INEEL/EXT-098-00996
SAND98-2208/2
DOE/SNF/REP-0033
Revision 0

Nuclear Dynamics Consequence Analysis (NDCA) for the Disposal of Spent Nuclear Fuel in an Underground Geologic Repository

Volume 2: Methodology and Results

Idaho National Engineering and Environmental Laboratory
Lockheed Martin Idaho Technologies Company
Idaho Falls, Idaho 83415

October 1998

This report was not produced under a quality assurance program that satisfies the requirements of the National Spent Nuclear Fuel Program and DOE/RW-0333P, Office of Civilian Radioactive Waste Management Quality Assurance Requirements Description. Therefore, the data in the report are not considered qualified and are not to be relied upon to address safety and waste isolation issues until an accepted qualification process has been completed.

Prepared for the
U.S. Department of Energy
Assistant Secretary for Environmental Management
Under DOE Idaho Operations Office
Contract No. DE-AC07-94ID13223

SANDIA REPORT

SAND98-2208/2 ● UC-900
INEEL/EXT-098-00996
DOE/SNF/REP-0033
Unlimited Release
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SF2900Q(8-81)

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ABSTRACT

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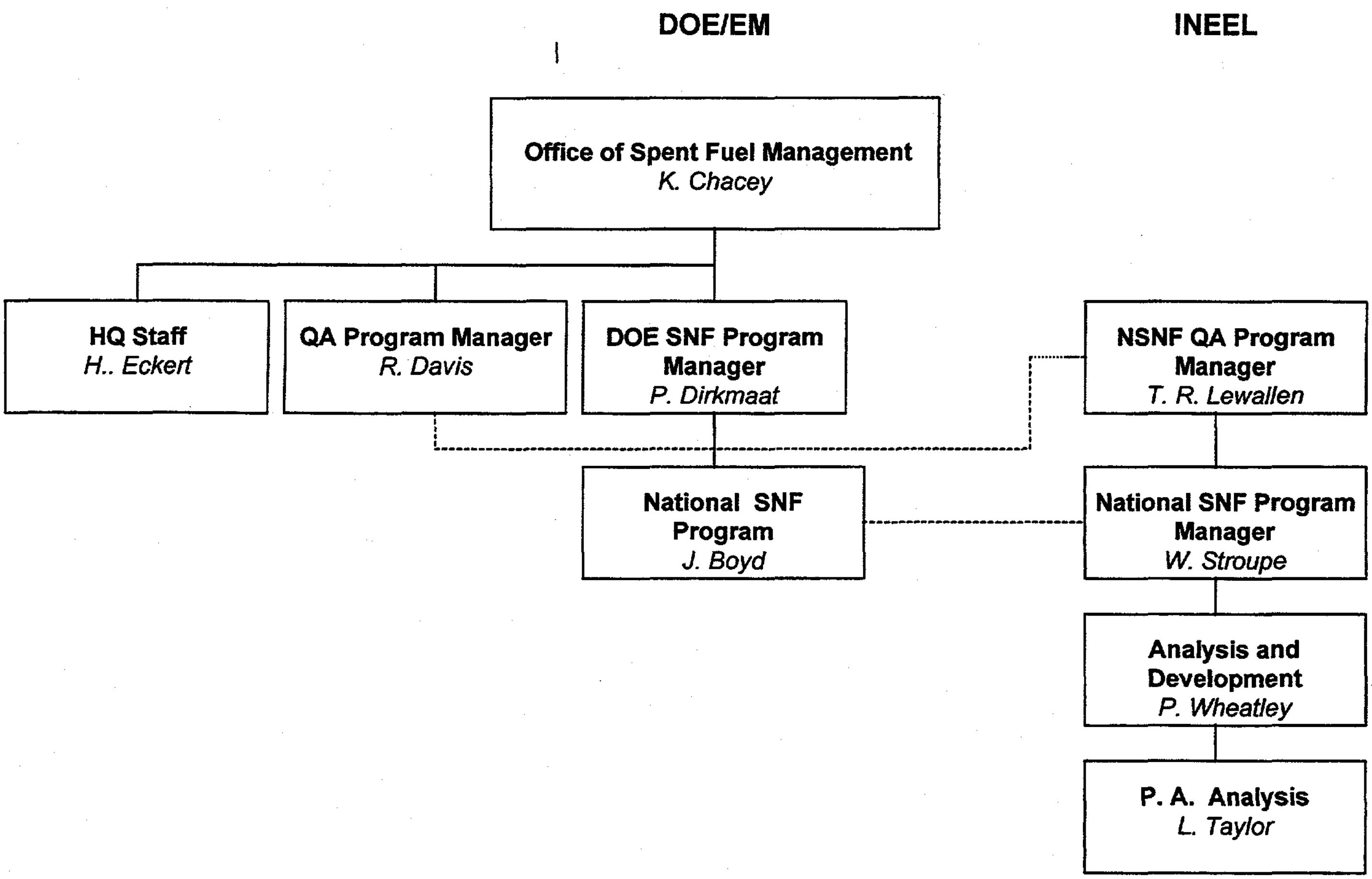

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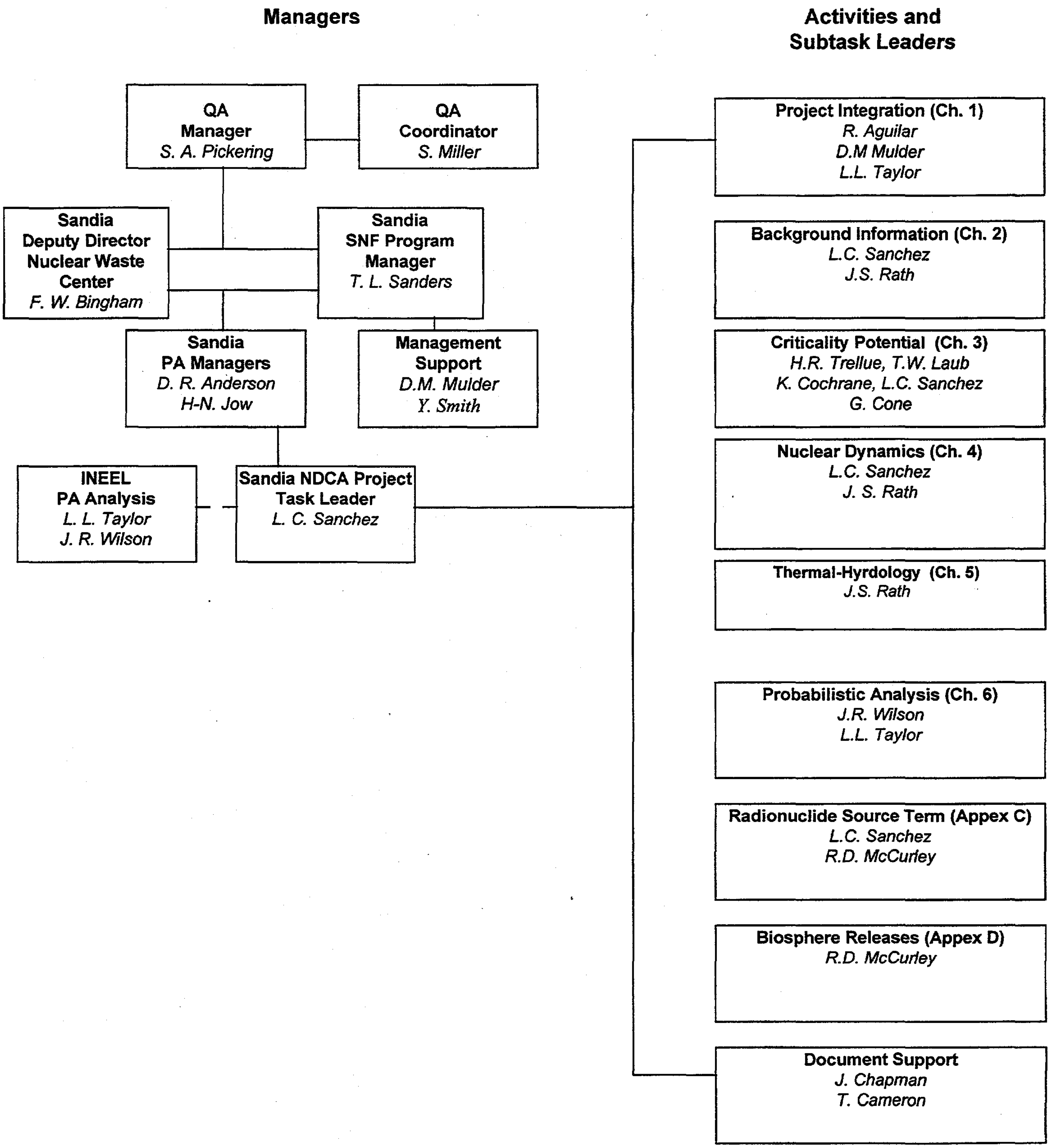

