	110	>7,000	6
Pu 240	2,600	45	2,600	45

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Water Flow into Waste Package

Water Influx Sensitivity

[packages needed to release 15 mrem/yr at drift wall - no geologic delay]

Nuclide	WP breach at 5,000 yrs Low Flow	WP breach at 5,000 yrs High Flow	WP breach at 1,000 yrs Low Flow	WP breach at 1,000 yrs High Flow
Tc 99	>7,000	>7,000	>7,000	3,100
I 129	>7,000	>7,000	>7,000	6,700
Np 237	>7,000	120	>7,000	40
Am 241	>7,000	65	>7,000	1
Pu 240	>7,000	2	>7,000	1

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Waste Form

Performance Sensitivities

- Dissolution rate of spent fuel
  - pre-exponential term
    $1.2 \times (10^3 \text{ to } 10^6)$ mg/m^{2}d
  - surface area (particle radius)
    0.7 to 3.0 mm

- Temperature dependence (link to failure time of waste package)

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Waste Form

Release Rate Sensitivity

[packages needed to release 15 mrem/yr at drift wall - no geologic delay]

Nuclide	WP breach at 5,000 yrs Low Rate	WP breach at 5,000 yrs High Rate	WP breach at 1,000 yrs Low Rate	WP breach at 1,000 yrs High Rate
Tc 99	>7,000	780	>7,000	230
I 129	>7,000	1,700	>7,000	490
Np 237	>7,000	95	>7,000	130
Am 241	>7,000	15	25	8
Pu 240	220	55	160	55

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Unsaturated Zone
Performance Sensitivities

- Retardation in Calico Hills vitric unit
  - Tc 99 (Rf = 1)
  - I 129 (Rf = 1)
  - Np 237 (Rf = 16 to 135)
  - Am 241 (Rf = 8×10^6 to 3×10^8)
  - Pu 240 (Rf = 1.7×10^3 to 1.4×10^4)

- Spatial extent of Calico Hills vitric unit below repository
  - approximately 50% of footprint
  - average thickness of 30 meters

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Unsaturated Zone
Retardation Sensitivity (CHnv)

[years for initial release into Unsat zone to exit Unsat zone]

Nuclide	Rf (low)	Rf (high)
Tc 99	450	450
I 129	450	450
Np 237	9,000	60,000
Am 241	>100K	>100K
Pu 240	>100K	>100K

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Saturated Zone
Performance Sensitivities

- Retardation in alluvium
  - Tc 99 (Rf = 1)
  - I 129 (Rf = 1)
  - Np 237 (Rf = 1 to 3900)
  - Am 241 (Rf = 7×10^4 to 7×10^7)
  - Pu 240 (Rf = 420 to 3.9×10^5)
- Extent of alluvium (1- 5 km)
- Matrix diffusion
  - "effective" fraction of matrix (0.01 to 0.10)

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Saturated Zone
Retardation Sensitivity

[years for initial release into Sat zone to exit Sat zone]

Nuclide	Alluv(1km) Rf (low)	Alluv(1km) Rf (high)	Alluv (5km) Rf (low)	Alluv(5km) Rf (high)
Tc 99	350	350	550	550
I 129	350	350	550	550
Np 237	950	76,000	1,050	>100K
Am 241	>100K	>100K	>100K	>100K
Pu 240	54,000	>100K	>100K	>100K

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Saturated Zone

Retardation Sensitivity *(with Mat. Diff.)*

[years for initial release into Sat zone to exit Sat zone]

Nuclide	Alluv(1km) Rf (low) Mat Diff (low)	Alluv(1km) Rf (low) Mat Dif (high)	Alluv(5km) Rf (high) Mat Dif (high)
Tc 99	300	600	700
I 129	300	600	700
Np 237	700	1,800	>100K
Am 241	>100K	>100K	>100K
Pu 240	45,000	>100K	>100K

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Summary

- Water flow into waste package
  - solubility limit and water flow important for Np 237
  - large number WP failures needed for I129 and Tc99 to be important (limited inventory)
- Waste form
  - degradation rate important
  - limited sensitivity to temperature (assuming minimum WP lifetime of 1,000 years)

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Summary (cont.)

- Unsaturated zone
  - Calico Hills vitric unit important for nuclides that are sorbed (e.g., Np237)
- Saturated zone
  - Np237 sensitive to variation in retardation
  - limited sensitivity to matrix diffusion
  - limited sensitivity to extent of alluvium (assuming a minimum of 1 km)

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Next Steps

- Understanding "system" performance will assist staff prioritization efforts
- Flexibility in selection of analysis method (and use of diverse methods) necessary because of system complexity, long time frames, and uncertainties
- Each analysis provides specific information and/or answers a specific question
- Continue to examine data based on insights

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T. McCartin, NRC Staff: In terms of the saturated zone, retardation is principally in the alluvium. We're assuming fracture flow in the welded tuff units.

M. Morgenstein, Geosciences Management Institute, Inc. (GMII): Could you go through again on the other one, what's driving retardation? Is it a combination then of matrix diffusion plus sorption?

T. McCartin, NRC Staff: This retardation is sorption in the alluvium.

M. Morgenstein, GMII: And is it mineralogically controlled? What's driving it? What minerals are driving sorption? In other words, what are the assumptions?

D. Turner, Center for Nuclear Waste Regulatory Analyses (CNWRA): The sorption coefficients for the TPA code have been calibrated to a model of sorption onto aluminosilicates and then we ran it over the range in water chemistries that are observed in the saturated zone near Yucca Mountain. That set up the probability distribution function for transport. Sorption coefficients were calibrated using site specific water chemistry at the site.

M. Morgenstein, GMII: The aluminum silicates are dominantly feldspars and/or clays?

D. Turner, CNWRA: For uranium they are clays. They're based on clay. It's also generated down here in San Antonio for plutonium and americium. They are based on data from the literature with sorption on to what I believe is an aluminosilicate.

M. Morgenstein, GMII: A final question, so this is based on the concentration of clays, essentially and aluminumoxy compounds? What site information do we have on concentrations?

P. Bertetti, CNWRA: We don't have that site specific information in this version of the model, but we now have quantitative x-ray diffraction data from Nye County boreholes in the alluvium and we're incorporating that into the next phase of the modeling effort.

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5. STAKEHOLDER PRESENTATIONS

5.1 Near-Field Environments and Corrosion

(Don L. Shettel, Geosciences Management Institute, Inc.)

Dr. Don Shettel (representing the State of Nevada) gave a talk about corrosion in near-field environments. The talk described various water environments within Yucca Mountain, and noted water types that include precipitation, unsaturated fracture flow, matrix pore water, and water in a thermal refluxing zone. Dr. Shettel described various in-drift chemical and physical processes, and focused on the processes of acid volatilization and hydrolysis of salts. He explained how residual salt solutions and condensates become acidic with thermal evaporative concentration. Deliquescence of salts causes accumulation of liquid on waste package canisters. During hydrolysis of salts, nitric acid vapor is given off. Dr. Shettel estimated a corrosion rate of 678 microns per year, which means that a hole could develop through 2 centimeters of Alloy C-22 in less than 30 years. Dr. Shettel concluded that in-drift processes are more complicated than the DOE admits, that corrosion rates are significantly higher for evaporating solutions and their condensates (0.1 to 1.0 millimeters per year (mm/yr), up to 10 mm/yr), that subboiling immersion testing of engineered barrier materials in groundwater is unrealistic and nonconservative, and that the vadose zone is not a good environment for a high-level waste repository.

Near-Field Environments and Corrosion

Presented to

Advisory Committee on Nuclear Waste

26 March 2003

By

Don L. Shettel, Ph.D.

Prof. A. Barkatt & Dr. A. Pulvirenti: Catholic University of America

Drs. J. Gorman & C. Marks: Dominion Engineering

Dr. R. Staehle

Geosciences Management Institute, Inc.

1000 Nevada Way, Suite 106

Boulder City, Nevada 89005

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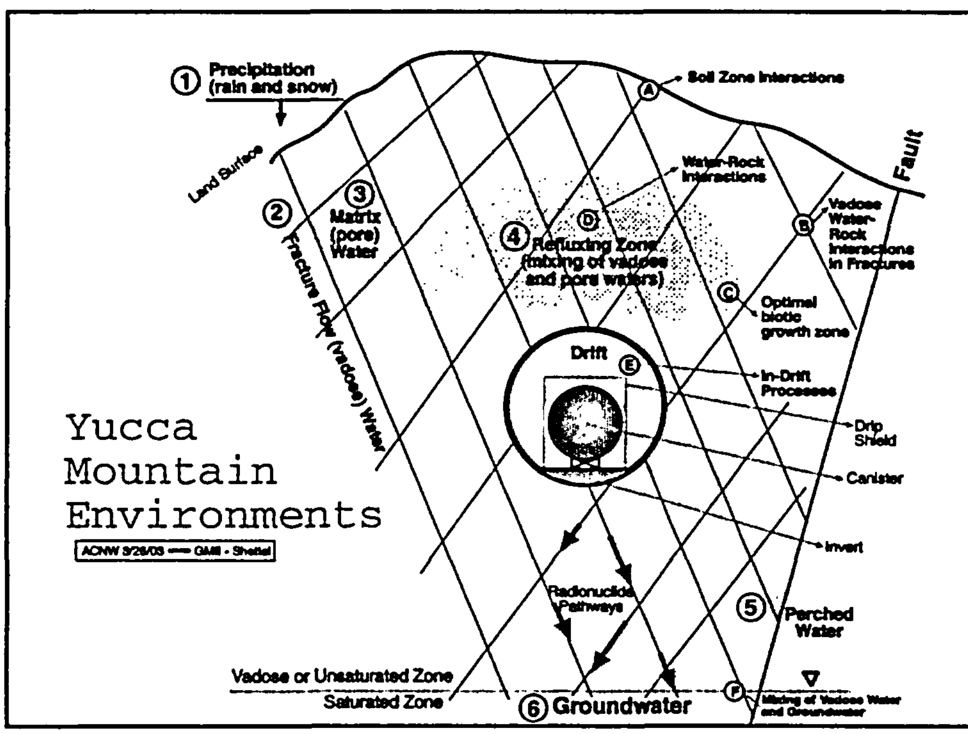


Yucca Mt. Water Types

1. Precipitation (rain and snow)
   dilute: Ca - HCO_3
   (NO_3 similar to SO_4 and Cl)

2. Fracture flow (vadose) water
   3 shallow samples: Ca-Na-HCO_3 to Na-HCO_3
   Composition is generally unknown

3. Matrix (pore) water in Vadose Zone
   shallow (above Repository Level): Ca - SO_4 + Cl
   deep (below Repository Level): Na - HCO_3

4. Refluxing Zone
   Heated mixtures can evolve
   Mixtures of most types (except GW & perched)
   (from concentrated solutions to dilute condensates)

ACNW 3/26/03 — GMII - Shettel

In - Drift Processes

- Dripping / flowing vadose waters from fractures
- Temperature & Rel. Humidity variations
- Dust & Evaporative salt build-up on EBS surfaces
- Rockfall
- Radiolysis
- Corrosion
- Other man-made materials (corrosion products)
- **Acid Volatilization**
- **Hydrolysis of Salts**

ACNW 3/26/03 - GMII:Shettel

Acid Volatilization

- HNO_3, HCl, & HF vaporize from thermally evaporated solutions
- $SO_4^{=}$ in residual solution precipitates as Sulfates
- Residual solutions lose "beneficial" inhibitors
- Residual solutions and condensates become acidic with thermal evaporative concentration

ACNW 3/26/03 - GMII:Shettel

Hydrolysis of Salts

- Hydrated salts form from thermal evaporation of dripping vadose water:
  Examples: tachyhydrite ($CaMg_2Cl_6 \cdot 12H_2O$)
  sinjarite ($CaCl_2 \cdot 2H_2O$)
- Deliquescence of salts causes accumulation of liquid on canisters
- Salts are hygroscopic, absorb moisture from drift atmosphere, and form acid solutions
- Brines are highly viscous and have low vapor pressure
- During hydrolysis: HNO_3 vapor given off

ACNW 3/26/03 - GMII:Shettel

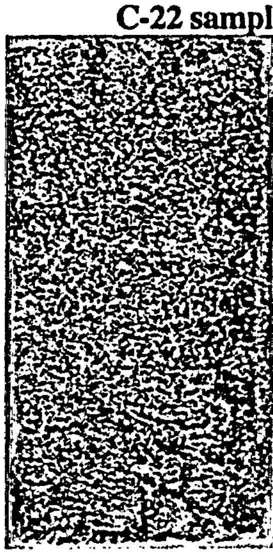
C-22 Disk E34 in Wet Residual Paste at 144°C for 29 days

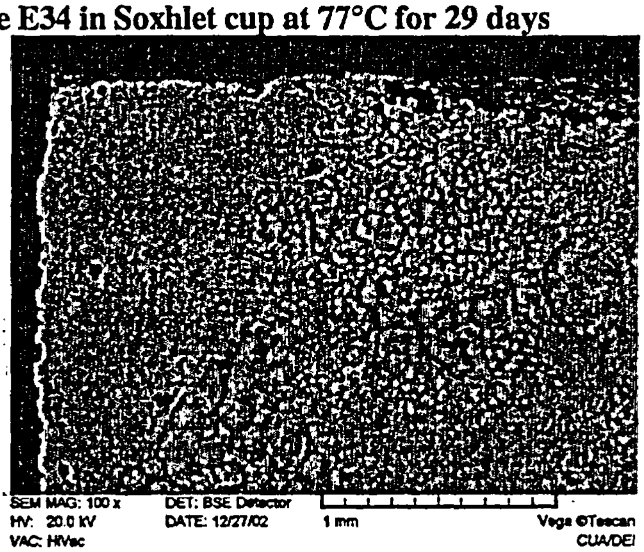
Initial solution: 12L of 1243X UZ pore water

Paste pH = 2.21

Gen. Corrosion Rate = 678 microns / y. (29.5 y for hole to develop in 2 cm thickness of C-22)

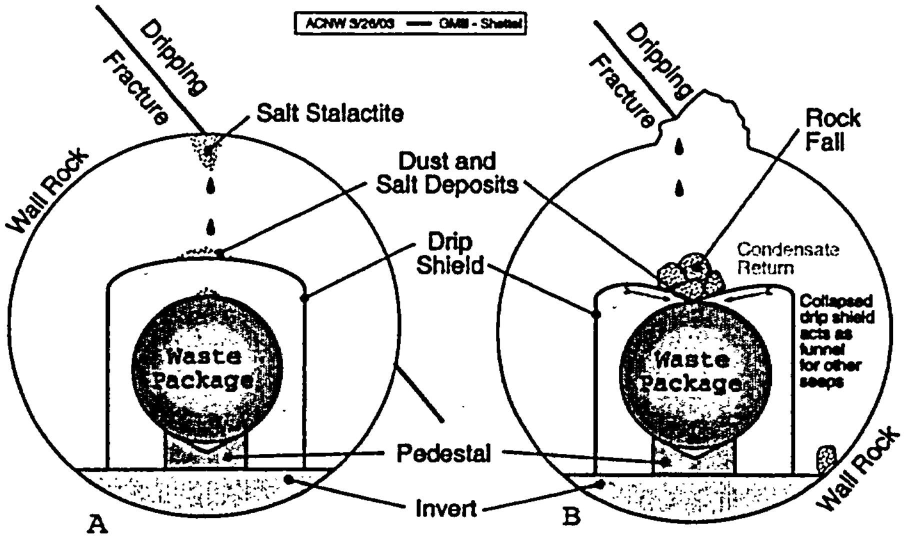
C-22 sample E34 in Soxhlet cup at 77°C for 29 days





1 cm by 0.5 cm slab exposed intermittently to a clear Condensate liquid of pH = -0.48
General corrosion rate = 938 microns/y (21 y to penetrate 2 cm thickness)

In-Drift Processes



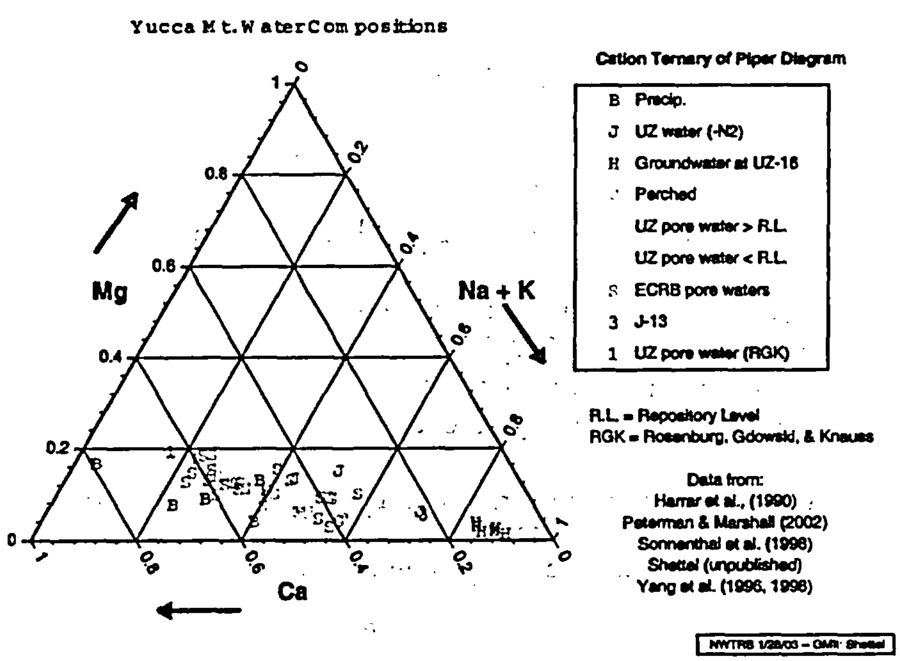
Cross Section of Emplacement Drifts

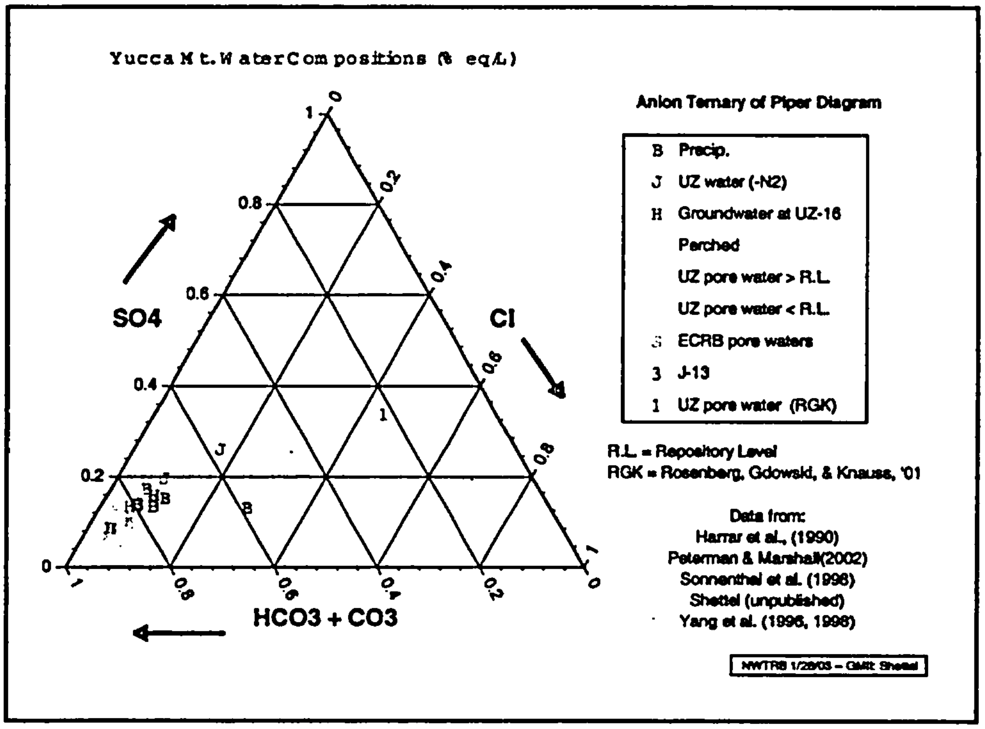
Conclusions

- Vadose (fracture and pore) waters occur at and above repository level. (No groundwater)
- In-drift processes are more complicated than thus far admitted (by DOE).
- Corrosion rates are significantly higher for evaporating solutions and their condensates (0.1-1.0 mm/y, up to 10).
- Sub-boiling, immersion testing of EBS materials in groundwater is BOTH unrealistic and non-conservative.
- Vadose Zone is NOT a good environment for a Repository?

Back Up Slides

For
D. Shettel





How Dry is the Repository?

There are 81 L of pore water per m^3 in Topopah Spring tuff (TS tuff is ~300 m thick)

- 24,300 L of pore water in each $1m^2$ column of tuff

- Current Percolation Flux: avg. 5 $mm/y/m^2$

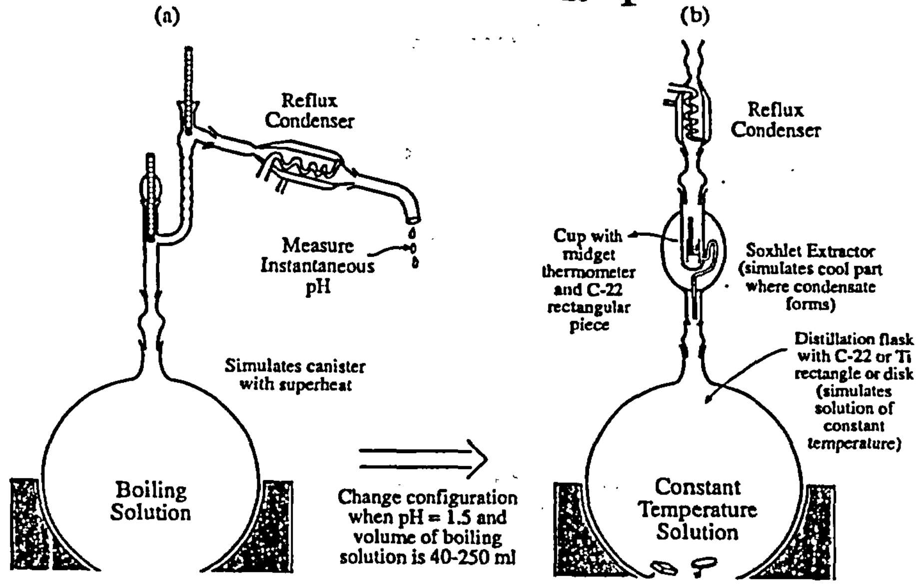
This is equivalent to 5 $L/y/m^2$
Spatial variability: 0-60 $mm/y/m^2$,
Equivalent to 0 to 60 $L/y/m^2$ over repository.

- Long Term Average Percolation Flux (last 1-10k Years)

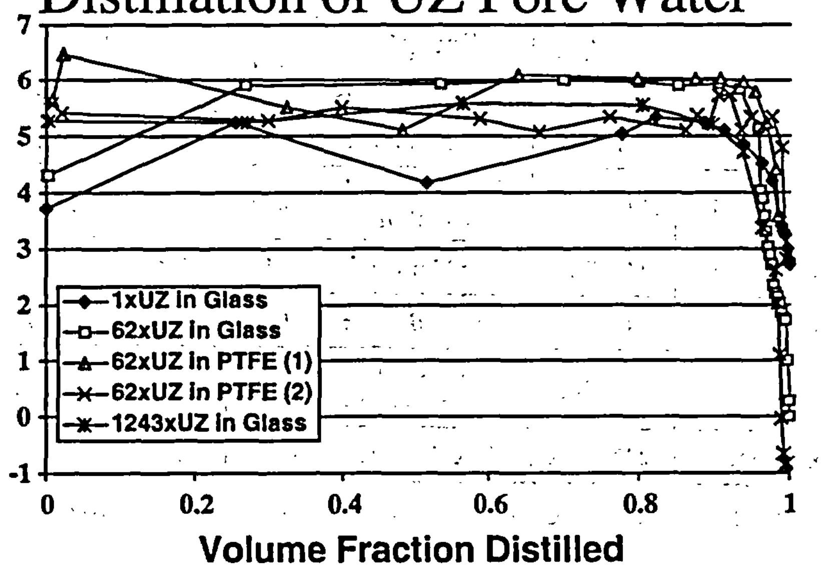
Avg. 6 $mm/y/m^2$, OR 6 $L/y/m^2$
Range: 2-20 $mm/y/m^2$, OR 2 to 20 $L/y/m^2$

Ref.: Peterman & Marshall, 2002; Yucca Mt. S&B Rpt.

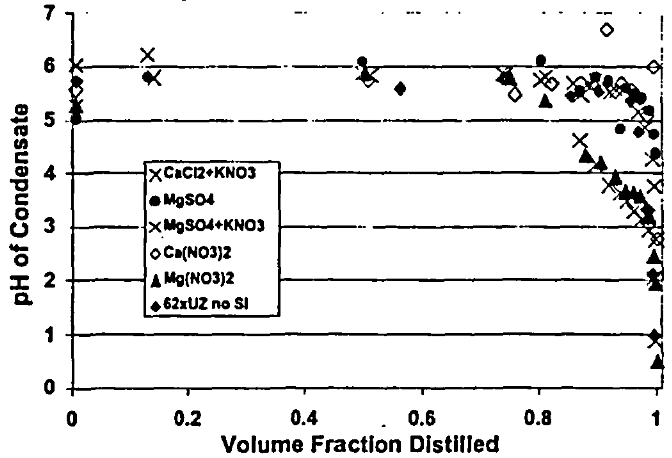
Distillation / Reflux Experiments



Distillation of UZ Pore Water



Distillation of Components of UZ Pore Water



Distillation / Reflux Experiments

Metal	Original Solution	Sample Environment	pH	Temp °C	Corrosion Rate
C-22	62xPore	Residual Paste	2.63	144	134
C-22 (#21)	1243xPore	Clear residual solution	0.22	144	10,943
C-22 (#21)	1243xPore	Soxhlet Cup	0.18	78	14
C-22 (#34)	1243xPore	Residual Paste	2.21	144	678
C-22 (#34)	1243xPore	Embedded in Residual solid	2.21	144	30
C-22 (#34)	1243xPore	Soxhlet Cup	-0.48	77	938

NOTES: 22-29 day tests. Corrosion rate based on weight loss, in micron/year.

Corrosion of Alloy 22 in Condensates

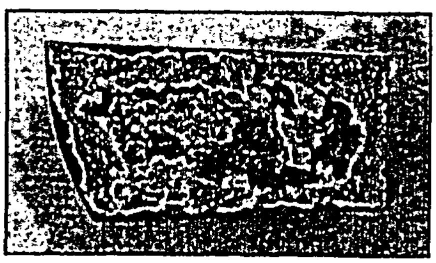
Original Solution	Condensate Type	Measured pH	Test Temp.°C	Corrosion Rate
62x Pore	Next-to-Last 30mL	1.62	130	15
62x Pore	Final 30 mL	0.59	130	406
1243x Pore	Next-to-Last 30mL	0.02	90	52
1243x Pore	Final 30 mL	-0.54	90	603

NOTES: 30 day immersion tests.
Corrosion rate based on weight loss, in microns/year.

Distillation / Reflux Experiments

Metal	Original Solution	Sample environment	pH	Temp °C	Corrosion rate†
Ti-7	1243xPore	Residual Solution	1.60	144	969
Ti-7	1243xPore	Residual Solid	1.6	144	36
T-7	1243xpore	Soxhlet cup	-0.88	78	114

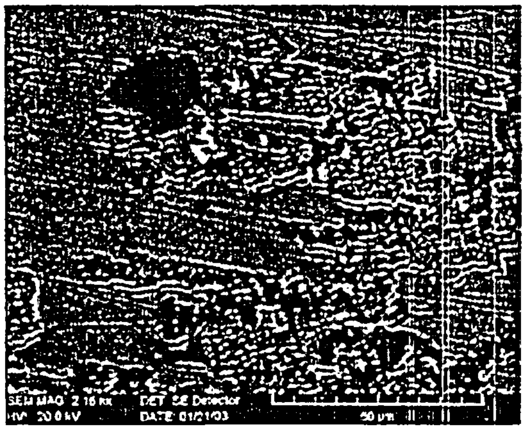
(Microns/year)



Ti-7 in Residual solution

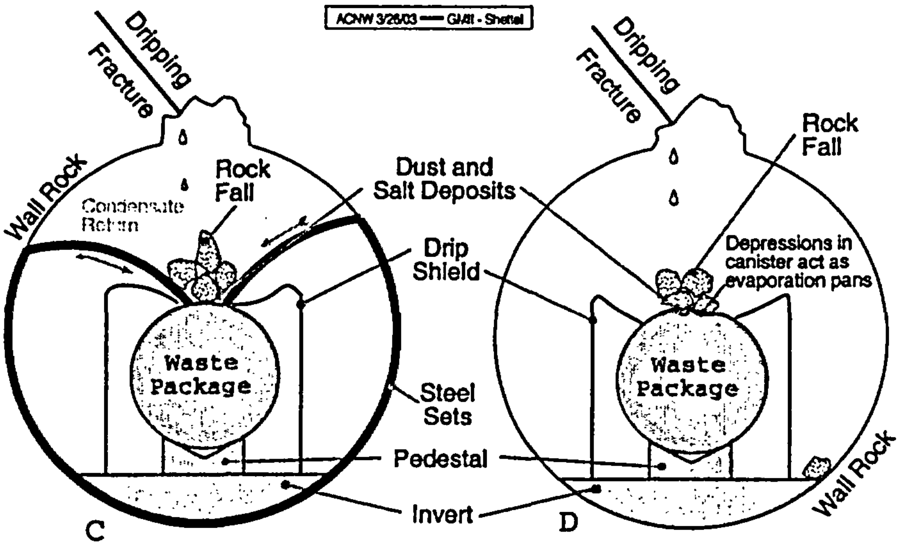
Importance of Solids

Solids that precipitate during distillations, including halite (NaCl), tachyhydrite ($CaMg_2Cl_6 \cdot 12H_2O$), and basic Mg oxy salts, are porous and heterogeneous. When allowed to deliquesce as a paste, may become aggressive as well.



Sample of C-22 embedded in a moist paste of residual solids from a distillation of 1243x Pore Water showed signs of tarnishing after 8 weeks at room temperature.

In-Drift Processes



Cross Section of Emplacement Drifts

J. Payer, Case Western Reserve University (CWRU): Just one comment. You have shown that it is possible to start with mixtures of ions and waters that are available here. And if you treat them by boiling them down, refluxing, things of that sort.

D. Shettel, Geosciences Management Institute, Inc. (GMII): We're not just starting with any composition of ions. We are starting with ones that are appropriate at and above the repository level.

J. Payer, CWRU: Yes. You are starting with ions that are present there and treating them. What I haven't seen yet, and I am not saying that it cannot exist, is how do those environments get generated on a metal waste package surface. Do you envision a small Soxhlet-type process?

D. Shettel, GMII: No, just by the solution that is dripping onto the canister and being evaporated and concentrated on a hot metal surface.

J. Payer, CWRU: I understand, but how do they get refluxed?

D. Shettel, GMII: The refluxing was up in the rock. That is a different matter.

J. Payer, CWRU: The highly acidic brines are up in the rock. That is where they form. Then do they drip onto the waste package?

D. Shettel, GMII: That is a possibility, but the loss would probably buffer the pH to limit that.

J. Payer, CWRU: I have heard these ideas in many different presentations. The part that's missing in my mind, and I'm not saying that it does not exist, or where it is, or where the boundaries are, is the description of how these environments form on a waste package or a drip shield, either on the top, or the bottom, or wherever. How would they form; would they persist; how much of it is there; if they go away, would they re-form. I think this is the real issue. There is no question that you can generate environments in a lab that will make Alloy C-22 and alloy titanium corrode very rapidly. That has been demonstrated.

D. Shettel, GMII: Right. These solutions can concentrate in the refluxing zone above the rock (i.e., above the drift in the rock). The essentially pre-concentrated solutions to some extent can then penetrate the fractures and drip onto the canisters where they can reach that final evaporation approaching near dryness or even complete dryness.

J. Payer, CWRU: The part that I cannot envision is how the condensation occurs. How are the acid vapors that are generated kept at that location on the metal surface? My picture is that it is an ambient pressure. Maybe you have recondensing to keep bringing back acid vapors. It seems to me you've got an open system where acid vapors could go wherever acid vapors are going to go, but they do not have to come back and be captured in the solution.

D. Shettel, GMII: That's right. They don't have to. But you have to remember, you can still keep dripping water down onto the canister and build up the salt deposits, and add moisture to that.

M. Morgenstein, GMII: Joe, let me interject for just a second. If you just take a fracture dripping onto say a titanium drip shield, the precipitate that you would get from the evaporation of that drip will have tachyhydrite in it. Period. You don't need recycling.

Left blank intentionally.

5.2 Evaporation, Reconstitution, and Water Chemistry

(John Walton, University of Texas at El Paso)

Dr. John Walton (representing Nye County, Nevada) gave a talk about the importance of evaporation and water chemistry in estimating corrosion for all engineered barrier materials. A theme of the talk was the concern that the U.S. Department of Energy (DOE) had not considered physical separation processes in its analyses. During evaporation, different minerals deposit at different locations. He showed salt separations in two examples–deposits from a sidewalk, and those near a desert spring. Dr. Walton believes that natural air movements within Yucca Mountain have not been fully considered, that the tunnel construction effects increase the air permeability of the rock, that the climate could be dryer than anticipated, and that the period of evaporation may last well beyond current projections.

Dr. Walton concluded that physical separation of minerals is certain to occur, that potentially aggressive environments could be created for titanium drip shields and Alloy C-22 waste packages, that these environs will have high spatial and temporal variability, and that biological and other chemical processes will also be important.