Figure P-2. Organizational Chart for NDCA Project

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G.M. Newman	GRM			Illustrations
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J. Sterbentz	INEEL			Criticality Analysis
L.L. Taylor	INEEL		Ch. 1, 2, 6, 7	Project Task Leader
J. Talley	TRI			Typing
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H.R. Trellue	LANL	RKeff	Ch. 3, 7	Baseline Criticality

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J. R. Wilson	INEEL		Ch. 6	Risk Analysis

GRM - GRAM Inc.
INEEL - Idaho National Environmental and Engineering Laboratory
LANL - Los Alamos National Laboratory
SNL - Sandia National Laboratories
TRI – Tech Reps Inc.
UNM - University of New Mexico / New Mexico Engineering Research Institute

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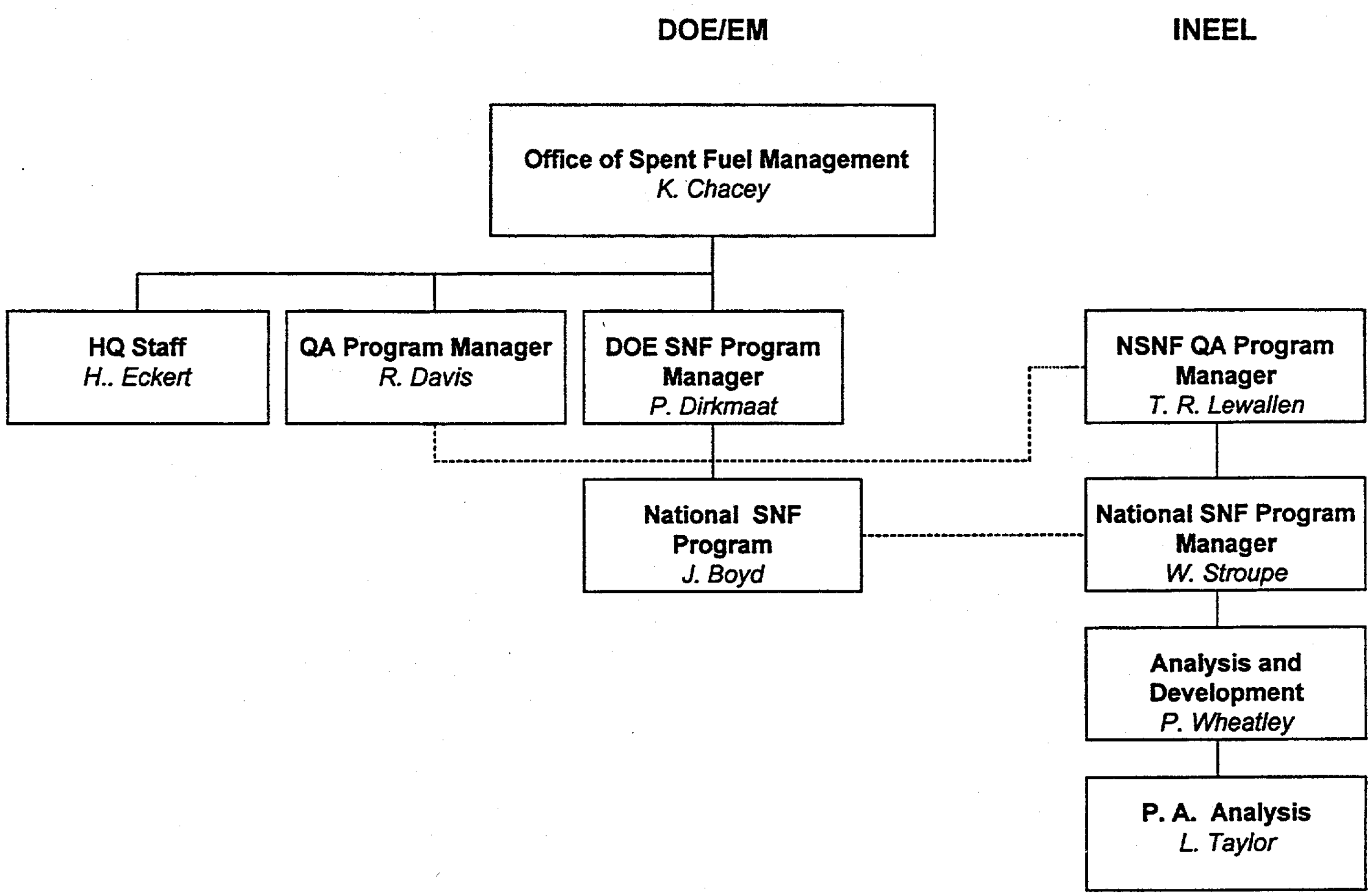

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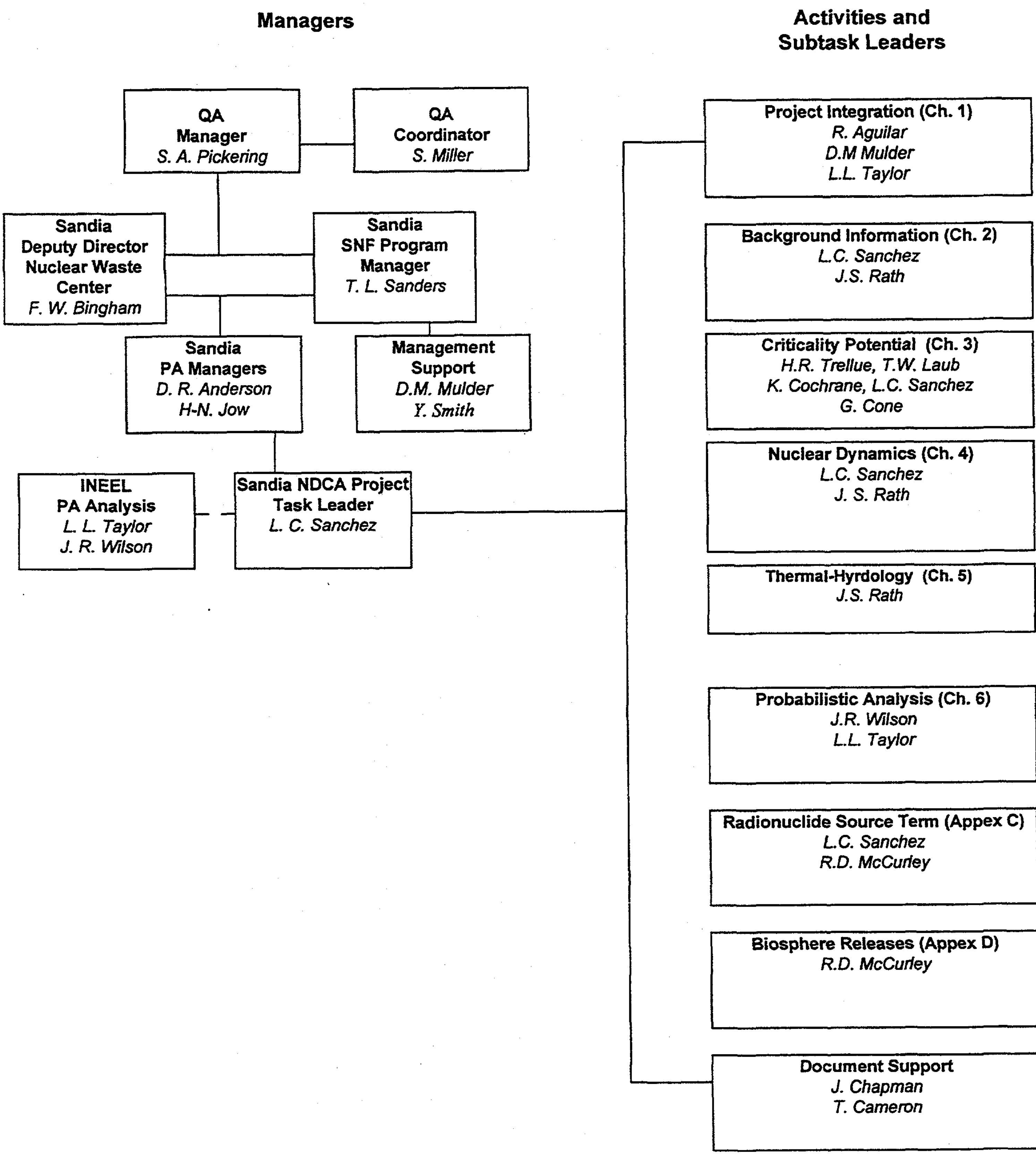