Nye County Department
of Natural Resources and Federal Facilities

Evaporation, Reconstitution, and Water Chemistry

John Walton, Ph.D., P.E. and Drew Hall
University of Texas at El Paso

ACNW
March 2003

Objectives

- Water chemistry important for corrosion of all EBS materials and in determining radionuclide mobility
- Important to consider all likely chemical, biological, and physical processes
- Physical separation processes are not being considered

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Evaporation

- Water generally moves during evaporation
- Minerals precipitate as water becomes concentrated
- Different minerals deposit at different locations
- Many potential situations
- Common in arid environments

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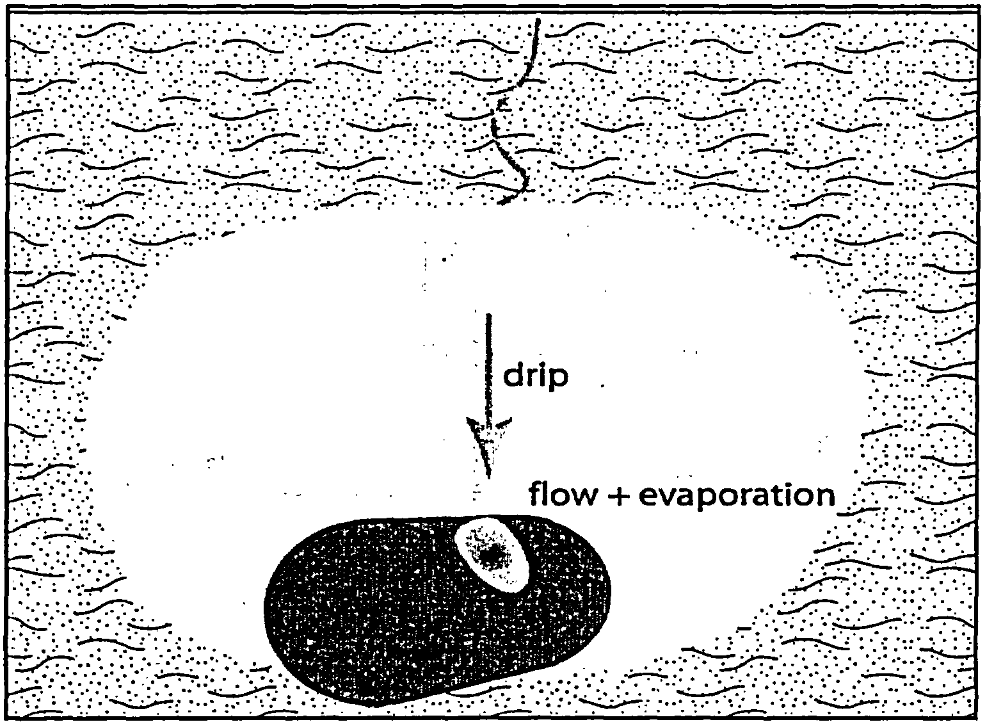
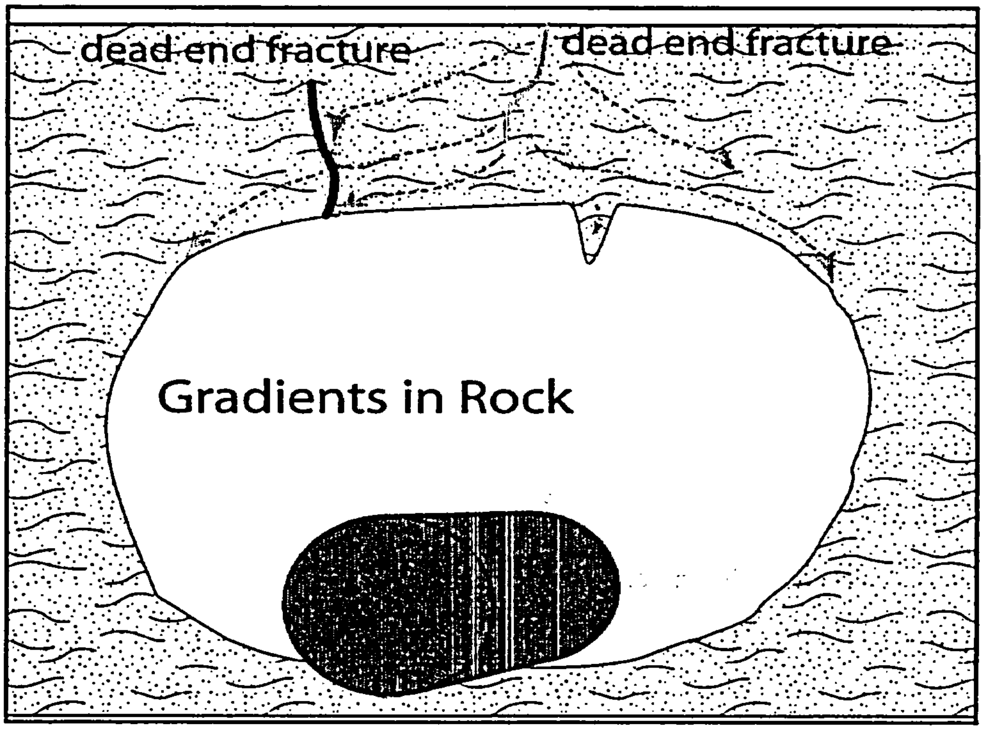
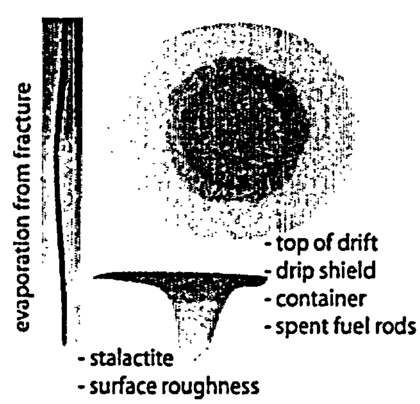


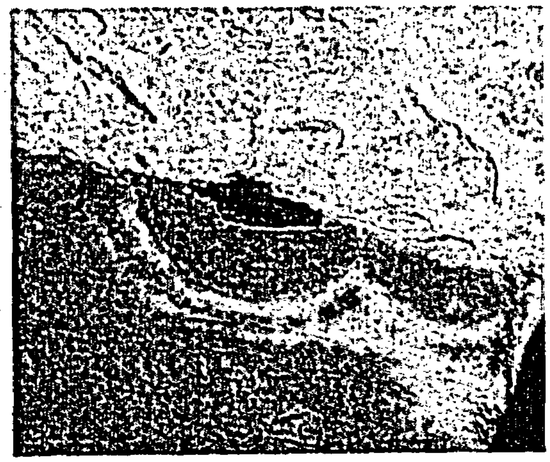


Physical Separation of Precipitates

- Mouth of fracture opens into drift
  - relative humidity gradient in fracture
  - solution most concentrated at mouth
- Vertical features on drift roof
- Radial flow from water source
- Dripping is not required for physical separation



Sidewalk Example



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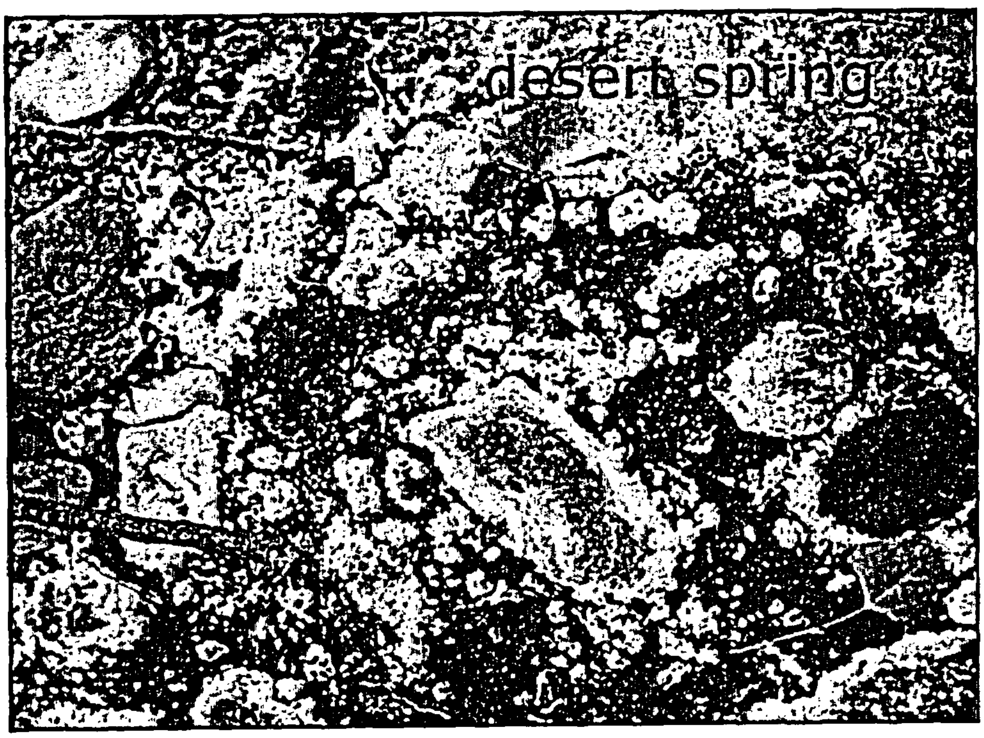

Model

- Simple equilibrium model
- Adequate for first look and semi-quantitative analysis
- Two endpoints:
  - single cell mixing tank (no separation)
  - infinite series of mixing tanks (maximum possible degree of separation)
- Reality likely to be intermediate and highly variable
- Simulation stopped at 10^6, 1 mg/kg concentration factor

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Interpretation

- Aggressive versus non-aggressive anions (~5 chloride :1 nitrate ratio)
- Drips can be problematic during evaporation and subsequent hydration as repository cools
- Separation in rock important as dust and during pluvial periods

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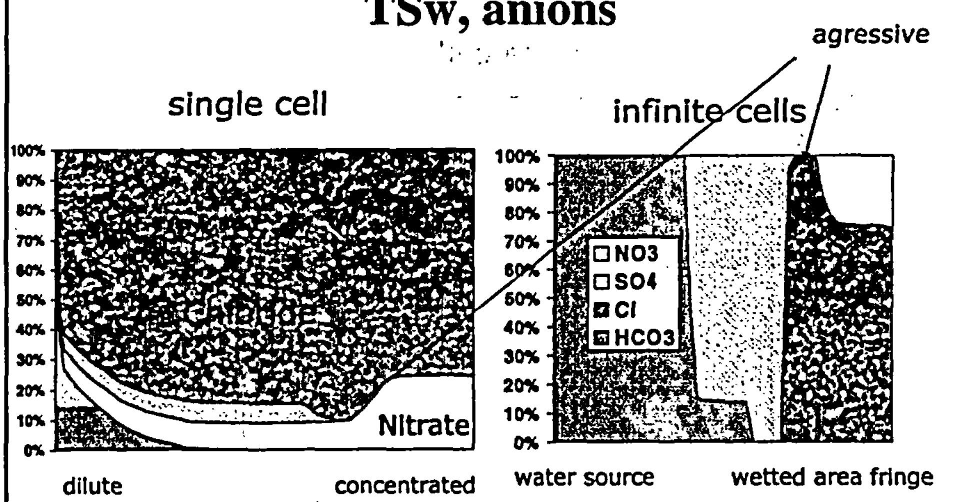
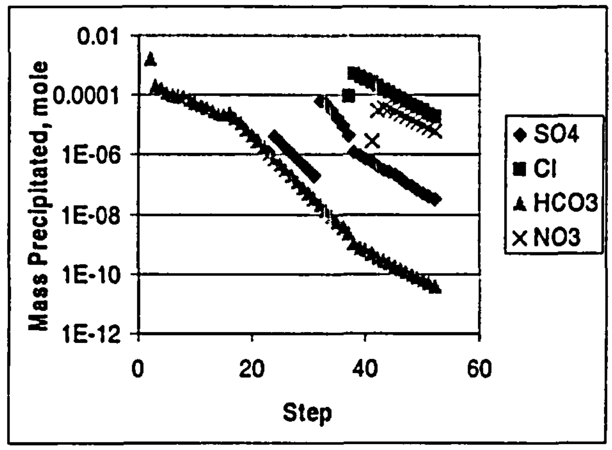
Source Waters

- Precipitation
- Paintbrush Non-Welded Tuff (PTn) Pore Water (above)
- Topopah Spring Welded Tuff (TSw) Pore Water (repository)
- 50:50 mix Precipitation & Paintbrush
- What else should we try?

TSw, anions



TSw, anions



dilute concentrated

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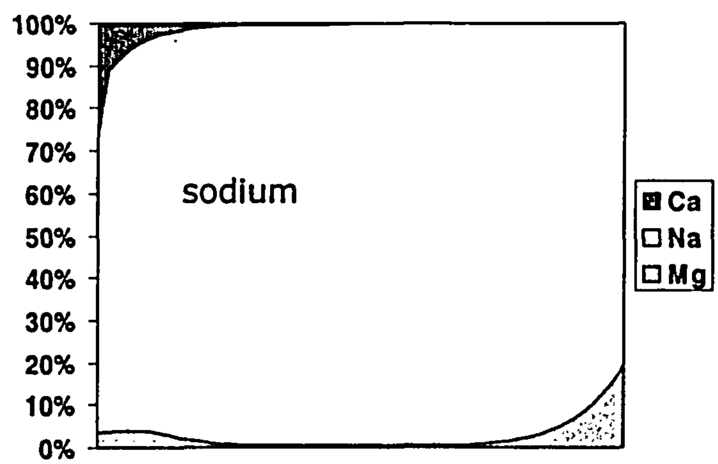
TSw, cations

single cell



dilute concentrated

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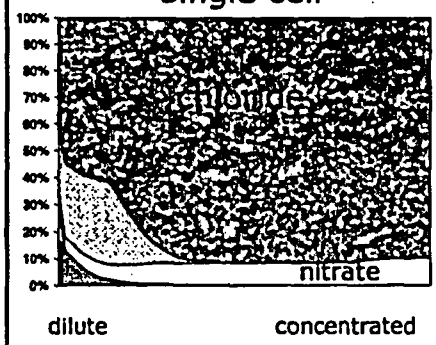
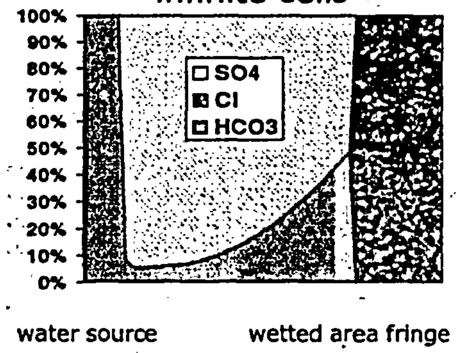
PTn, anions

single cell



infinite cells



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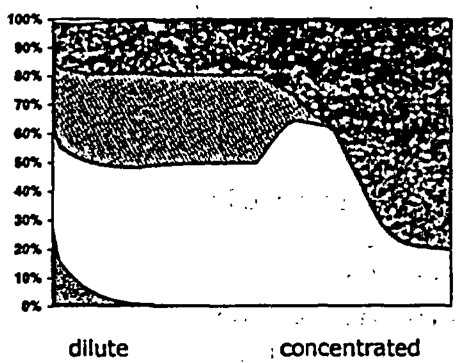
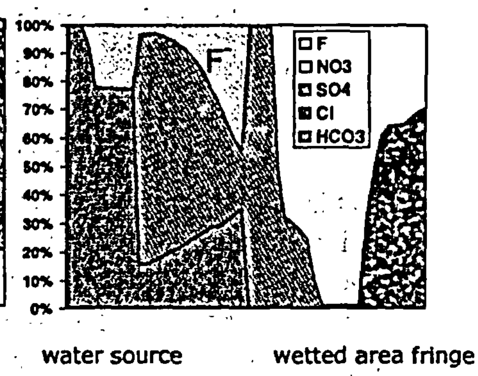
Precipitation, anions

single cell



infinite cells



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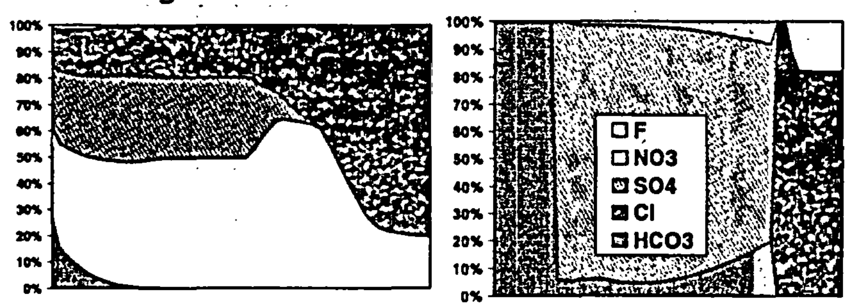
Precipitation & PTn, anions

single cell　　　　　　infinite cells



dilute　　concentrated　　water source　　wetted area fringe

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Relative Humidity (timing)

- Natural breathing of mountain not fully considered
- Construction increases air permeability
- "Conservative" models predict high relative humidity
- Climate could be dryer than anticipated
- What is conservative? Are high infiltration and high relative humidity always conservative?
  - no, alternating wet and dry is more problematic
  - ignoring dryer repository scenarios is non conservative
- Evaporation period likely to last well beyond current projections

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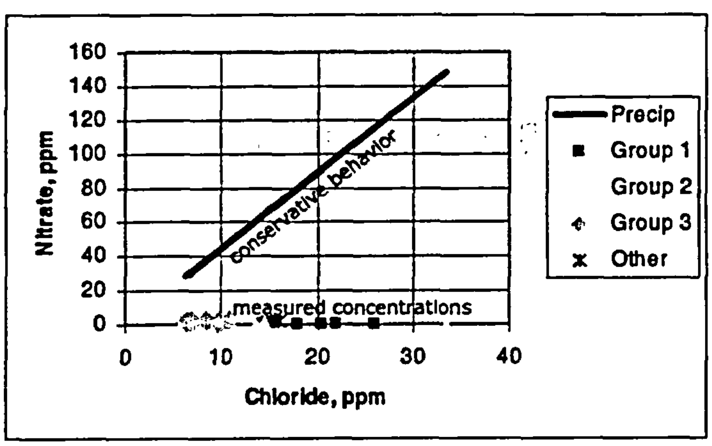
DOE Nitrate Assumption versus Data from Wells



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Conclusions

- Physical separation is not "likely" it is certain to occur
- Produces wide range of anticipated water chemistry
- Potentially aggressive environments for Titanium, Alloy-22, cladding, alteration, solubility
- High spatial and temporal variability
- Extends indefinitely in time
- This work only examines a subset of total anticipated variability in water chemistry: biological as well as other chemical processes will also be important.

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Backup Slides

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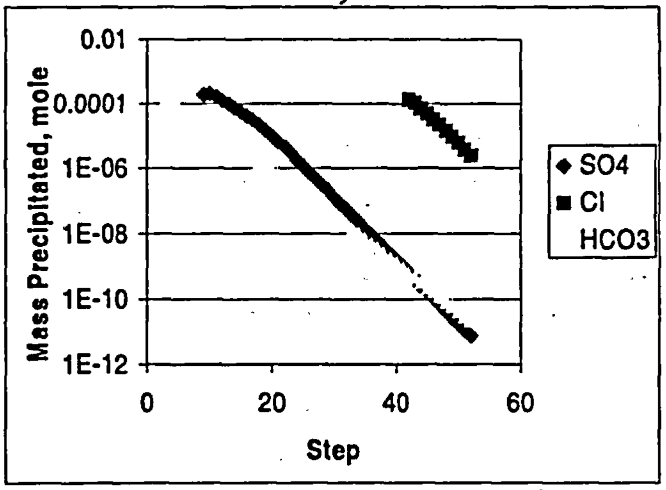
PTn, anions



dilute concentrated

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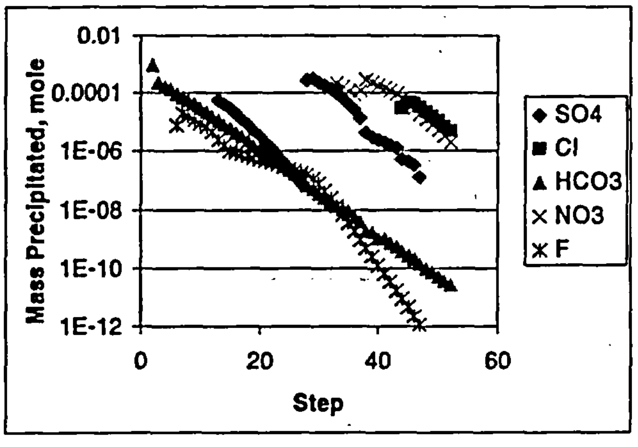
Precipitation, anions



dilute concentrated

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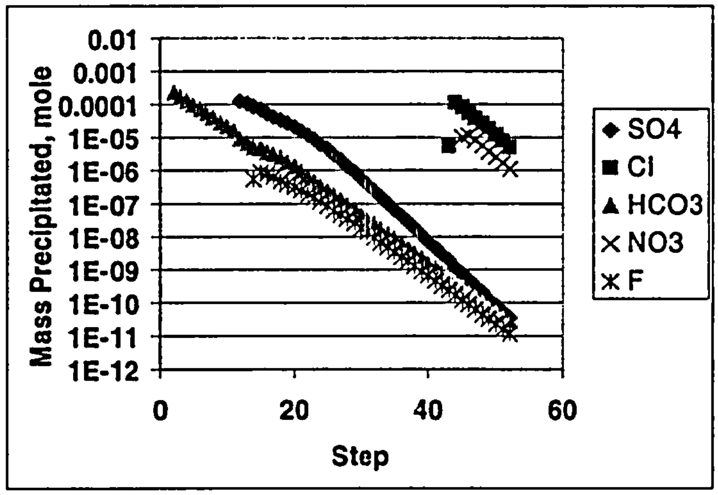
Precipitation & PTn, anions



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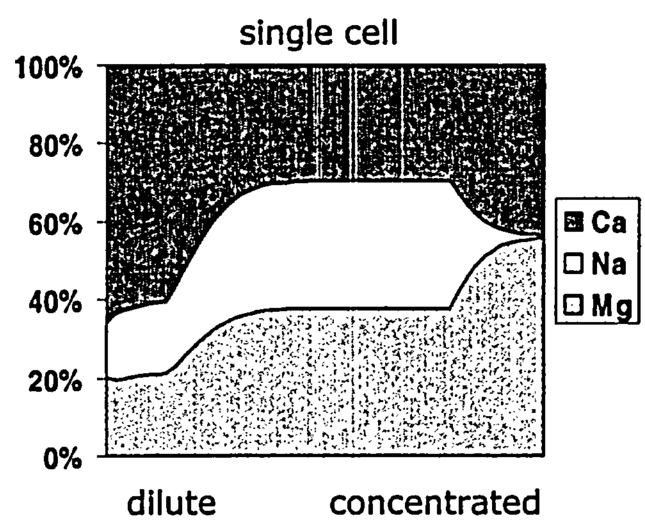
PTn, cations



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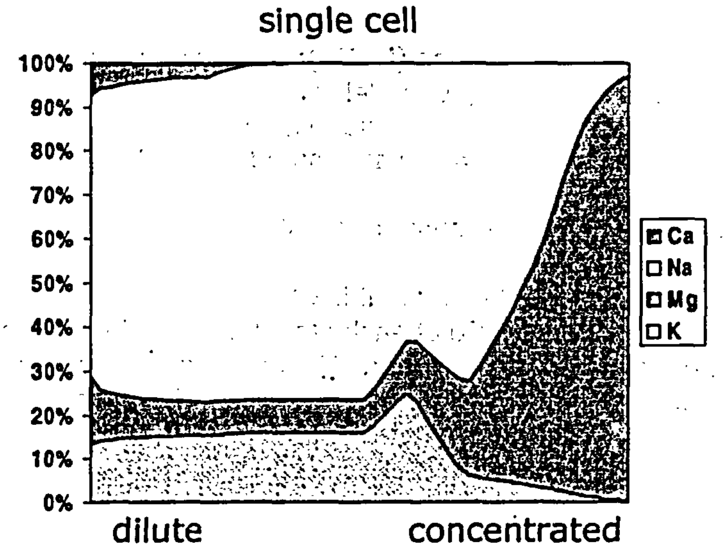
Precipitation, cations



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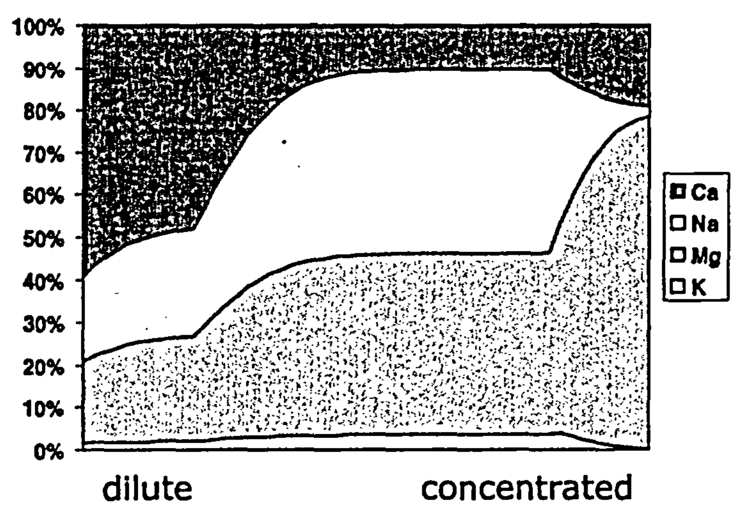
Precipitation & PTn, cations



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J. Payer, Case Western Reserve Univ. (CWRU): John, just a question. I believe the approach and the goals of this work are right on, so I applaud you for that. How do you deal with the issue of what is going to precipitate, and when it precipitates, and the thermodynamic database and brines, and things of that sort? It is always a challenge, so my question is, just what do you do?

J. Walton, University of Texas at El Paso (UTEP): I was careful to label what we did as semi-quantitative. We used a very simple model, which dd not tally for activity coefficients. We just took the common salts that people have said might be there and put those in the list. When these are super-saturated they precipitate immediately. So it is very simplistic.

J. Payer, CWRU: As single salts or mixtures of salts?

J. Walton, UTEP: Mixtures precipitate, and that is why, when you rehydrate them, you get chloride and nitrate coming together. So at each step, for example, sodium chloride and sodium nitrate are going to precipitate together. Things are allowed to precipitate together, but there is nothing like a salt solution or anything as complicated as that.

5.3 Clark County, Nevada–What Is Our Concern, and Why Are We Still Concerned? Temperature, Coupled Processes, Corrosion

(Engelbrecht von Tiesenhausen)

Mr. Englebrecht von Tiesenhausen (representing Clark County, Nevada) gave a talk that focused on the concerns by Clark County regarding temperature, coupled processes, and corrosion. He referred to a letter to the U.S. Nuclear Regulatory Commission (NRC) Chairman Meserve (dated August 13, 2001) that recommended continued exploration of the chemical issues associated with repository design, such as a "hot" versus "cold" repository, or the use of backfill. Mr. von Tiesenhausen expressed concerns that the DOE has selected the "hot" repository option for the design to be proposed in a license application. He was also concerned that DOE is still using concentrated J-13 well water for seepage brines. He noted that a previous State of Nevada presentation to the Board on Radioactive Waste Management (of the National Academies) indicated that evaporation of concentrated unsaturated zone pore waters will produce acidic environments, while evaporation of J-13 well waters will produce more benign alkaline environs. Rock dust, with its major and minor chemical constituents, will also influence the chemistry of evaporated solutions. Mr. von Tiesenhausen concluded that fully coupled thermo-hydro-chemical processes may be impossible to model at this time, that chemical environs of the waste packages are likely to be very complex, and that predicting long-term corrosion of Alloy C-22 using J-13-based waters is probably not realistic.

Clark County Comments

What is our concern, and why are we still concerned.

Temperature

Coupled Processes

Corrosion

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ACNW Guidance

Letter to Chairman Meserve:

August 13, 2001

Recommendation 1

The staff should continue to explore the chemical issues associated with major repository design changes such as a "hot" versus "cold" repository or the use of backfill.

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DOE White Paper on Thermal Operating Modes (2/02)

- Uncertainty in total dose is larger than the difference between operating modes
- At the total system level the difference between HTOM and LTOM is not significant.

NWTRB Concerns

- Current analyses may indicate that temperature does not affect repository performance and levels of uncertainty or that current TSPA models are not sufficiently sensitive to capture the differences between higher and lower temperature operating modes (Cohon 2001)

Concerns Persist

- DOE has selected the HTOM option for their repository design, to be carried forward to LA.
- DOE is still using concentrated J-13 water for the seepage brines. (TRB 1/28/03)

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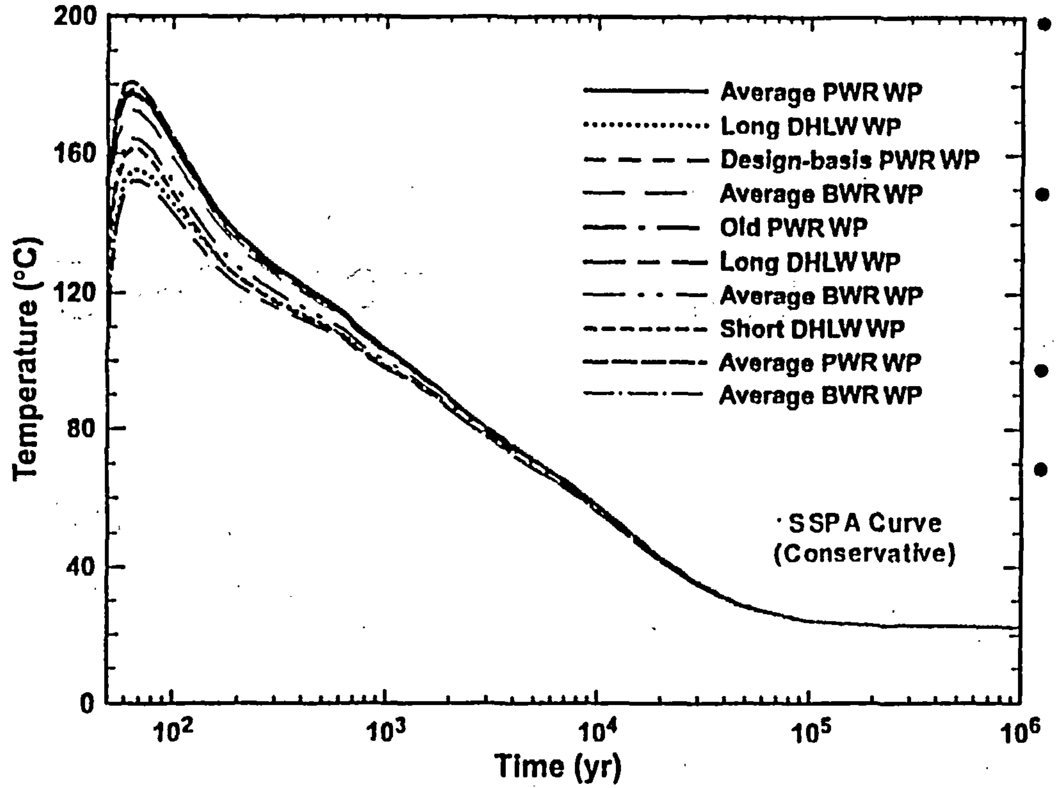
In-Drift Environment – Temperature



- Analysis from Supplemental Science and Performance Assessment (SSPA)
- Predictions for waste packages (WPs) at center of repository (hottest)
- Assumes all WPs are instantly emplaced
- A more realistic sequential emplacement process will lower WP temperatures by approximately 30°C

Epistemic Issues
Coupled Processes

- "I think the process is still at an early stage" (12/18/02)

- Beyond our understanding of the mechanisms at this time (7/25/02)

State of Nevada Presentation

- Made to the Board on Radioactive Waste Management (12/12/02)
- Continued evaporations of concentrated and aqueous UZ pore water solutions produce acidic environments.
- Similar evaporations of J-13 well water produce generally alkaline environments.

Water Chemistry in the Near Field

- Influence of dust
- Contribution from vadose zone water, pore water, and rock chemistry.
- Construction water

Dust Chemistry

- Mean major and minor element compositions <60 mesh
- Mean major and minor element compositions of 10 size classified dust samples
- Water soluble components in dust samples
- Mean trace element compositon

Table 1—Mean major- and minor-element compositions of <60-mesh dust samples collected in 2001 from the Exploratory Studies Facility, Yucca Mountain, Nevada.

	<60-mesh bulk analysis,			<60-mesh soluble ions,	
	Mean	*Stdev*		Mean	*Stdev*
	Weight percent			Micrograms/gram	
SiO_2	69.09	*3.25*	Ca	607	*258*
Al_2O_3	11.84	*0.55*	Mg	34.2	*21.9*
FeO	3.30	*1.73*	K	204	*87*
Fe_2O_3	1.16	*0.52*	Na	363	*98*
MgO	0.32	*0.13*	Si	81.7	*49.2*
CaO	1.83	*1.17*	Cl	181	*56*
Na_2O	3.25	*0.11*	Br	29	*15*
K_2O	4.37	*0.21*	F	15	*9*
TiO_2	0.16	*0.04*	NO_3	418	*351*
P_2O_5	0.09	*0.03*	SO_4	816	*472*
MnO	0.11	*0.02*	PO_4	20	*24*
Br	0.0049	*0.0022*	As	0.096	*0.036*
Cl	0.1185	*0.0397*	Pb	0.0012	*0.0007*
F	0.0739	*0.0433*			
S	0.05	*0.04*			
CO_2	0.21	*0.17*			
C organic	1.46	*0.63*			
H_2O-	0.45	*0.23*			
H_2O+	2.53	*0.86*			
SUM	99.99	*0.80*			

Table 2- Mean major- and minor- element compositions in weight percent of 10 size-classified dust samples collected in 2002 from the Exploratory Studies Facility, Yucca Mountain, Nevada. The mean composition of the rhyolite member (Tptp) of the Topopah Spring Tuff[6] is shown for comparison. Dashes (---) indicate that element was not analyzed.