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T. Cameron	TRI			Text Editing
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1.0 INTRODUCTION

1.1 Overview

Sandia National Laboratories' (SNL's) Nuclear Waste Management Program (NWMP) Center is assisting the National Spent Nuclear Fuel Program (NSNFP), sponsored by the U.S. Department of Energy's Office of Environmental Management (DOE/EM), in the development of a safe and cost-effective technical strategy for the interim management and ultimate disposition of domestic and foreign spent nuclear fuels (SNFs) that are in DOE's jurisdiction. Major NSNFP project efforts at the NWMP Center include; (1) analysis of transportation systems used for DOE-owned SNF, (2) the assessment of the post-closure performance of a geologic repository for the SNF, and (3) the assessment of the probability and consequences of post-closure nuclear criticality within the geologic repository. These preliminary analyses will be used to identify if DOE's SNF are ready for placement in the Yucca Mountain Site (YMS) repository. The purpose of this report is to analysis the consequences due to post-closure nuclear criticality in a repository from a risk perspective. The current regulations for nuclear criticality in the YMS repository can be found in 10 CFR 60. However, these regulations are vague with respect to its application to nuclear criticality. The regulations in their current form require the application of the criticality safety limit ($k_{eff} < 0.95$) for the "isolation" of the disposed SNF (see Section 2.1.1). This may imply that safety limits are requested for post-closure times, even though humans could not possibly be in the immediate vicinity of the disposed SNF. This report does not analyze nuclear criticality from the criticality safety limit approach. Instead, this report identifies the risks associated with post-closure criticality without the application of the criticality safety limit enhancements. Because the estimated risks can be identified to be minimal, the results from this report can be used as the basis for arguments that post-closure criticality consequences are insignificant and that criticality safety limits are not necessary for post-closure time frames. Risk limits for the screening arguments are expected in the 40 CFR 197 regulations (see Section 2.1.2), which have yet to be promulgated. The performance goal of this report is to show that the risks due to post-closure criticality are less than the round-off of the overall risk identified in the performance assessment of the repository.

The information listed below in the remainder of this sub-section will present general information on: DOE's fuel types, nuclear criticality, applicable regulations and the link between repository performance assessment and the nuclear criticality consequences issue.

1.1.1 DOE Fuel

The safe disposal of defense (DOE-owned) spent nuclear fuels (DSNFs) presents a multitude of technical challenges (Crowley, 1997). To meet these challenges, preliminary analyses are necessary for the proposed disposal of these fuels. The current U.S. strategy for waste isolation calls for SNFs to be encapsulated in multiple metal-barrier waste packages for disposal in a geologic repository at the Yucca Mountain Site near Las Vegas, Nevada. The current package design also incorporates the co-disposal of DSNF with DHLW (defense high-level waste). As currently designed, the SNF packages may eventually corrode and begin releasing radionuclides into the surrounding environment within a few ten-thousand years after emplacement (DOE, 1996). The physical and chemical processes that could potentially lead to the release of radionuclides into the surrounding repository matrix through the unsaturated zone above the repository and into the groundwater have been established (TRW Environmental Safety Systems, Inc., 1995; Rechard, 1995b). Previous performance assessment (PA) studies suggest that the key radionuclides: technetium-99 (^{99}Tc; 213,000-yr half-life), iodine-129 (^{129}I; 16 million-yr half-life), and neptunium-237 (^{237}Np; 2.14 million-yr half-life) are soluble and mobile in groundwater (DOE, 1996; TRW Environmental Safety Systems, Inc., 1995). These fission product isotopes dominate the repository releases during a 100,000-yr post-closure time frame. In addition, the long-lived fissile isotopes of uranium-235 (^{235}U; 703 million-yr half-life), plutonium-239 (^{239}Pu; 24,100-yr half-life; decays to ^{235}U), and uranium-233 (^{233}U; 159,200-yr half-life) and daughter products (e.g. ^{226}Ra and ^{210}Pb) must be considered in any scenarios of transport and accumulation away from the waste packages. See Appendix C for repository inventory of radionuclides from disposed SNF and HLW and Ref. Rechard 1998 for detailed discussion on repository performance measures.

1.1.2 Post-Closure Nuclear Criticality Issues

The primary technical challenge for the performance assessment (PA) of a geologic repository is the acquisition of defensible, scientifically based models and data necessary to assess the long-term behavior and performance of the proposed repository. The models and data must include information on the physical characteristics of the flow system, the mechanisms and rate of fluid flow, the interaction of water with SNF packages in the repository, and the transport of radionuclides through the unsaturated and saturated zones (Crowley 1997; Rechard 1995b). The PA results are expressed as doses due to repository radionuclide released to the biosphere. A Nuclear Dynamics Consequence Analysis (NDCA) may be used to demonstrate that the occurrence of a post-closure nuclear power excursion (i.e., nuclear criticality) results in inconsequential additional releases to the biosphere if the SNF is disposed in a underground geologic repository. A primary criticality concern is highly enriched uranium (HEU) fuels since they comprise a significant portion (approximately 27%) of the DSNF packages slated for geologic disposal. Waste disposal canisters for the DSNFs will be intermixed with commercial packages in the repository and are designed to maintain subcritical conditions with appropriate margins of safety for pre-closure times. However, water influx and the resulting corrosion over time in a geologic repository environment could potentially alter the waste canisters and the SNF itself and increase the potential for criticality unless the package designs and fissile payloads ensure subcritical conditions for post-closure times.

This study investigated both the potential for criticality and the consequences of a post-closure nuclear excursion in the proposed repository. With respect to nuclear reactivity behavior (i.e., neutron multiplicity or growth), packaged fissile material will respond differently when stored in a geologic repository environment than when it is used in an engineered nuclear reactor core. These behavior differences result in vastly different time scales for important reactivity parameters controlling a nuclear power excursion.

This report does not study the post-closure aspects of criticality safety of the disposed SNF, as implied in the 10 CFR 60 regulations (the impact of post-closure criticality safety limits on SNF loading, in waste canisters, is being analyzed by criticality experts, see DOE-RW, 1997; 1998). This report only analyzes the risks associated with post-closure criticality consequences, with the intent of developing the basis for post-closure criticality FEP's screening arguments (see Appendix B for details). The screening arguments will indicate that, from a risk perspective, the consequences due to post-closure criticality of disposed SNF, without the use of criticality enhancements, are insignificant (i.e., they are less than the estimated round-off of expected performance assessment for the repository). Thus, the application of the criticality safety limit ($k_{eff} < 0.95$) for post-closure timeframe would not result in any measurable reduction of risk.