	60- to 200-mesh		200- to 325-mesh		<325 mesh		Tptp	
	Mean	*Stdev*	Mean	*Stdev*	Mean	*Stdev*	Mean	*Stdev*
SiO_2	71.02	*2.54*	68.53	*2.57*	67.92	*2.19*	76.29	*0.32*
Al_2O_3	12.71	*1.25*	12.45	*1.00*	12.22	*0.59*	12.55	*0.14*
FeO	0.97	*0.85*	1.80	*1.24*	2.52	*0.85*	0.13	*0.05*
Fe_2O_3	1.22	*0.51*	1.16	*0.63*	0.93	*0.44*	0.97	*0.07*
MgO	0.27	*0.21*	0.39	*0.23*	0.38	*0.21*	0.12	*0.02*
CaO	1.32	*0.57*	1.85	*0.65*	2.26	*0.65*	0.50	*0.03*
Na_2O	3.40	*0.52*	3.25	0.47	3.18	*0.38*	3.52	*0.11*
K_2O	4.63	*0.54*	4.39	*0.38*	4.34	*0.29*	4.83	*0.06*
TiO_2	0.21	*0.10*	0.22	*0.10*	0.19	*0.06*	0.11	*0.00*
P_2O_5	0.09	*0.16*	0.25	*0.54*	0.16	*0.27*	<0.05	---
MnO	0.10	*0.02*	0.10	*0.02*	0.10	*0.01*	0.07	*0.01*
Br	0.0024	*0.0021*	0.0037	*0.0028*	0.0040	*0.0018*	—	---
Cl	0.0815	*0.0503*	0.1243	*0.0713*	0.1507	*0.0610*	0.0167	*0.0041*
F	0.1099	*0.1103*	0.1595	*0.2077*	0.1194	*0.0813*	0.0383	*0.0080*
S	0.04	*0.03*	0.06	*0.06*	0.09	*0.05*	<0.05	---
CO_2	0.40	*0.39*	0.59	*0.37*	0.91	*0.36*	0.01	*0.00*
C (organic)	0.43	*0.31*	0.85	*0.52*	1.36	*0.64*	—	---
H_2O-	0.42	*0.27*	0.49	*0.30*	0.55	*0.28*	0.24	*0.07*
H_2O+	2.09	*1.27*	2.99	*1.29*	2.69	*0.78*	0.40	*0.09*
SUM	99.48	0.42	99.45	0.99	100.05	*0.52*	99.79	

Table 3-Mean compositions in micrograms/gram of water-soluble components of size classified dust samples collected in 2002 from the Exploratory Studies Facility, Yucca Mountain, Nevada

	60- to 200-mesh		200- to 325-mesh		<352-mesh	
	Mean	*Stdev*	Mean	*Stdev*	Mean	*Stdev*
Ca	380	*275*	686	*389*	1079	*541*
Mg	37	*17*	45	*17*	68	*32*
K	231	*67*	237	*95*	273	*76*
Na	215	*77*	311	*166*	402	*170*
Si	114	*69*	105	*82*	117	*57*
Cl	102	29	171	97	209	93
Br	8	*5*	16	*15*	13	*9*
F	13	*6*	10	*9*	3	6
NO_3	184	*77*	358	*169*	645	*489*
SO_4	402	*215*	732	*383*	984	*350*
PO_4	28	*52*	12.1	*6.2*	13.0	*4.9*
Pb	0.0027	*0.0012*	0.0031	*0.0013*	0.0019	*0.0006*
As	0.051	*0.025*	0.056	*0.040*	0.073	*0.040*

Table 4—Mean trace-element composition in micrograms/grams of size classified dust samples collected in 2002 from the Exploratory Studies Facility, Yucca Mountain, Nevada. The mean trace-element composition of the rhyolite member (Tptp) of the Topopah Spring Tuff[9] is shown for comparison.

	60- to 200-mesh		200- to 325-mesh		<325 mesh		Tptp	
	Mean	*Stdev*	Mean	*Stdev*	Mean	*Stdev*	Mean	*Stdev*
As	7.200	*5.820*	7.610	*2.930*	8.840	*1.750*	5.220	*1.810*
Ba	382.000	*563.000*	428.000	*470.000*	326.000	*232.000*	51.000	*14.000*
Be	4.030	*1.040*	3.880	*0.680*	3.780	*0.540*	3.410	*0.150*
Bi	0.220	*0.200*	0.190	*0.130*	0.260	*0.210*	0.060	*0.040*
Cd	1.846	*2.907*	0.769	*0.703*	0.694	*0.220*	0.066	*0.034*
Co	1.900	*1.030*	3.250	*1.490*	4.140	*1.410*	0.230	*0.060*
Cr	43.100	*20.300*	58.900	*24.600*	81.900	*18.20*	9.290	*3.590*
Cs	4.820	*2.630*	4.990	*2.380*	5.000	*1.520*	4.250	*0.350*
Ga	20.600	*1.900*	20.000	*1.700*	19.900	*1.500*	15.700	*0.600*
Li	32.500	*9.900*	39.700	*9.600*	45.700	*7.900*	26.500	*9.000*
Mo	8.500	*5.200*	11.800	*6.700*	13.400	*4.800*	2.400	*1.000*
Ni	17.200	*9.200*	29.900	*12.500*	42.300	*8.600*	1.400	*0.400*
Pb	34.400	*8.600*	34.500	*5.200*	33.700	*1.900*	26.900	*1.300*
Rb	171.000	*42.000*	172.000	*27.000*	180.00	*17.000*	185.000	*13.00*
Sb	2.250	*1.780*	3.740	*2.830*	3.520	*1.430*	0.320	*0.060*
Sc	3.360	*1.500*	3.910	*1.830*	3.900	*1.620*	2.390	*0.110*
SR	92.500	*76.000*	143.300	*100.500*	136.500	*71.500*	26.500	*3.300*
Th	19.500	*5.200*	21.100	*3.600*	22.300	*2.200*	25.700	*2.100*
Tl	1.060	*0.300*	1.250	*0.440*	1.320	*0.430*	1.120	*0.2100*
U	3.480	*1.330*	3.530	*0.920*	3.570	*0.600*	3.920	*0.400*
V	8.130	*4.760*	13.230	*11.790*	12.290	*10.460*	0.070	*0.610*
Y	49.400	*29.000*	49.00	*10.400*	52.400	*5.900*	29.900	*3.400*
Zn	189.000	*110.000*	294.000	*162.000*	365.00	*189.000*	36.000	*5.000*
La	45.200	*27.400*	60.800	*35.800*	58.900	*25.200*	41.800	*5.700*
Ce	89.800	*46.000*	118.100	*56.600*	122.700	*41.800*	76.500	*8.700*
Pr	9.580	*4.440*	11.560	*5.000*	11.530	*3.640*	9.990	*1.070*
Nd	35.500	*15.800*	42.200	*17.200*	42.300	*12.500*	33.020	*3.340*
Sm	6.910	*2.390*	7.540	*1.490*	7.650	*1.120*	6.820	*0.530*
Eu	0.720	*0.660*	0.900	*0.680*	0.840	*0.460*	0.320	*0.030*
Tb	1.050	*0.420*	1.070	*0.150*	1.120	*0.100*	1.190	*0.110*
Gd	6.200	*2.440*	6.450	*0.830*	6.700	*0.670*	7.050	*0.550*
Dy	6.840	*2.710*	6.860	*1.100*	7.230	*0.680*	6.910	*0.510*
Ho	1.420	*0.580*	1.410	*0.240*	1.480	*0.150*	1.480	*0.110*
Er	3.920	*1.540*	3.930	*0.670*	4.120	*0.430*	5.020	*0.390*
Tm	0.580	*0.200*	0.590	*0.100*	0.620	*0.060*	0.870	*0.070*
Yb	3.380	*1.070*	3.490	*0.530*	3.640	*0.340*	4.160	*0.320*

Conclusions

- Fully coupled THC processes may be impossible to model at the present time
- Chemical environments on the waste package are likely to be extremely complex
- Predicting long term corrosion of Alloy 22 using J-13 based solutions is probably not realistic

E. von Tiesenhausen, Clark County: My point is that I don't think the knowledge base is there to look at fully coupled thermo-hydro-chemical corrosion processes at these high [repository] temperatures. The environments are going to be extremely complex. And with that degree of complexity, I do not know if it's even possible to arrive at the reasonable bounding analysis.

B. J. Garrick, ACNW Member: Okay. Engelbrecht, you have identified a number of areas where you think better data would give us much better knowledge with respect to the adequacy of the site. Do you have any views on the feasibility of such data being obtained in a reasonable time? Are we talking about a problem here that is, from your perspective, solvable, or are we talking about something that would take 100 years to do?

E. von Tiesenhausen, Clark County: I do not think it would take 100 years, but certainly with the time frame available, and the temperatures under consideration, I do not think it is possible to get that data. I think if the DOE had started by funding programs at the universities to look at thermodynamic issues and kinetic issues, that we might be a little further ahead. I do not think that with the license application supposedly going forward, the data can be had.

D. Bullen, Iowa State University: This novel idea to go to low temperatures is very interesting. How low is low enough in your opinion, Engelbrecht?

E. von Tiesenhausen, Clark County: That is a very difficult issue. You look at the DOE's low temperature design and the average is around 80°C. That may not be good enough as an average, but it may be good enough as an upper bound.

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5.4 Tribal Representative

(Atef Elzeftawy)

Dr. Atef Elzeftawy (representing the Las Vegas Paiute Tribe) read a statement into the record regarding tribal concerns. He stated that the Tribe should be allowed to play a major role in the Yucca Mountain program, and that the Tribe has major concerns about the policies and technical direction of the Yucca Mountain project and the DOE, U.S. Environmental Protection Agency, and NRC roles in the program. For example, the Tribe believes that the DOE's TSPA should not be accepted as the method of testing and evaluating the suitability of the Yucca Mountain site. The Tribe seeks no adverse impact on the health of the tribal population or on the economic development of its Snow Mountain Reservation.

LAS VEGAS PAIUTE TRIBE
NEVADA

Presentation
To
ACNW
Of the
UNITED STATES NUCLEAR REGULATORY COMMISION
March 26,2003
Washington, D.C.

TRIBAL CONCERNS

1. **NO** Government –to-Government consultation or interaction according to Presidential Executive Orders.

2. We **(Federally Recognized Tribe)** should be allowed to play a major role in the Yucca Mountain Program as stated in the NWPA and its amendments in terms of policy and technical direction.

3. We started to get some fragmented information, now and then, from NRC? **WHY?**

4. We have **MAJOR CONCERNS** about the policies and technical direction of the Yucca Mountain Project and the DOE, EPA, and NRC role in the program. Few listed below;

   - NRC should have the independent role as specified in the NWPA, which means that the NRC should not modify its CFR to fit the technical problems of the DOE Yucca Mountain program. And if the NRC does, that is **NOT** acceptable to the Tribe,

   - Accepting the DOE total system performance computer assessment (TSPA) as the method of testing and evaluating the suitability of the Yucca Mountain Site is **NOT** acceptable to the Tribe, and

   - NRC should assess the Yucca Mountain Site as **GEOLOGIC SITE** for high-level radioactive waste repository and **NOT** an engineering site.

5. We simply **DO WANT** to have no adverse impact on the Tribal Population health and our economic development of our Snow Mountain Reservation.

Atef Elzeftawy, Las Vegas Paiute Tribe: Before I go on, I want to make one comment on [Ms. Gloria Hernandez's] behalf. We would like to say thank you, on the record, for the Chair of the U.S. Nuclear Regulatory Commission who generously gave about an hour, an hour and a half, of his time in Las Vegas to meet with the Chairman and Vice Chairman of the Tribe in the presence of John Greeves [NRC Division of Waste Management]. And I'd like also to say thank you to Marty Virgilio and John Greeves for taking the time to meet with us. And another compliment for [NRC] Commissioner Merrifield, who took the time and spent four or five hours with us visiting Las Vegas and visiting our land.

Ms. Gloria Hernandez writes, "No government-to-government consultation or interaction according to the Presidential Executive Order." The Tribe of the United States Government would like to have its standard upgraded to be treated equally to the States. They do in many instances, and she also writes, "As a federally recognized Tribe, we should be allowed to play a major role in the Yucca Mountain Program as stated in the Nuclear Waste Policy Act."

Another point that Ms. Hernandez makes is that "We started to get some fragmented information now and then from the NRC. We haven't got a thing from the DOE, even though we knocked on their doors a couple of times." When I explained to her about the background of the site, her point was that if the site was put together as a geologic repository, it should be a geologic repository, not an engineering repository. They are firm on that.

Looking at the DOE total performance assessment, when I explained to her in layman terms about the modeling and the total system performance, she wrote, "Accepting the DOE Total Performance Computer Assessment as a method of testing and evaluating the suitability of the Yucca Mountain site is not acceptable to the Tribe." In other words, do not do it by the computer and say it looks fine. You should have data. You should have things that really supplement that decision when it comes to the politics of it.

She also said, "They feel–that's the Council–they feel that the NRC and NRC staff should play their independent role as specified in the Nuclear Waste Policy Act," which means that the NRC should not modify the CFR to fit the technical problem with the DOE Yucca Mountain Program. And if the NRC does, that is not acceptable to the tribe.

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5.5 When Realism Is and Is Not Needed in TSPAs

(John Kessler, Electric Power Research Institute)

Dr. John Kessler gave a talk about realism in performance assessments. He pointed out that conservatism (as opposed to realism) is often easier to defend, especially during licensing proceedings. It serves to provide boundaries for license conditions and maintains a connection to performance confirmation. However, conservatism may distort the relative importance of individual barriers. Dr. Kessler gave an example of this from the diffusive release model in the Electric Power Research Institute's (EPRI) TSPA code. The EPRI model assumes excellent contact among all regions of the engineered barrier system, but in reality, spent fuel would not be in close contact with the rock walls of tunnels. The EPRI model also assumes continuous water pathways through the engineered barriers, but in reality, pathways would be much more limited. Dr. Kessler showed model results that illustrate how an estimated 10,000 year dose is strongly affected by the conservative diffusion model. He concluded that better relative unsaturated/saturated zone performance would be apparent if he had used a more realistic diffusive release model. Dr. Kessler said that it is reasonable to replace uncertainty with pessimistic assumptions to establish robustness for the adjudicatory process, to provide boundaries for license conditions, and to provide "reasonable expectation" levels of confidence for compliance with regulations.

When Realism is and is Not Needed in TSPAs

John Kessler

Manager, HLW and Spent Fuel Management Program

EPRI, Inc.

Presented to the ACNW, 26 March 2003

EPRI

Outline

- Why realism is useful
- Why full realism is not always necessary
- How much realism is needed for a TSPA used for Yucca Mountain licensing purposes?
  - Process by which improved realism can be achieved

Slide 2 - Kessler ACNW, 26 March 2003

EPRI

TSPA Regulatory Requirements

- 10 CFR 63.2 on what a TSPA should do
  - Identify FEPs and sequences of events (over 10,000 years) and their probabilities of occurrence
  - Examine the effects of the above on "performance"
  - Probability-weighted dose estimates (plus uncertainties) to the RMEI
- Identification and defense of multiple barriers
- **Main regulatory requirement: *reasonable expectation* of compliance with individual dose limits and MCLs**
  - Different from "reasonable assurance"
  - ***Conservative approaches OK as long as there is still compliance***

EPRI

TSPA as a Tool for Management and Understanding

- Evaluate existing knowledge
  - Develop uncertainties/variabilities
    - Provide estimate of range of possible behavior
    - Best if uncertainties/variabilities are not biased
- Identify which parts of the system (FEPs) "matter"
  - I.e., "significant" change in the probability-weighted dose ("dose risk") estimates
    - BSC used ±1 millirem per year ("Risk Prioritization..." report) – seems reasonable
  - Use to develop candidate barriers
- ***If the barrier (or FEP) "matters" and the uncertainty is high, then it should be the focus of attention***

EPRI

Counter Uncertainties with Conservatism (i.e., Pessimistic Assumptions)?

- Advantages
  - Often easier to defend – especially during licensing
    - Is sufficiently robust for the adjudicatory process
  - Serves to provide boundaries for license conditions
    - Connection to Performance Confirmation
- Pitfall
  - May distort which part(s) of the system "matter"
    - Will distort the relative importance of individual parts (barriers)
    - Example on next few viewgraphs: effects of conservative approach to near-field diffusion

Slide 5 - Kessler ACNW, 26 March 2003

EPRI

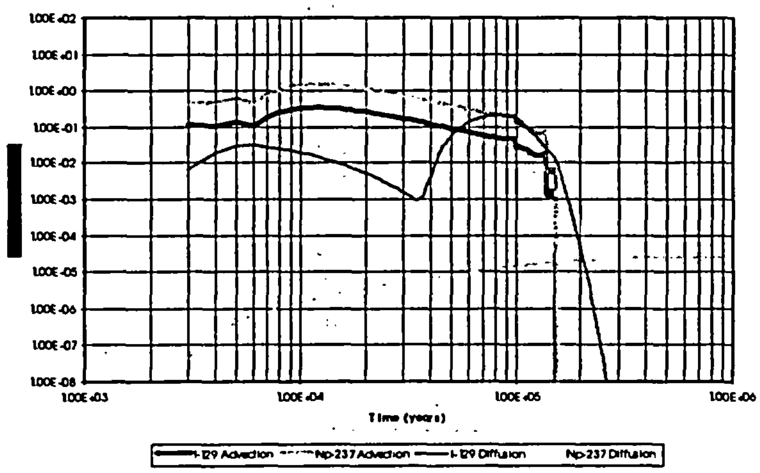
Conservative (Pessimistic) Example: Diffusive Release Model in EPRI's IMARC-7 TSPA Code

- Background
  - Few containers expected to be actively dripped on
    - Limits release due to advection
  - Most containers will eventually be in humid air conditions
    - Thin films of water coating exposed surfaces a possibility
    - Facilitates release due to diffusion
- EPRI's (current) pessimistic assumptions about diffusive release
  - Excellent contact between all EBS regions (spent fuel, cladding, container interior walls, invert, surrounding rock
    - Reality: poorer contact
  - Multiple continuous water pathways through EBS
    - Reality: more limited continuous pathways

Slide 6 - Kessler ACNW, 26 March 2003

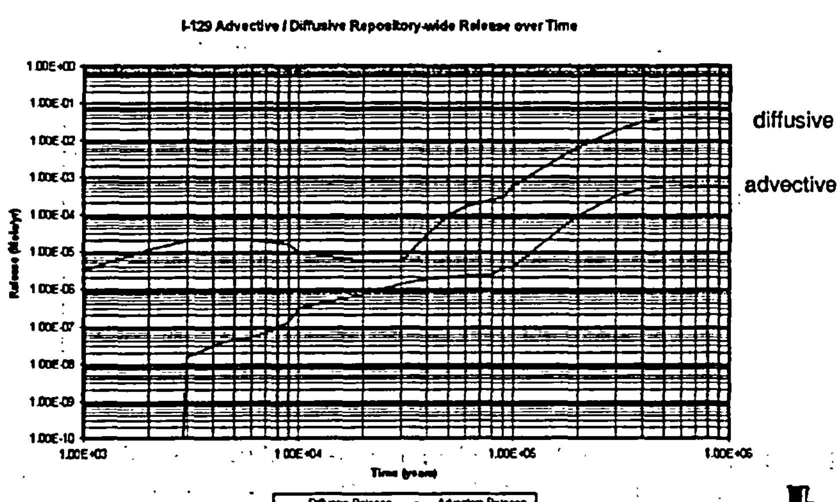
EPRI

Single "Failed" Container Advective and Diffusive Release from EBS



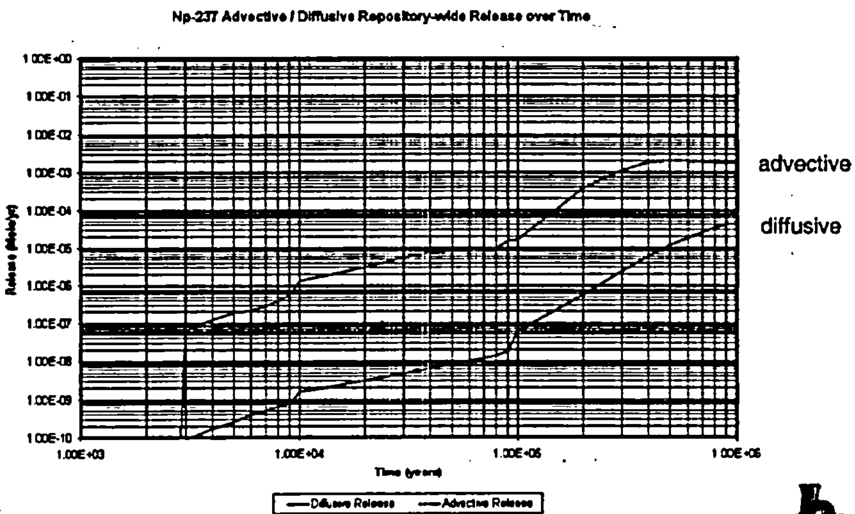
EPRI

Repository-Wide I-129 Advective and Diffusive Release from the EBS



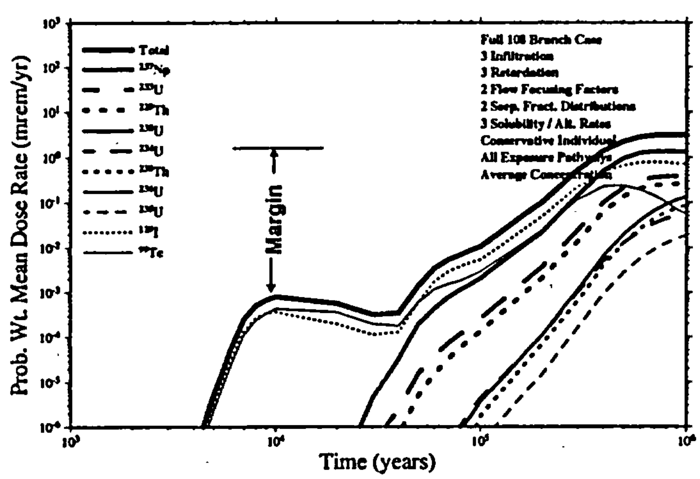
EPRI

Repository-Wide Np-237 Advective and Diffusive Release from the EBS



EPRI

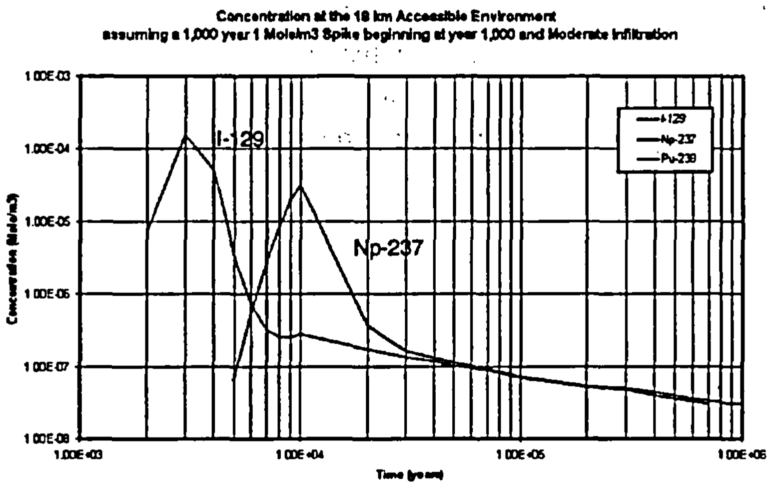
EPRI Base Case Dose Risk Result ("Normal" Release Scenario)



Peak 10,000-year dose risk: ~10^{-3} mrem/yr (~10^4 times lower than Part 63 limit)
10,000-year estimate strongly affected by conservative diffusion model!

EPRI

Overestimating I/Tc Release Affects Relative Importance of the UZ/SZ
Example: Radionuclide Travel Times in UZ/SZ



Pu below 10^{-8} M

Slide 11 - Kessler ACNW, 26 March 2003

EPRI

Summary of UZ/SZ Travel Times

- UZ below repository: 1200 to 3000 years
  - Radioelement- and infiltration rate-dependent
    - I/Tc (diffusive release-dominated): lower end of the range
    - Np/Pu (advective release-dominated): higher end
- SZ: 500 to >>9000 years
  - Radioelement- and discharge rate-dependent
    - I/Tc (diffusive release-dominated): lower end of the range
    - Np/Pu (advective release-dominated): higher end
- **Conclusion: better relative UZ/SZ performance would be shown if a more realistic diffusive release model were used**

Slide 12 - Kessler ACNW, 26 March 2003

EPRI

Relevance of Pessimistic Approaches

- YMP is *not* fundamentally a research project
  - Purpose is not to know everything about everything
- Purpose is to provide "reasonable expectation" the Yucca Mountain system will protect human health

Slide 13 - Kessler ACNW, 28 March 2003

EPRI

OK to Leave High Uncertainty (or Replace with Pessimistic Assumptions) if:

- It doesn't "matter" to overall performance
  - Corollary: we need to be confident ("reasonable expectation") that we know some parts do NOT matter
- Compliance can be demonstrated anyway (use of margin)
  - Replacement with a more realistic model would only result in more margin (EPRI diffusion example)
  - Additional work could be done to increase confidence *if desired*
    - Performance Confirmation
    - Analogue studies
  - Pessimism can be replaced with more realism at the time when more confidence is required (perhaps at a later stage of repository development)

Slide 14 - Kessler ACNW, 28 March 2003

EPRI

Conclusion: Pessimism (Conservatism) has its Place

- Realism is important for management purposes
  - Identifies what is "important" without bias
  - Use to focus resources
- Some pessimistic approaches will need to be built into the TSPA model for licensing purposes
  - To establish robustness for the adjudicatory process
  - To provide boundaries for license conditions
  - To provide "reasonable expectation" level of confidence on compliance with regulations

J. Kessler, EPRI: Conservatism has its place in performance assessments. Realism is important for management purposes. If the management needs to identify what is important without bias, they need to do that to focus resources. Some pessimistic approaches will need to be built into the TSPA model for licensing purposes. The DOE will need to establish robustness for the adjudicatory process. It is an adjudicatory process. That is reality, in a sense. That is what is going to be required, to provide boundaries for license conditions, and to provide a reasonable expectation level of confidence and compliance with regulations.

The idea is that even when we have uncertainties, which will always be there to some extent, in the end, the NRC needs to be satisfied with the reasonable expectation that regulations will be complied with. Sometimes that will involve the use of conservatism.

J. Garrick, ACNW Member: John, I think an even more significant conclusion is that you have demonstrated the value of embracing the notions of uncertainty. You've demonstrated the value of knowing that if something is four, five, six, or seven orders of magnitude uncertain, but is a couple of orders of magnitude below what is driving the risk, the analysis is adequate. To me, that's the most important issue. It's not so much knowing whether you are pessimistic or conservative. It's knowing what the uncertainties are.

D. Bullen, Iowa State University: I really enjoyed your presentation, although I have a question about your pessimism/conservatism analyses. As you do a TSPA or TPA, how do you convince yourself that you are not masking an effect, that is, over-simplifying the results, leading you to a conclusion that may or may not be physically real? How do you address those types of concerns as you look at, for example, the source term issue that we are trying to address here?

J. Kessler, EPRI: We do lots of sensitivity studies. We try to use expert judgment in the sense that, in some cases, you don't have a good handle on what the realistic value is, or the best estimate value is. In some cases, you may have a better handle on near bounding cases, rather than bounding cases. We'll use judgment to suggest that it is probably in this range. We might use that value or range of values in what we think is probably a better estimate of what reality might be, rerun our sensitivities, and try to get some understanding as to what got masked or what got out of balance in terms of relative importance. We do this so that we can understand what are the most important parts of the system in terms of their effect on dose risk.

G. Hornberger, Chairman, ACNW: In other words, you do a more realistic analysis to see whether or not your conclusion is justified.

J. Kessler, EPRI: That is what I'm saying. In some cases, we try to do it. One would hope that, behind the scenes, the DOE has been doing what they think is more realistic modeling to get a handle on what the important parts of the systems are, at least from a management standpoint.

R. Latanision, MIT: I, too, enjoyed hearing your comments. I would like to take a very specific case and see how you would deal with this. And I'm thinking particularly of the reasonable expectation of what the environment would be in terms of the waste package. How would you deal with determining what is a realistic expectation in terms of the environment?

J. Kessler, EPRI: Well, I need to back off and ask myself first, why do I care? Why do I care to get the chemistry right? How does it matter to me? Again, I go back in our case to our own set of barriers which are similar enough to what the DOE or the NRC is thinking about in terms of barriers. I want to know what is the ultimate impact on those barriers, so in the global sense

I'll say I care about chemistry because it affects the corrosion of some of the things in the near-field. It is going to affect solubilities and all things like that, so what I care about is how long my waste package will last. How much release will they get and how will it affect solubility limits? How might it affect retardation, in the sense that these are the main indicators of performance of some of the barriers? After that, what we do is look at how this might impact corrosion.

R. Latanision, MIT: Given that there is evidence that the environments generated by extreme condensation are very corrosive, from your perspective, is this an issue that the project ought to be exploring in a different way, perhaps, or in more detail than it is today?

J. Kessler, EPRI: The project ought to be exploring what they think are plausible conditions that could lead to significant degradation of what they think might happen to their container performance. I mean, if they feel that this is plausible, they should have some sort of—

R. Latanision, MIT: Reasonable expectation.

J. Kessler, EPRI: Of course, that is for NRC to decide. But the point is, the DOE needs to come in with their own case as to why they feel what Don [Shettel] and John [Walton] presented is or is not reasonable. Certainly, that would have an effect on what estimates the DOE is making for container corrosion.

R. Ewing, Univ. of Michigan: Great presentation, but of course, I disagree with the results a bit more than some of the others. I would say that what you've described is not an iterative PA process, but more a circular process. In the extreme, what I mean by that is, if you design an analysis that's chemistry-free, and you do a sensitivity analysis, it is no surprise that chemistry doesn't matter. Certainly for licensing, you have to identify what matters most, what the uncertainties are, and be able to identify and recognize when you make bounding or conservative calculations. Then you do the sensitivity analysis. But behind all of that is the assumption that you have a useful model.

You start with a model. If your analysis does not show X, Y and Z, it does not mean that they are not important. It could be that the model is not very useful for analyzing the system. At the end, you mention natural analogs. What I always propose is that when we have these complicated models, we pull out the modules and test them either against real laboratory data or natural systems, and we design experiments to challenge the efficacy and usefulness of the models.

J. Kessler, EPRI: I'm opposed to that.

R. Ewing, Univ. of Michigan: Yes, but you put this at the end in italics, "if necessary." It seems to me it's absolutely necessary from step one.

J. Kessler, EPRI: It is necessary from step one in some areas. You may want to call this circular or whatever, but I must protest the comment about chemistry-free.

R. Ewing, Univ. of Michigan: I didn't say your model was chemistry-free. I used an example that many of these models are nearly chemistry-free. It was an example. If you leave something out and do a sensitivity analysis, don't be surprised that what you left out turns out not to be important.

M. Morgenstein, Geosciences Management Institute, Inc.: I'm having major problems with the simplest things like going toward the concept of natural analogs when we have not actually sat at the site and done an accurate characterization. Don't you want to know and understand the site before you go to Africa to look at Oklo? Granted there is information at Oklo that would help us in certain aspects, but if we do not know what the chemistry of the site is, what the chemistry of the near-field is, what is the difference of what happens at Oklo?

J. Kessler, EPRI: You may be right, you may be wrong.

R. Ewing, Univ. of Michigan: Here we disagree. I must interject that. But what I am really proposing is that there can be many places in the world, separate from the site itself, where we could ask very specific questions, take parts out of the performance assessment, and try it out.

J. Kessler, EPRI: If those things are relevant to what we need to know to provide confidence, then that would provide additional confidence. My take on what Maury said was that if there is something about doing a model, benchmarking against Oklo, that will give us what we need to know about our models, and that provides confidence in a particular model that underlies an important barrier, then it is useful to do. It needs to meet all those criteria before we go do it.

R. Ewing, Univ. of Michigan: Now as a reviewer or as a scientist looking at any performance assessment, and not picking on any particular person, I inevitably would be able to find some difficulties. That is natural in life, but how many mistakes do I have to find before we abandon the analysis or the site? How would I know when I have finally reached the point where I can say the analysis is not very good?

J. Kessler, EPRI: If you talk about what's the importance of the mistake.

R. Ewing, Univ. of Michigan: There you use your model. However, if I don't accept your model, then we are in this loop.

6. WORKING GROUP ROUNDTABLE PANEL DISCUSSION ON TSPA/TPA

6.1 Summary of Panelist Comments

The five expert panelists (Payer, Ewing, Bullen, Morgenstein, and Latanision) participated in a panel discussion that was moderated by ACNW Member Garrick.

Dr. Ron Latanision (Massachusetts Institute of Technology) focused on temperature issues because all of the modes of corrosion degradation, including uniform corrosion rates and the rates of localized corrosion, are affected by temperature, as well as by the environmental chemistry and state of stress of the material.

Dr. Joe Payer (Case Western Reserve University) posed a number of questions about the importance of the environment when evaluating corrosion. Given a population of environments and a range of corrosion resistance for a material, the issue is where they overlap because that is where corrosion can occur. Can these conditions be correlated with a real repository? How, when, and where will the corrosive conditions occur? How much corrosion will there be? Will the adverse environments persist? Dr. Payer noted that one of the things lost in most testing and thermodynamic modeling is that researchers point to a given condition and describe what can happen under that condition. But in real systems, the aqueous solutions are not constant—they evolve. With respect to waste package environments, if they contain something that can consume the acidity, then the solution will become more alkaline. If something can consume the hydroxyl ions, the environment will become more acidic. Dr. Payer observed that we know about these processes—it is just a matter of working them in. Will these environments form? Will the environments persist? If they don't persist, if they go away because the package becomes dry in that area, could they re-form and start again?

Dr. Maury Morgenstein (Geosciences Management Institute, Inc.) focused on the vadose zone environment. He said that it is a very complex area that we do not understand at present—the very basics of the hydrogeochemistry. He noted that water entering the soil zones within the region could likely have highly variable chemistry in spatial terms. This water will evolve as it migrates down through the vadose zone and through the repository environment. Dr. Morgenstein referred to a basic lack of understanding of the hydrochemical system, and noted that engineered barrier system items, such as alloy C-22 and titanium-7, can react with water that has been altered by the temperature of the system and the variations of the dynamics of the system as it changes through time. He believes that the project is probably moving too fast to be able to collect and acquire the needed information. He noted that there are obviously degrees of retardation offered by the natural system, but it is not clear that these degrees of retardation are sufficient to meet licensing requirements. He also noted the importance of using vadose zone pore water chemistry, rather than the chemistry found in the saturated zone.

Dr. Dan Bullen (Iowa State University) covered a broad range of issues, including evolution of waste package design and changes in the understanding of how much water moves through Yucca Mountain. He focused on thermal- and biosphere-related issues. Dr. Bullen noted the difficulty of dealing with uncertainties if the models do not include key processes that relate to those uncertainties. For example, the DOE Supplemental Science and Performance Analysis examines both high- and low-temperature operating modes. But dependence of corrosion on temperature is not included in some calculations, and this alone can have a significant effect. In some cases, there is no simulation of localized corrosion because the localized corrosion model was not used because data needed to support it were not available at the time.