1.1.3 Dismissal of FEP's Through Screening Arguments

The work presented in this report contributes to the features, events, and processes (FEPs) screening process, which is associated with repository performance assessment (Rechard, 1998). The performance assessment is a structured methodology to determine the long-term behavior of a geologic system for disposal of nuclear waste. Formally, the performance assessment can be defined as a structured plan of investigation in which (1) features, events, and processes (FEPs) associated with the system are identified and ranked according to the degree that they affect system behavior, (2) the effects of significant FEPs on system performance are examined by means of mathematical models, taking into account all known uncertainties in model formulations and model parameters, and (3) the results of system performance, including the uncertainty of those results, are presented in probability distributions for system performance measures (EPA, 1985). The specific event (or process) under consideration is the development and subsequent consequences of a post-closure critical condition in or near a geologic repository containing DSNF. The screening criteria for criticality scenarios are identified in Figure 1.1.3-1. Decision box 2 is concerned with the likelihood of occurrence of each criticality scenario. Decision box 3 is concerned with the physical consequences of each individual type of scenario, assuming that they occur.

Earlier work on criticality scenarios associated with DSNF in a tuff repository conservatively estimated an upper bound of 10^{-4} for the probability of any criticality event occurrence in a 10,000-yr period (Rechard, 1995b). However, given the currently available information on the Yucca Mountain repository environment, values for criticality event probabilities cannot be determine without significant uncertainties. Therefore, our current effort is focused on assessing the physical consequences of a criticality occurrence under the highly unlikely conditions and circumstances required for the assembly of critical mass in a repository setting. The Environmental Protection Agency (EPA) had previously established in 40 CFR 191 a 10,000-yr compliance time frame (Rechard, 1995a) for assessment of the FEPs. This regulation has been remanded and is expected to be superceded by the to-be-promulgated 40 CFR 197. It is anticipated that the current 10,000-yr regulatory compliance period may be increased further, but the screening limits for the FEPs are expected to be comparable to previous limits in 40 CFR 191. Specifically, in 40 CFR 191, the agency [EPA] assumes that such performance assessments need not consider categories of events or processes that are estimated to have less than one chance in 10,000 of occurring over 10,000 years (equivalent to 10^{-8} /yr). Furthermore, the performance assessments need not evaluate in detail the releases from all events and processes estimated to have a greater likelihood of occurrence. Some of these events and processes may be omitted from the performance assessments if there is a reasonable expectation that the remaining probability distribution cumulative releases would not be significantly changed by such omissions (EPA 1985, Appendix B). The NCDA project uses a probability screening limit of 10^{-8} /yr and an arbitrary consequence limit of 10^{22} fissions for a single criticality event. Since the consequence limit for individual excursions is difficult to ascertain due to significant uncertainties in the criticality models, risk limits are ultimately used as performance goals in this report. Thus, this report will compare the criticality risks to the round-off of the repository performance assessment, assumed to be 1 % (see Figure 1.1.3-2).

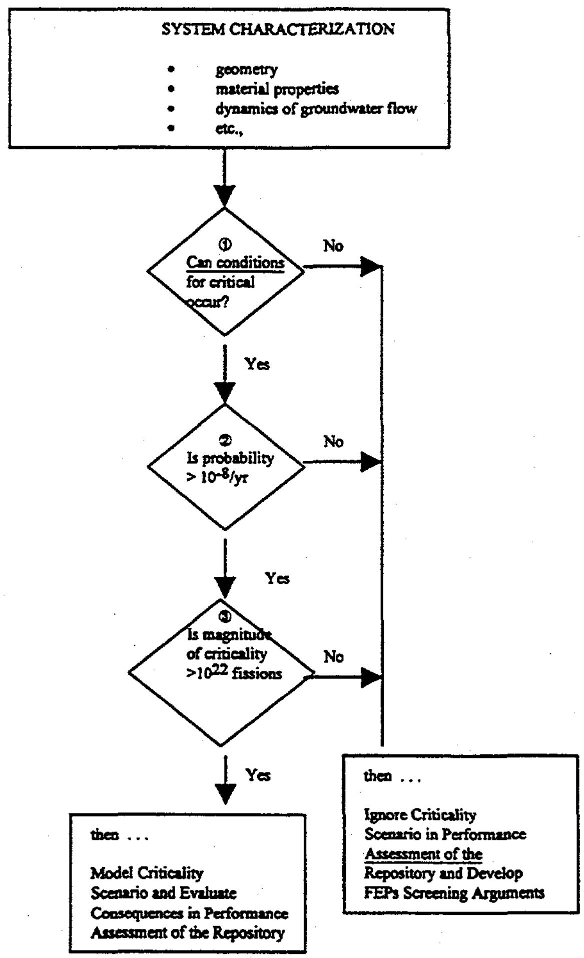


Figure 1.1.3-1 Screening process for criticality FEPs (features, events, and processes) using probability (decision box #2) or criticality consequences (decision box #3).

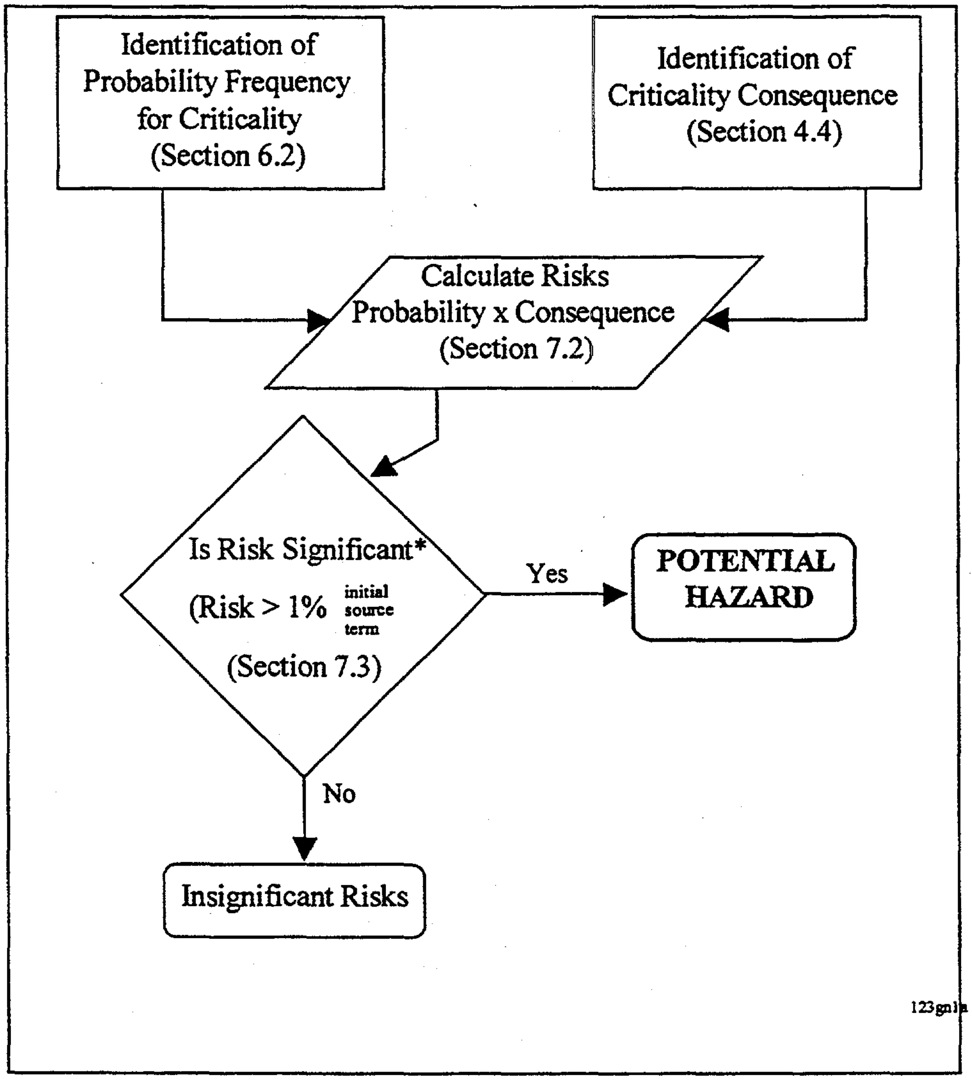


Figure 1.1.3-2 Flowchart of calculations used to identify risks due to criticality and comparison to assumed round-off of the initial source term.