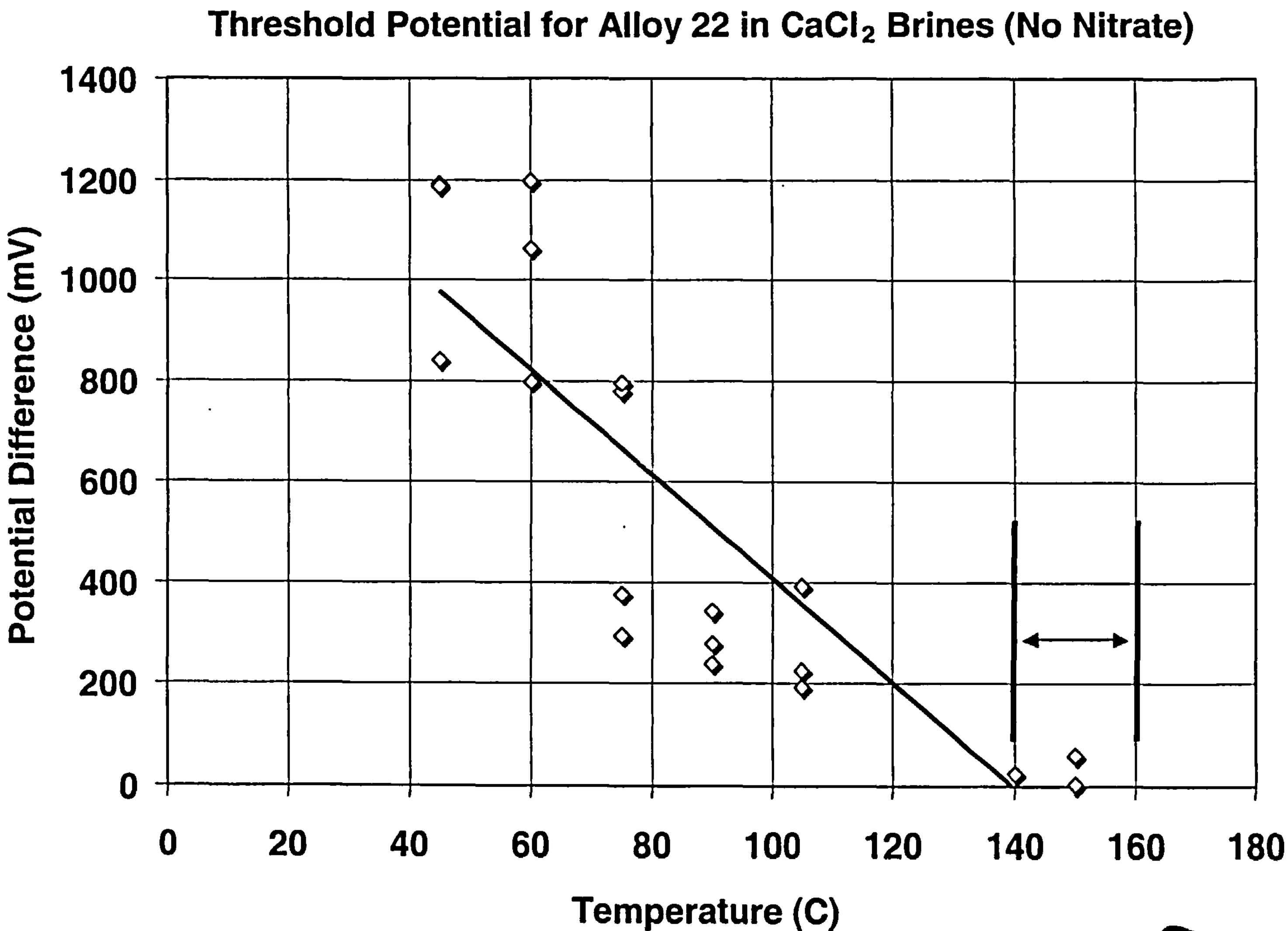
Dr. Bullen feels that a cooler repository design may be desirable, not only because it is less difficult to model, but because it is more closely related to the current ambient conditions at Yucca Mountain. In other words, the less the mountain is perturbed the better. Perhaps a cooler design would not produce the high chloride concentrations and high salt concentrations that have been discussed as a concern. Dr. Bullen expressed concern about the 3000 acre feet of water dilution factor because it might be masking some significant problems associated with the biosphere model. He felt that the model is not realistic and not conservative because a small source of water with a high concentration that is not significantly diluted may give a significantly greater dose than that which is predicted with a greater dilution factor.

Dr. Rod Ewing (University of Michigan) noted that if he had either DOE's or NRC's job, the first thing he would do is a performance assessment because the performance assessment informs one about how things are connected. But although the exercise would be informative, the results would almost certainly be wrong. Dr. Ewing noted that the modeled system is quite nonlinear. The fact that the one-off and one-on analyses can be done so readily suggests that the modeled parameters are probably not coupled well enough. Dr. Ewing noted that evolution of repository boundary conditions over time would be challenging to model (e.g., water chemistry, temperature, porosity, permeability, etc.). He said that the chemistry of this system may be the dominant driving force in terms of the end result. Although the TSPA computer code has chemistry in the model, from a geochemical point of view it is at a somewhat primitive level. Further, the remarkable extrapolation over time of all the processes makes for a very tough problem.

How to deal with these problems? Dr. Ewing feels that if we look at the TSPA and the TPA computer codes in a very natural and understandable way, in terms of modeling, "they've evolved into a corner, talking one to the other." What is missing, and not part of the license application process, is the broader context in terms of what can be done by modeling. Dr. Ewing presented the analogous case of future climate modeling and the difficulties in that arena. A key question in climate modeling is how can we extrapolate results before the uncertainty hinders the ability to make a policy decision. In the waste arena, the question should be, How far can results be extrapolated before the uncertainty is so large we cannot reasonably determine whether the regulation has been complied with?" Dr. Ewing suggested that it would be informative to look around at other systems, particularly complex systems, and ask what the limitations are to see if we're fooling ourselves. Dr. Ewing concluded that he does not understand how the uncertainty of long-term extrapolation will be handled, and he sees a need for better ways to judge the adequacy of models and modeling.

6.2 Presentation Materials Used by Ron Latanision (MIT) During the Roundtable Panel Discussion on TSPA/TPA

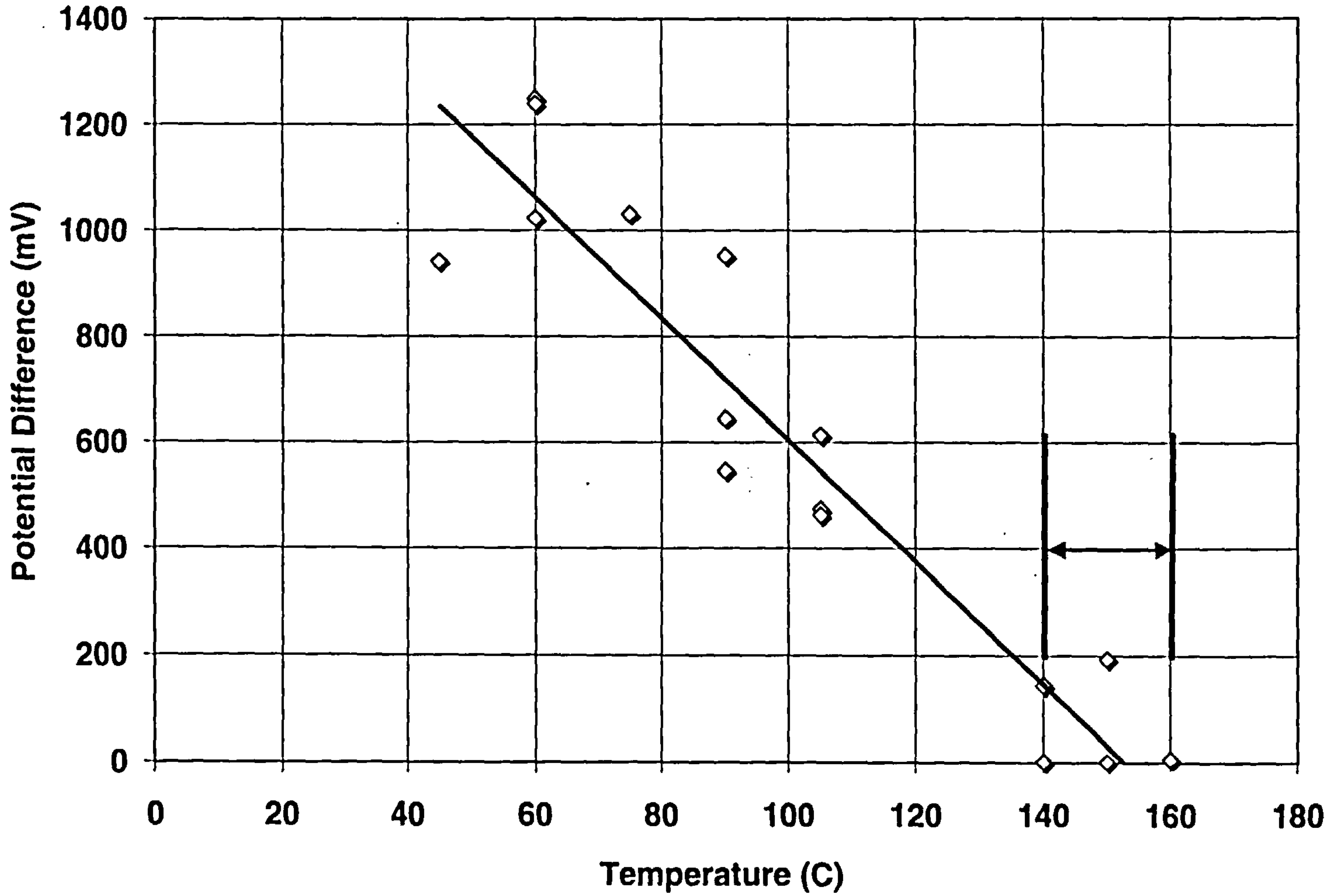
CP of Alloy 22 in $CaCl_2$ Brines (No Nitrate)



CP of Alloy 22 in $CaCl_2$ Brines ~~(No Nitrate)~~

(Continued)

Threshold Potential for Alloy 22 in $CaCl_2$ Brine (Nitrate Added)



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6.3 Closing Remarks by Keynote Speaker Joe Payer (CWRU) During Roundtable Panel Discussion on TSPA/TPA

[Edited comments with notations to slide numbers used in presentation]

In my summary comments, I want to expand upon a couple of things we've said. I think it is a reasonable follow-on to what Ron Latanision said in his remarks, and the concerns that any of us that deal with corrosion have about the prediction of long-term performance in potentially hostile environments. I showed this diagram yesterday, and I think it captures the reality of materials selection where localized corrosion is being considered. (Slide 1) If the field on the left represents the environment, the population of environments, and if the field on the right represents the population of the corrosion resistance of a material, the issue is where they overlap. The overlap zone indicates the material/environment combinations where corrosion can occur. If there is a zone of susceptibility (overlap), then corrosion can occur, and a primary concern is to describe those environments for the material. But that is not enough.

The next questions are—Can we correlate those conditions in the susceptibility zone with real repository conditions? How do they form? When, where, and how much corrosive environment is formed? Will the environments persist? One of the things that is lost in most of our testing modes, and in most of the thermodynamic modeling (e.g. on a potential (Eh) vs. pH diagram), is the fact that the environment on the metal surface can change with time. People point to a given potential-pH condition on the diagram and use this point to describe how the material will behave—it will corrode, or it will be immune, or it will be stable. In real systems, there are trajectories of potential and pH with time because the solutions are not constant.

And so, while this is a useful foundation, we should build on it or extend it. If there is a process on the metal surface that is consuming the acidity, then the environment becomes more alkaline. If there is something that is consuming hydroxyl ions, the environment will become more acidic. We know the chemical and electrochemical processes that can occur on the surface, and it is a matter of working the consideration of changes in the environment into our analysis.

Will the corrosive environments form? How much, where, and how often? Will the environments persist? If they do not persist, any corrosion will stifle or arrest, and no further corrosion damage will occur. The arrest of corrosion can result by the environment moving out of the susceptibility zone, or the metal surface becoming dry. Should the conditions move again into the susceptibility zone, then corrosion processes could restart.

The next slide (Slide 2) shows a predicted temperature/time behavior for waste package surfaces from the time of closure of the repository out to one million years. The temperature/time behavior can be coupled with other information to give the relative humidity as a function of time (Slide 3). Based on our knowledge, assumptions, and analysis of what is on the package, we can make a judgment as to whether the metal surface will be wet or dry at a given relative humidity. At low relative humidity, the metal will be dry; at intermediate relative humidity, the metal may be dry or may be wet; and at high relative humidity, the metal almost certainly will be wet. The variability at intermediate relative humidity is due to the influence of what is on the package surface and the surface condition. If a deposit on the surface is hygroscopic, the surface will be wet at a lower relative humidity. The influence of deposits on the metal surface need be considered in order to determine the wet/dry condition.

The use of material/environment diagrams to illustrate the susceptible zones for localized corrosion is expanded upon in Slide 4. Again, the diagrams define the populations for environment and material. For this case, consider a given material and vary the temperature from high temperature (T1) to low temperature (T2). The field for the material (e.g. Alloy 22), does not change. The field for the environment is affected by temperature and moves right or left as indicated by the diagrams. At a high temperature (T1), moisture cannot form and the metal surface will be dry. At this condition, there is no wet environment and there will be no corrosion. At lower temperatures, moisture can form on the metal surface. As the temperature decreases for T1, there is a temperature at which moisture forms on the surface (T2). In the diagram, an overlap of fields is shown which defines a susceptibility zone for corrosion. As the temperature decreases, we would expect the environment field to move to the left (less corrosive) and the susceptibility zone to get smaller. I think we would agree that there is some lower temperature, whatever that temperature is, at which the environment and material fields separate. This condition is shown at T4 and T5, and no corrosion will occur.

The diagrams define a temperature range in which the material is susceptible to localized corrosion. At higher temperatures, no corrosion occurs because the metal is dry. At lower temperatures, no corrosion occurs because the material has sufficient corrosion resistance to avoid localized corrosion. Based on the temperature/time prediction for waste package surfaces, the temperature zone of susceptibility could be correlated to a time period of susceptibility.

Where there is a susceptible zone, a region of overlap, there are question marks shown. There are two questions. Is there water available? Will the chemistry persist? Further questions include—If the corrosive environment forms, will it persist? On what locations of the waste package will it form? What is the rate of damage during this period? I think we have logic and a rationale for dealing with the occurrence of localized corrosion. An important concern is whether we have sufficient data and understanding to apply this logic.

Allow me to extend this treatment further. [Slide 5] A family of subfields can represent the entire environment and the entire material fields. That is to say, there are subsets of environments and subsets of materials. I think it is clear from the various presentations of the DOE, the NRC, the State of Nevada, and some others, that we are really talking about a family of waters. In the figure, I suggest that the ambient waters at Yucca Mountain would be to the left side. This is all qualitative at this point, but the family of waters would be skewed to the left side for the ambient waters. The carbonate/mixed ionic brines move toward the right, and these are the types of waters on which a lot of the testing has been done by the DOE project. The highly acidic, concentrated halide brines would be farther to the right. Again, this is qualitative, but that is the general movement.

The subsets of the material field are also indicated in Slide 5. Shifts in the material field to the left and right will affect the presence and size of any susceptibility zone. The material subset for the base metal in a solution-annealed condition would be farthest to the right (i.e., most corrosion resistant). Several factors can move the material resistance field. Increased concentrations of chromium, nickel, and molybdenum in the alloy increase the corrosion resistance and move the material resistance field to the left, away from a susceptible zone. This effect is demonstrated by a comparison of the corrosion resistance of 316 stainless steel, Alloy 825, and Alloy C-22. The corrosion resistance increases from 316 stainless steel to Alloy 825 to C-22 as the chromium, nickel, and molybdenum concentrations increase. The high nickel-chromium-molybdenum alloys, such as Alloy C-22, are the most corrosion resistant materials examined for Yucca Mountain conditions. As the materials resistance field shifts to the right, the extent and likelihood of overlap is less, that is, the susceptible zone gets smaller or does not exist. Welds and their associated heat-affected zone can be more susceptible to corrosion, and that will move the materials field to the left. Thermal aging can result in the precipitation of phases or ordering in the alloy, and that also will shift the materials field to the right. The same logic and questions prevail as with the environments discussed above. The questions include—Is there an overlap of fields resulting in a susceptible zone? If there is a susceptible zone, how often will these conditions occur on waste packages surfaces and how long will they persist?

Some comments from my keynote address are reiterated in Slide 6. Sometimes you come to a workshop and just reinforce your predispositions, and other times you learn things and modify your thoughts. In my case, this workshop has been a combination of both. An underlying issue is the water as the primary accessor, meaning it is the primary agent that can cause penetrations in the waste packages. Should penetrations occur, then the questions become when, how many, and how much water enters the waste package. Once water gets into the package, it will continue to provide access by moving through penetrations in the cladding that encapsulates the spent fuel. Once in contact with the spent fuel, the water becomes the mobilizing agent. Through reaction with the spent fuel and alteration products, radionuclides can be released. Water then acts as a transport agent. The radionuclides are transported in moisture either in thin films by diffusive transport, or in droplets and flow by advective transport. The form and amount of water is again a primary determinant of the transport processes. So it all comes back to the water—it is not the only thing that's important, but water is a very critical part when you are talking about the source term.

Summary comments are made in Slide 7. Annotations have been made based on some points that I have taken from our discussions here. The blue italicized comments are items I added for this summary. In order to address the source term, I think we are still talking about water contacting the waste package, the waste package lifetime, releases of waste form and alteration, mobilization, and transport. Those are logical boxes. You could divide these categories or add other ones, but I think the slide presents a reasonable flow and organization for the processes of interest.

Using this water contact in the waste packages, we know that condensation on cooling is going to occur, and we know that it is likely that dripping will occur sometimes in some places. How much? Where? How often? These are the key questions? Waste package lifetime is crucial, and we know we are going to get full containment for some period of time. Is that a long time or a short time? We know that penetrations will ultimately occur, certainly if we are looking over tens of thousands and millions of years. With localized corrosion, penetrations could occur much sooner. After penetrations have occurred, water will access the waste package and contact the internals. The waters are likely to corrode any carbon steel internals, and that will produce iron oxides. The water is likely to corrode any aluminum that is in the waste package. Zirconium cladding may be attacked by corrosion or hydrogen damage from contact with waters.

Once water gets to the spent fuel, it can react and release radionuclides by uranium dioxide corrosion and formation of alteration products. Rod Ewing has been telling us a lot about that, and he could tell us a lot more. What is going to happen as far as retardation in those waste and corrosion products, and as the radionuclides move on to the invert? Once the waste form has degraded, we seem to have a good handle on the inventory of radionuclides and how that inventory changes over time. The issues are where are they solved, where they are dissolved, where they are sorbed, and where they are desorbed. It is my opinion that the DOE and NRC models have identified these relevant processes, and they have identified a lot of detail below that set of processes. The question is and the issues include—How sound is the technical basis in the data to support models of data to support that analysis? How solid are the models in providing an understanding and confidence? However, I think the structure makes sense, and I would not suggest that we abandon this and start again. Thank you.

Left blank intentionally.

6.4 Presentation Materials Used by Joe Payer During the Roundtable Panel Discussion on TSPA/TPA

Susceptible Zone for Localized Corrosion

? ? ?

Correlate with Repository Conditions

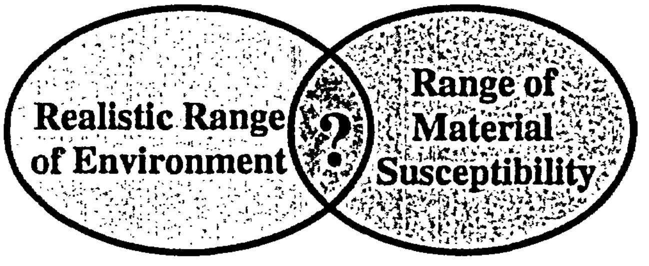
How do these form?

When, where, how much?

Will environments persist?

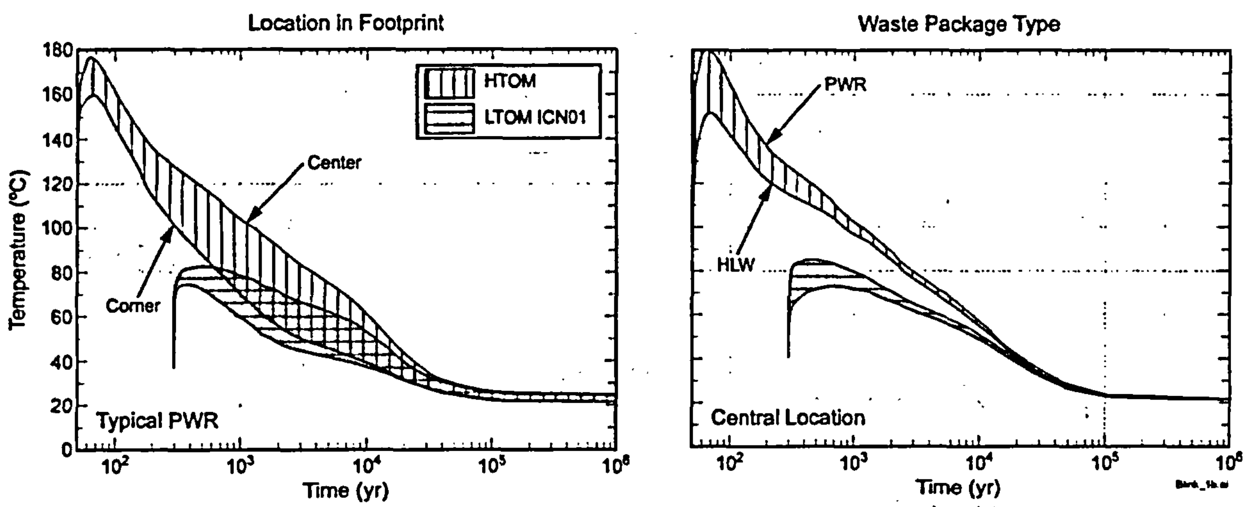
Can they reform?

- Water must contact WP
- Water must remain on WP
- Corrosive species must be present to form electrolyte
- Material must be susceptible to corrosion under these conditions
- Conditions must persist over sufficiently long time



Slide 1

Example Thermal Load Time Profiles



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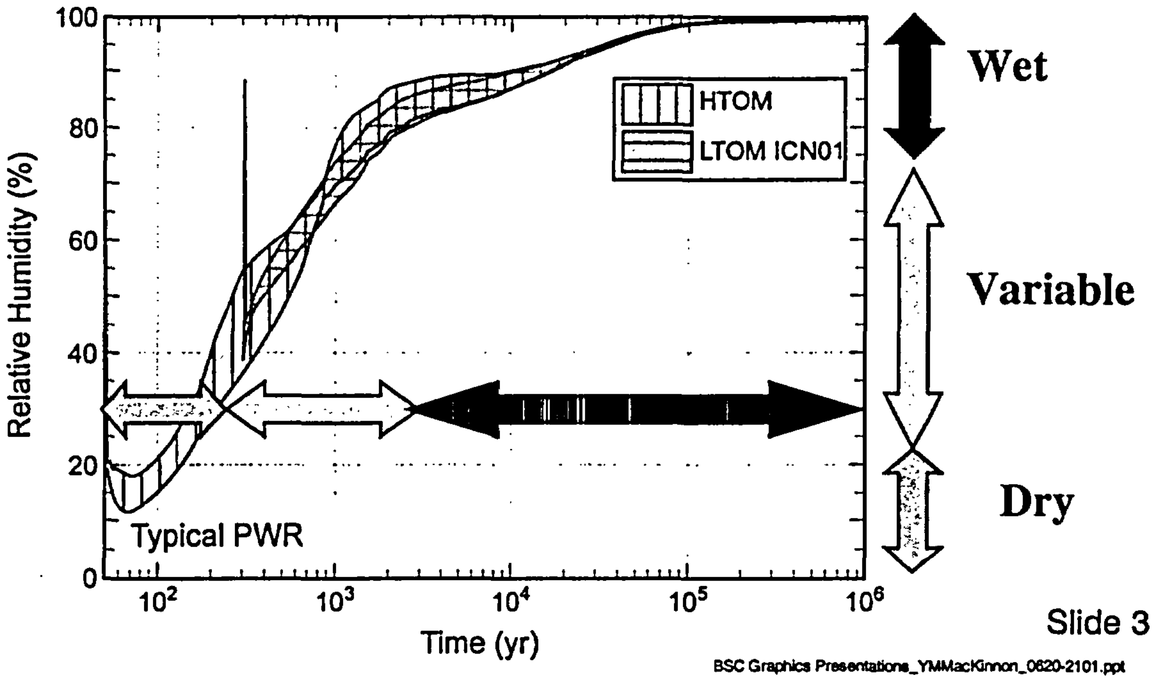
Slide 2

Example of Equilibrium Humidity and Its Connection to Moisture on Surfaces



Slide 3

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140th ACNW Meeting March 25, 2003

Realism in Long Term Corrosion and Source Term; J.H. Payer

Susceptible Zones Scenario

Environment | **Material**

T1-Metal surface is dry, No corrosion

T2-Aggressive solutions possible

T3-Aggressive solutions possible

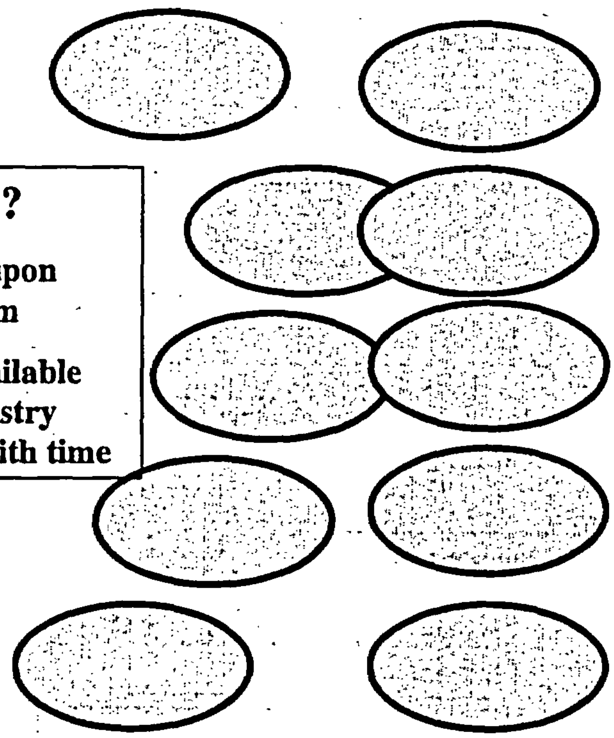
???

Depends upon water chem

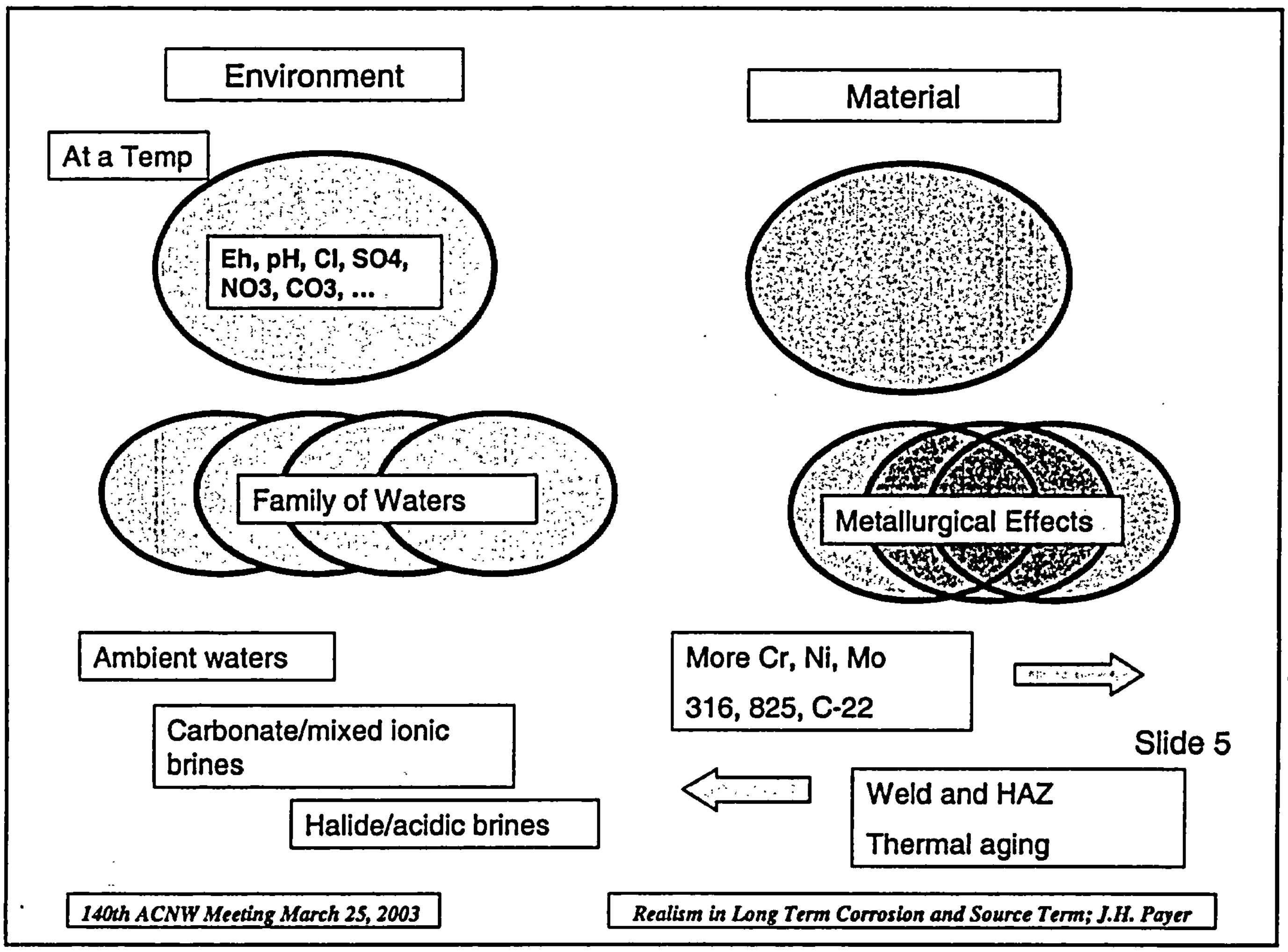
Water available and chemistry changes with time

T4-No localized corrosion

T5-No localized corrosion



Slide 4


Environment
Material
At a Temp
Eh, pH, Cl, SO4, NO3, CO3, ...
Family of Waters
Metallurgical Effects
Ambient waters
Carbonate/mixed ionic brines
Halide/acidic brines
More Cr, Ni, Mo
316, 825, C-22
Slide 5
Weld and HAZ
Thermal aging
140th ACNW Meeting March 25, 2003
Realism in Long Term Corrosion and Source Term; J.H. Payer

Understanding Water is a Key Component of Understanding Yucca Mountain

Water is the primary accesser, mobilizer and transporter

Waters on waste package surface (access)
- -when, how much, chemistry
- -determines corrosion behavior

Waters into waste package (access/mobilize)
- -when, how much, chemistry
- -form, frequency and distribution of penetrations

Waters in waste package (mobilize)
- -on clad, waste form and internals
- -determines radionuclide mobilization

Waters from waste package and drift (transport)
- -when, how much, chemistry
- -determines radionuclide transport

Slide 6

Summary/***Summary***

Note: Blue, bold, italics are summary comments on day 2 of meeting.

Goal is for a set of models that capture reality—important processes, controlling factors and performance relevant to conditions at Yucca Mountain.

Water Contacting Waste Package ***Condensation on cooling; Dripping sometimes in some places***

Waste Package Lifetime ***Full containment for a period, penetrations occur, water accesses WP internals***

Releases from Waste Form and Alteration ***UO2 corrosion, alteration, retardation in WP precipitates and corrosion products and invert***

Mobilization and transport of Radionuclides ***Inventory of radionuclides with time, solubility, incorporation, sorption,***

From WP, through invert and into rock; UZ and SZ.

DOE and NRC models have identified the relevant processes

Issues are technical basis (models and data), understanding, confidence

Slide 7

140th ACNW Meeting March 25, 2003

Realism in Long Term Corrosion and Source Term; J.H. Payer

PUBLIC COMMENTS

Dr. Atef Elzeftawy (representing the Las Vegas Paiute Tribe) discussed how the researchers in the Manhatten Project looked at uncertainty in their theoretical work and ultimately demonstrated the results. This was their equivalent of "performance assessment." He also mentioned quantum mechanics theory and that the physicist Feynman said that it wasn't clear what quantum mechanics is, and that it was not understood in all details, but that it works. Dr. Elzeftawy observed that if we can come up with performance assessment models that work, that helps the decisionmaking process.

Ms. Judy Treichel (Nevada Nuclear Waste Task Force) observed that it was "refreshing" to hear the "knock down, drag out" discussions, but felt that they did not last long enough. She described the different perspectives of Yucca Mountain seen by farming families living in the Amargosa Valley who get their water from wells and consume many of their own agricultural products ("they don't have to just eat tomatoes and cucumbers, they can eat pistachios, they can drink the milk from the cow who drinks out of the same tap"). From their perspective, their risks will be assigned by someone else. Ms. Treichel stated that her real fear relates to the biases of the various presenters and that she is worried that "NRC is sort of pushing to make this thing [Yucca Mountain] okay." She feels that the NRC would like to have Yucca Mountain, and that people who don't have to live with Yucca Mountain would be "way more eager to have uncertainty or to feel that it can be accepted than other people." Ms. Treichel was skeptical that the process was "totally fair."

Dr. Roger Staehle described examples of mechanical failures that have made an impression on him, including helicopter rotor blades and nuclear reactor pipe failure. He noted the very complex nature of Yucca Mountain with regard to surface chemistry, temperature, and mathematics. He recommended a bounding approach to the problem to make predictions, taking into consideration a "reasonable" set of worst cases, but not a worst case. He further recommended that the DOE use this set of worst cases as a basis to make progress with modeling.

Mr. Steve Frishman (representing the State of Nevada) noted that John Kessler had a viewgraph that said pessimism can be replaced with more realism at a time when more confidence is required, perhaps at a later stage of repository development. Mr. Frishman said there is no room for this staging concept under the current regulation. The NRC's rule as it stands today is not a staged rule. The confidence that is necessary is the "confidence that can be elicited through demonstration at the time a construction authorization is issued, if it is to be issued." Mr. Frishman noted that the TSPA computer code is not just a useful tool for understanding what is known or not known. He stated that under the licensing rule the outcome of the performance assessment is the statement of compliance (or not). One of Mr. Frishman's concerns is that performance assessment results will be translated into a decision for reasonable expectation or reasonable assurance that can lead to another level of subjectivity.

Dr. Garrick noted that the ACNW "does its best to address the technical issues and is not the body that makes the decision about whether or not a license is in compliance. ACNW members are not license experts, are not regulation experts. ACNW is here to complement the regulatory process and focus on what is going on from a technical standpoint."

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11. ABSTRACT *(200 words or less)*

The Advisory Committee on Nuclear Waste (ACNW) held a working group session at its 140th meeting on March 25-26, 2003, regarding NRC and DOE performance assessments: assumptions and differences. A panel of five expert engineers and scientists participated in this working group session. The purposes of this working group session were to: (1) identify areas in the analyses that may warrant increased realism, (2) increase ACNW's understanding regarding the onging performance assessments, (3) understand the different approaches taken by NRC and DOE, and (4) provide a point of reference for a follow-on working group on performance confirmation. The main idea of this working group session was to gain further knowledge on how the NRC and DOE are achieving appropriately credible and realistic performance assessment models.

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