1.1.4 Regulations

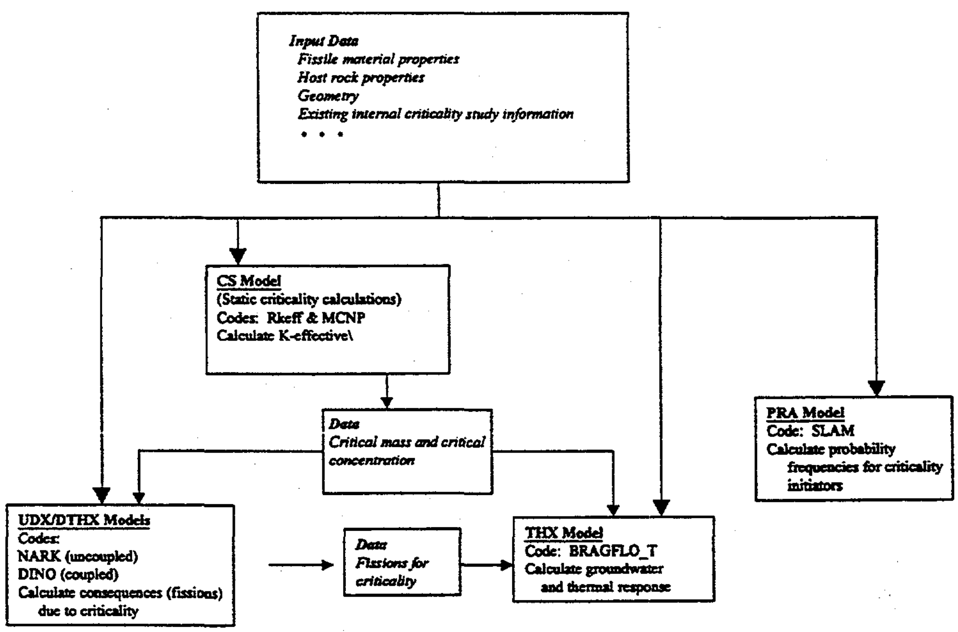
As discussed in McLaughlin 1996, the 10 CFR 60 regulations are vague and can be interpreted to mean that "criticality safety" (i.e., the $k_{eff} \leq 0.95$ constant) should be applied to SNF canisters placed in a geologic repository for all time (operational phase and post-closure). This subcritical limit is principally meant to protect personnel working in the vicinity of fissile materials. In order to assure that subcritical limit is not exceeded as waste packages corrode and their contents migrate from their original locations during post-closure times would require severe limitations upon fissile material loading in each waste package. The limitations would be dependent upon whether credit over the regulatory timeframe could be taken for criticality mitigation mechanisms such as neutron poisons in the waste packages. From a PA perspective, it is only the repository operational period from the initial SNF disposal phase to the closure of the repository that need be considered for criticality safety concerns, after which only consequences need be analyzed. Also, the risks associated with post-closure criticality in a geologic repository are minimal since it is not possible for humans to be immediate vicinity of any post-closure criticalities. Thus, there is no risk-based justification for subcriticality safety measures to be applied for post-closure times. This is important because the economic considerations are highly related to the definition of criticality. For this report criticality safety measures are assumed for the operational phase, but no enhancements beyond post-closure is used. The logical approach to criticality analysis, from a repository PA perspective, is:

(1) Perform criticality safety analysis only for the maximum period of time that humans would be in the immediate vicinity of the disposed SNFs (during the "operational phase" of the repository). Criticality safety limits are principally meant to protect personnel working in the vicinity of the SNFs. (Analysis in this area is currently being performed by DOE/RW.)

(2) Perform risk analysis calculations that would identify the long-term risk to future generations of humans due to consequences of possible criticality excursions. These risk calculations would estimate doses that could result from the additional radionuclides (fission-yield products) generated by any additional fissions produced by possible nuclear excursions. A significantly large inventory of radionuclides already exists from commercial SNF and DSNF prior to the disposal in the proposed repository (12.5 billion curies at the anticipated time of disposal, see Appendix C). Additional radionuclides generated from any future critical excursions would constitute only a small fraction in comparison to the initial inventory. Furthermore, it would be exceedingly difficult to produce a critical assembly in a geologic repository setting. A critical assembly would require many unlikely events (fissile material dissolution, groundwater transport, common collection point of drain leachate plumes from multiple failed packages, etc.,).

1.1.5 Measures of Criticality

For the NDCA project, post-closure conditions are assumed not to apply enhancements that would ensure the criticality safety limit of $k_{eff} < 0.95$. Thus k_{eff} may approach delayed critical conditions (i.e., $k_{eff} = 1.0$). Since there are a multitude of scenarios that could possibly result in a criticality, the analysis of post-closure criticality must be a probabilistic one. The most meaningful way to estimate the risks associated with post-closure criticality, is to calculate the additional fissions, on a yearly average basis, due to criticality and then compare them to the number of fissions needed to generate the initial source term inventory. The additional fissions can also be used to estimate the contribution to the key fission yield products (e.g., ^{99}Tc, ^{129}I, and ^{237}Np) which may have an impact (though small) in the estimated doses in the biosphere. The number of additional fissions may be estimated by multiplying the expected number of fissions per criticality times the probability of obtaining a critical configuration times the expected number of criticalities (or excursions) due to that configuration. The calculations for assumed nominal post-closure criticality risks are shown in Figure 1.1.5-1, which identifies the probability frequency and consequences of criticality. This figure identifies the fundamental principle for risks determined from the five different NDCA models.



RISKS = CONSEQUENCES X FREQUENCY

Figure 1.1.5-1 Flowchart of NDCA models and data exchange.

1.1.6 Approach to Criticality Analysis

As can be identified in Figure 1.1.5-1, the risks associated with post-closure criticality are fundamentally dependent upon the critical fissile mass. The geometries analyzed were all assumed to be wet (i.e., moderated systems) since groundwater is considered necessary for canister corrosion, subsequent breach and movement of fissile material. Thus, the static criticality calculations performed for the NDCA project were performed using systematic calculations to determine the quantity of fissile mass necessary to yield a critical assembly for a given fissile concentration. These criticality search calculations (termed "buckling search") identified that very large fissile material concentrations are necessary when fissile is transported by groundwater and reconcentrated in near-field and far-field locations even in ideal geometries (see Section 1.1.7). Criticality calculations for *in situ* geometries (degraded and semi-degraded waste canisters) were not performed as part of the NDCA project because enough existing calculations, for use in the PRA model, were available. Also not analyzed as part of the NDCA project were autocatalytic criticality scenarios, under-moderated dry and over-moderated wet assemblies. The under-moderated dry scenarios have been investigated by other researchers and have been identified to be essentially impossible to generate since groundwater is essential for the mechanisms needed to transport and reconcentrate fissile material. The over-moderated wet scenario were not analyzed because the maturity level of this scenario is immature at the present time (updates to the PRA model are under development and their results will be presented in the near future). Current nuclear dynamics results indicate that nuclear excursions would shut-down due to prompt feedback effects prior to over-moderated (groundwater movement) effects. Thus, an over-moderated wet system would have very large positive feedback effects (e.g., void coefficient) to be of concern. This scenario may be "screened out" if the PRA model can show that it highly unlikely.

Also not analyzed in this report is the identification of nominal reactivity insertion rates. The identification of this parameter is difficult due to the uncertainties in the groundwater and corrosion models used in repository performance assessments. Instead of analyzing a multitude of scenarios in order to estimate a viable range for reactivity insertion, the NDCA project performed sensitivity studies using a wide range for the initial reactivity insertion. The range of reactivity insertion values used included values as high as multi-"cents" of prompt reactivity insertion. This choice is expected to exceed nominal values since groundwater transport, under all but highly unlikely conditions, occurs at very slow rates and the self-shutdown mechanisms would cease nuclear chain reactions prior to development of sizable net reactivity insertions (on the order of one cent of reactivity). There are scenarios for very rapid reactivity insertions that could be postulated (e.g., events such as sudden groundwater insertion into a partially degraded waste canister due to rock fracturing above the canister in combination with perched water reservoirs). However, they are expected to be unlikely and the analysis of these special scenarios is beyond the intended scope of this study. Future updates to the PRA model will study these some of these scenarios to identify their probability. It is not expected that their associated risks (probability times consequences) will be significant.

1.1.7 Criticality Geometries

Internal, near-field, and far-field geometries were considered to determine the neutronic interaction of the stored fissile material with the geologic media. Internal geometries consist of in situ processes occurring within the SNF canisters themselves. Near-field geometries consider fissile material removed from the canisters and accumulated in rust slumps or concrete inverts in the emplacement drifts. Far-field geometries consider processes occurring at least one tunnel-diameter distance away from the SNF canisters.

- The **internal (*in situ*) model** used in this analysis used several geometries corresponding to different levels of degraded or reconfigured SNF assembly geometry. The NDCA project did not perform static criticality calculations for these geometries since existing computational results were available (see Sections 3.2 and 6.1 for discussion).
- The **near-field model** used in this analysis used perfect hemi-sphere geometries that contained a complex mixture of underground water with either rust (representing a corroded waste package) or concrete (representing corroded inverts). These geometries corresponds to an optimally or near-optimally moderated system since a non-optimal system would require substantially higher fissile concentrations than what is possible due to the canister loading.
- The **far-field model** used in this analysis assumed that for a nuclear excursion (supercritical state) to occur in the geologic repository, the most likely scenario is that of a high-moderation, slow assembly (e.g., Oklo natural nuclear reactor, Smellie 1995, or a critical event in an aqueous solution, Stratton 1989). In these situations, the moderator material is generally assumed to be a complex mixture of underground water, the geologic medium (such as salt, granite, tuff, or clay) and other gases resulting from the underground water or brine chemically reacting with the metallic canister. Far-field geometries assumed a perfect spherical model consisting of the fissile, moderating, and host rock materials.

1.1.8 Links to 97 PA

A detailed illustration of how Nuclear Criticality analysis is incorporated into the repository PA process is shown in Figure 1.1.8-1. As can be seen, the preliminary steps in the process are the identification of the possible scenarios that could ultimately contribute to repository risks (i.e., releases from the repository to the accessible environment). Also, Figure 1.1.8-1 indicates the use of criticality excursion consequences and probability and frequency FEP screening arguments. As identified in Section 1.1.3, FEPs can be screened out (i.e., identified as being reasonably insignificant) if the probability of occurrence is less than 10^{-8} /yr, the consequences are insignificant, or both. Obviously, if criticality has a significant cumulative effect on the releases from a repository, the consequences of criticality must become a standard subpart of the PA consequence modeling.

If the identification of the consequences of nuclear excursions is not enough to screen out the criticality FEPs or to satisfy the governing regulator, then the probability and frequency (yielding cumulative occurrences) will also be needed. This (possible future) analysis is difficult to perform. The most straightforward approach is to use PA computational results to identify first occurrences of nuclear excursions in the various repository regions: internal, near-field, and far-field. Follow-up calculations can then be used to determine the expected frequencies for the re-occurrence of an excursion. This process would require use of many of the PA codes and significant computational resources. A possible approach that would streamline the analysis may be to model only the basic physics related to a criticality (i.e., corrosion mechanisms, groundwater transport, precipitation, etc.) in a single consolidated code. Thus, if the key input parameters are (Monte Carlo) sampled (see Appendix B), the output database could be analyzed for the probabilities, frequencies, and the associated uncertainties for internal, near-field, and far-field criticalities.

The last important feature of Figure 1.1.8-1 is the inclusion of criticality consequences in the PA consequence modeling.

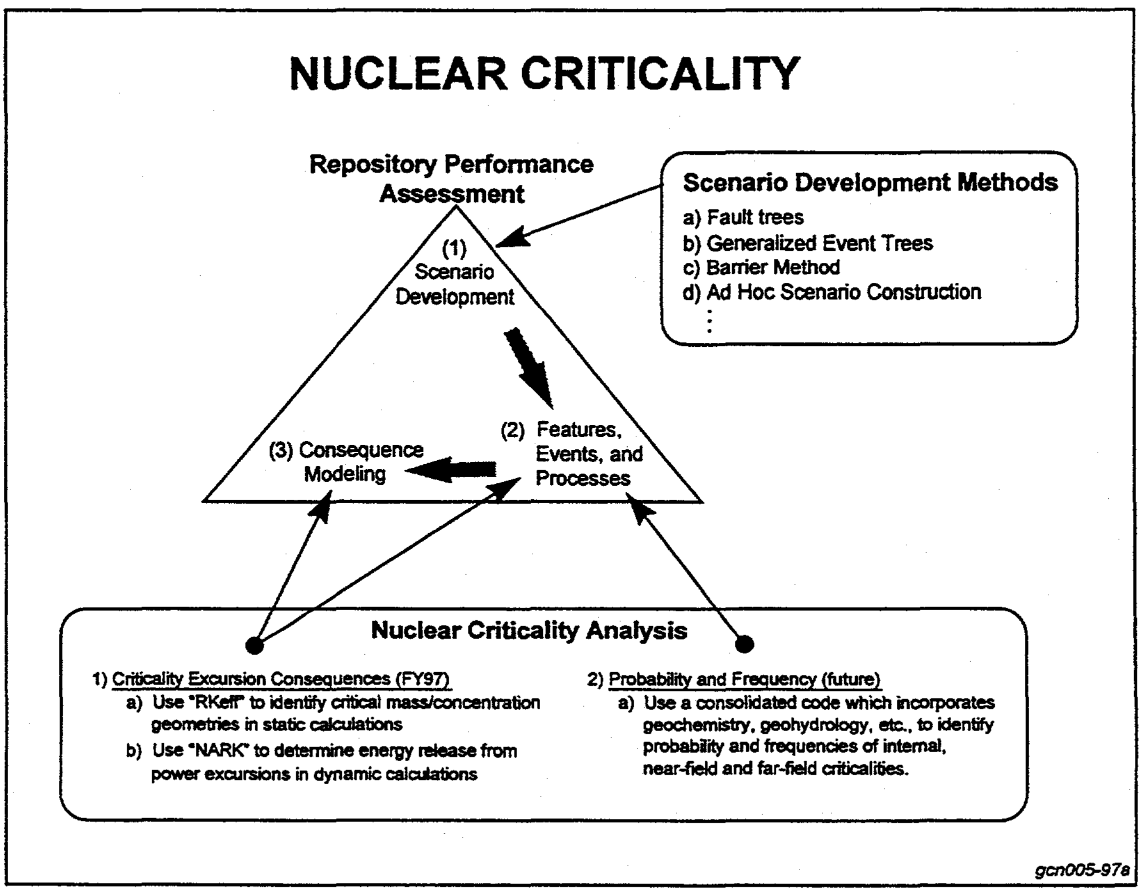


Figure 1.1.8-1. Integration of nuclear criticality analysis into repository performance assessment.

1.2 NCDA Technical Objectives

The nuclear dynamics of a delayed supercritical system deals with time-dependent reactivity, which ultimately controls the neutron population, neutron flux, power, and temperature of a nuclear fission assembly. The analysis of the nuclear dynamics of a system and their consequences is accomplished by modeling the entire nuclear energy system and incorporating feedback mechanisms to compute the time-dependent reactivity. The combination of stored fissile material stored in underground geologic moderating materials is an example of a potentially supercritical system that could produce a self-sustaining nuclear chain reaction if a critical mass is assembled by the integration of the materials. Therefore, a comprehensive Nuclear Dynamics Consequence Analysis (NDCA) of such a system is necessary to determine the following:

1. Whether or not a self-sustaining nuclear reaction is capable of occurring,
2. If a nuclear reaction does occur, whether or not the reaction will be promptly shut down by the Doppler effect before any significant energy releases can occur.

1.2.1 Uncoupled Versus Coupled Models

A major technical objective of the NDCA project is to test the hypothesis that the consequences of a nuclear power excursion of a critical assembly modeled only with uncoupled nuclear dynamics (neutronic effects only) envelop those derived with fully-coupled nuclear dynamics (coupling of neutronics and thermal-hydrology effects).

1.2.2 Excursion Behavior

The second major objective of the NDCA project is to identify what mechanisms actually control the transient power behavior and how these impede an unrestricted power excursion. This objective will be accomplished by conducting analyses and performing calculations that will determine the following:

(1) the power time history of post-closure criticalities,
(2) the integrated number of fissions (energy) experienced,
(3) and the thermal hydrology response of the geologic media due to a criticality.

The completion of these objectives provides a comprehensive evaluation of the consequences of a criticality excursion and their potential effects on a long-term repository performance. The consequences of criticalities, expressed as additional fissions in the repository, can then be directly compared to the fissions associated with the original burnup of the disposed radionuclides.

1.2.3 Risk (consequences x probability)

The risks associated with post-closure nuclear criticality are computed simply as the product of excursion consequences and probability. This is identified in Figure 1.1.5-1, where the probability is comprised of several subcomponents. It is the product of the probability frequency of criticality initiators (determined from the PRA model), the annual frequency of criticality due to groundwater and thermal responses (from the THX model), and an assumed duration of time for continuous cycles of excursions. The latter term corresponds to a maximum length of time that criticalities could continuously be cycled before host rock pores become clogged or some other mechanism occurs that restricts continuous criticalities. Since this term can not be accurately estimated at the present time, results for range of values is presented in Section 7. Also because the calculation for risk is mathematical linear, the example risks results in Figure 1.1.5-1 can be scaled linearly with input values for this term (e.g., for a assumed duration of 1,000 years (ten times the example value), the results in Figure 1.1.5-1 could simply be multiplied by a factor of ten).

1.3 NDCA Models

Five models were used in the NDCA computational effort to model SNF that exhibit negative thermal feedback effects. These models were needed to perform the large number of calculations for nuclear criticality potential, consequences of an individual nuclear excursion, probabilities for initiation of a criticality, and probability frequencies for repetitive criticalities. These models, with the exception of the PRA model, use computational codes contained in the Repository Nuclear Code System and include four deterministic models along with one probabilistic model were used for the NDCA screening process of FEPs in the PA of a geologic nuclear waste repository. The deterministic models were used to calculate the consequences (e.g., total fissions, peak energy, added fission products, etc.,) associated with a criticality event occurring in the waste repository. The probabilistic model estimated the frequency (probability) of a criticality event. The results of the deterministic and probabilistic codes were then combined to calculate the risk of a criticality event. Figure 1.1.3-1 gives an overall schematic of the screening process using deterministic and probabilistic methods.

The five models used in the NDCA screening process are:

1. **CX model:** The CX model uses two major computational codes, RKeff and MCNP, to determine the necessary fissile mass, concentration, and geometry size to achieve criticality. This model is described in detail in Chapter 3.

2. **UDX model:** The UDX model uses the NARK code to identify the duration, power history, and total number of fissions of a single excursion independent of groundwater effects. Further information of this model is given in Chapter 4.
3. **DTHX model:** The DTHX model is a combination of the THX and UDX models coupled together to form the DINO code. DINO determines nuclear excursion behavior considering both the nuclear dynamics and repository response. The DINO code is computational intensive and was only used for a small set of analyses. Chapter 4 gives a description of this model.
4. **THX model:** The THX model uses the BRAGFLO_T code to determine the maximum frequency of nuclear excursions in a far-field scenario by simulating the groundwater and thermal responses to a nuclear excursion. A further discussion of this model can be found in Chapter 5.
5. **PRA model:** The PRA model consists of a fault/event tree method to identify time-dependent events such as groundwater infiltration, container and SNF cladding degradation, dissolution of fissile material, and transport of fissile material to other geologic locations. Simulations of the repository behavior were performed using the SLAM code. The results of this model gave estimations for the probability of criticality initiators and a subsequent critical event. This model is described in detail in Chapter 6.

A detailed schematic of the flowchart for data transfer between the above models is given in Figure 1.1.5-1.

1.3.1 Criticality Potential (CX) Model

The CX model uses two major computational codes: RKeff (generated as part of the NDCA project) and MCNP (an existing industry standard code for neutral particle transport). The RKeff code was developed as a pre- and post-processor for eigenvalue (static criticality) calculations which identify the criticality potential of a fissile assembly. The code requires up to twelve input variables including: fissile mass, fissile concentration, model geometry shape, and saturation in the rock matrix. RKeff generates complete MCNP input files that are then used to identify whether an assembly of fissile material is subcritical, critical, or supercritical. Results are processed to identify critical fissile mass and concentration values necessary for given geologic conditions to result in a critical assembly. The critical mass and concentration values are then used in the THX, UDX, and DTHX models. The CX calculations were performed in a four step process:

A. A 3-D MCNP model is generated for a baseline case study, which has a set of fixed parameters such as fissile material, enrichment, host rock type, and geologic quantities such as porosity and saturation. Then, for a fixed fissile concentration, a series of static criticality (eigenvalue) calculations were performed for various masses. These values are plotted in a two dimensional curve termed a "criticality curve". A typical criticality curve can be seen in Figure ES-2.

B. A new fissile concentration value is identified and the processes in Step A are repeated. This is performed for a multitude of concentration values and the results represent a two-dimensional parametric study of k_{eff} as a function of fissile mass and fissile concentration. The results can be plotted as three dimensional curves termed "criticality surfaces", which are accumulations of criticality curves. Typical results can be seen in Figure ES-3.
C. Using results from Step B, a criticality buckling search is performed. This corresponds to the identification of sets of minimum fissile mass and concentration values that are necessary to yield a critical assembly (i.e., $k_{eff} = 1.0$). The results can be plotted in a 2-D curve termed a "criticality S-curve". Typical results from this step can be seen in Figures ES-4 and ES-5.
D. A set of S-curves (from Step C) can be obtained for a variation in a baseline parameter such as fissile enrichment. The results are plotted in a 3-D curve termed a "criticality saddle". Typical results can be seen in Figure ES-6.

From the above description it can be recognized that the development of criticality S-curves and saddles requires a large computational effort since each point on these curves corresponds to an eigenvalue search. In this study, key S-curves were generated for fissile material in near-fields and far-field configurations.

The code "RKeff" was created to allow the user to perform a systematic set of static criticality calculations. The code will produce eigenvalue solutions to the Boltzmann Transport Equation (Duderstadt, 1976) solved with a Monte Carlo Code for Neutral Particle Transport (MCNP) (Briesmeister, 1986). RKeff generates a systematic set of MCNP input files that allow a sensitivity analysis for the criticality constant (k_{eff}) of a limited number of near-field, and far-field geometries (for most common configurations of fuels/geometries typical of DOE HEUs). These sensitivity analyses are used for "buckling searches," correlative to performing a series of calculations that identify the dimensions of a critical assembly of thermal mass. These series of calculations will yield "S-curves." Several S-curves can be generated for the most common host rock/fuel combinations anticipated in the proposed repository for SNF. An example of an S-curve for a system of pure ^{239}Pu and water is shown in Figure 1.3.1-1, compares RKeff/MCNP calculations with published values (Clayton, 1980). As illustrated in the figure, it is possible to create a critical system with as little as 509 g of ^{239}Pu. Likewise, Figure 1.3.1-1 shows that it is not possible to generate a critical system with a fissile loading concentration less than 0.008 kg ^{239}Pu per liter of solution.

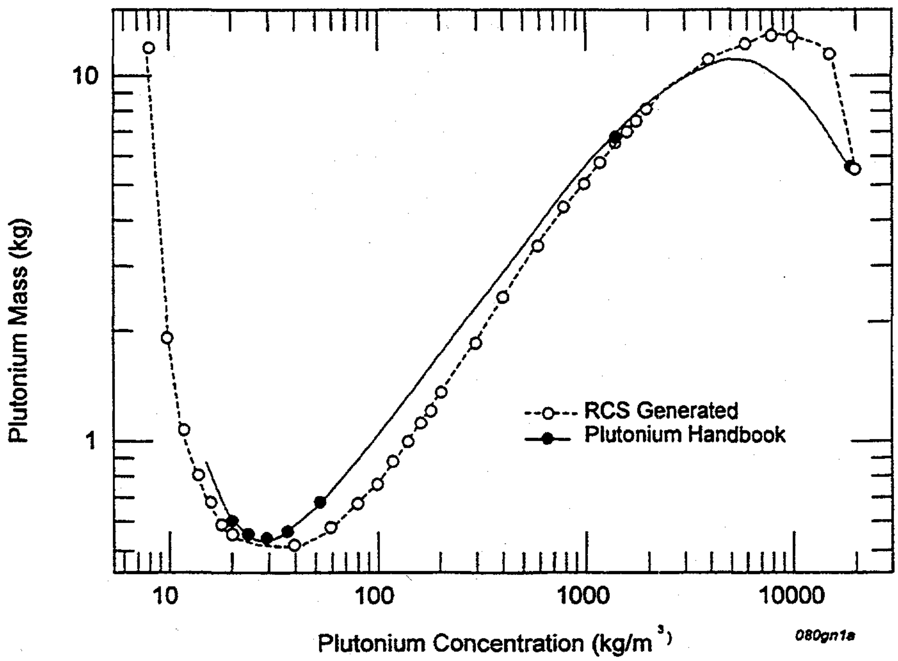


Figure 1.3.1-1 Criticality S-curve computed using RKeff and MCNP (identified as RCS generated). Computed values for critical fissile mass and concentrations compared to published values (Clayton, 1980).

For the NDCA project, S-curves were generated for the following scenarios:

(1). Near-field geometry comprising
   a. a hemispherical slump of a corroded storage cask (rust/TFM composition, see Appendix E)
   b. an inverted hemispherical assembly of corroded concrete/TFM composition (corresponding to an accumulation of fissile material in a corroded section of concrete insert, see Appendix E).

(2) Far-field geometry comprising a sphere of reconcentrated TFM (because of solubility, colloid transport, chemical precipitation, etc.) in yielded volcanic tuff typical of the Yucca Mountain Site.

RKeff contains over 20,000 lines of standard FORTRAN77 language code and runs on multiple platforms.

1.3.2 Uncoupled Nuclear Dynamics (UDX) Model

The UDX model uses the computational code NARK, which was generated as part of the NDCA project. This code was developed to determine the transient behavior (nuclear dynamics) of the neutron population in a critical assembly (uncoupled from groundwater effects) by using the point-reactor model. NARK uses modern self-adaptive and self-diagnostic numerical algorithms to solve sets of ordinary differential equations (ODEs). Input parameters include: fissile material type, delayed neutron lifetimes, half-lives of delayed neutron groups, initial conditions (power, reactivity, and select output from the RKeff code (e.g., fissile mass). Output from NARK is used to identify the power history of a nuclear excursion, total number of fissions from the excursion, and the duration of a single excursion.

The code "NARK" was created to model the kinetic and dynamic behavior of nuclear excursion. The dynamics analysis includes both uncoupled and coupled nuclear dynamics. Uncoupled nuclear dynamics includes prompt and delayed neutron feedback mechanisms, and coupled nuclear dynamics incorporates impeded feedback mechanisms due to coupling with groundwater transport. The NARK code solves both stiff and non-stiff ordinary differential equations (ODE) with the use of self-adaptive solvers. Hence, the code allows for modeling of both prompt and delayed nuclear excursions. NARK contains over 37,000 lines of standard FORTRAN77 language code and will also run on multiple platforms.

We have performed a multitude of nuclear dynamic calculations for various combinations of fissile mass, thermal feedback coefficient (i.e., fuel-Doppler and moderator-Doppler), and neutron generation times. This wide range of calculations can be performed because of the NARK code's use of modern, self-adaptive ODE integrators, which minimize the number of time steps requiring evaluation. These nuclear dynamics calculations show that nuclear excursions of DOE-owned SNFs experience prompt thermal feedback shut-down mechanisms that minimize energy releases and yield insignificant additions to the YMP SNF inventory.

1.3.3 Fully-Coupled Nuclear Dynamics (DTHX) Model

The DTHX models is comprised of the THX and UDX models coupled together resulting in the code DINO. This computational code was generated from the NARK and BRAGFLO_T codes. It models fully-coupled (neutronics and repository response) far-field nuclear dynamics excursions. Since this computational code was large and is computationally intensive, it was used for a small set of analysis runs. The output was compared to results from NARK (uncoupled nuclear dynamics) and identified that NARK results give conservative estimates of the transient behavior of the neutron population during an excursion. Thus large parametric studies for excursion consequences could be obtained with uncoupled nuclear dynamics results.

1.3.4 Thermal-Hydrology (THX) Model

The THX model uses the computational code BRACFLO_T, which is an existing SNL code. The THX model is used to determine the thermal and groundwater response of far-field geologic media to a nuclear excursion. The code used is an experimental version (using high spatial resolution) of the BRAGFLO_T code. BRAGFLO_T is a transient thermal hydrology and groundwater flow code that has been used for analysis of the Yucca Mountain Site. THX was used to analyze the transient 2-phase flow of groundwater and gas resulting from typical excursions determined by the NARK code. The results identified the time behavior of temperature for the fissile assembly zone and the groundwater saturation. From these results, the maximum frequency of occurrence of nuclear excursions could be estimated for far-field scenarios, should one ever be generated.

1.3.5 Probabilistic (PRA) Model

The PRA model uses the Monte Carlo simulation code SLAM. This is an existing INEEL code which is used to model probabilities for time-dependent events such as groundwater infiltration, canister degradation, SNF cladding degradation, dissolution of fissile material, radionuclides, neutron poison material, etc., and transport of the material to other geologic locations. For the PRA analyses, fault/event tree methodology was combined with the use of the Monte Carlo simulations performed with SLAM (see Chapter 6 and Appendix H). Although there is good confidence in the computational code used in the model, there is considerable uncertainty in the input data used at this time. Current work in this area should yield updated model results, which are expected to published in the near future (the updated results will supercede the PRA models results presented in this report). The most important result produced from this model is the estimated probabilities for initiation of a criticality.

When fission occurs in a fissile mass, whether it is caused by uranium or plutonium, the event results in the production of energy, fission fragments, neutrons, and various types of radiation (gamma, beta, etc,.). For aboveground nuclear excursions, it is the prompt radiation production from fission that is of greatest concern because it could be lethal to humans in the immediate vicinity. During post-closure times in an underground repository, humans would not be present at the time when future corrosion/groundwater mechanisms could dilute, transport, and reconcentrate fissile material to possibly produce conditions yielding a nuclear excursion. Thus, the doses from (post-closure) prompt fission radiation are not a concern for geologic repository designs. The doses of concern would only be those delayed doses produced through the transport of the additional radioactive fission yield products to the accessible environment. The dose contribution due to additional excursions can be shown to be insignificant in comparison to the dose contribution associated with the initial repository radionuclide inventory (see Appendix C for source term values). By the time that sufficient fissile material has accumulate to cause a criticality, the water would probably have transported away significant quantities of the radionuclides from the original inventory and they would dominate the doses released to the biosphere.

The effects of prompt (mainly neutron and gamma) exposure on humans for aqueous excursions of approximately 10^{17} prompt fissions would results in fatalities for humans in the immediate vicinity (several meters) of an unshielded criticality assembly. The spatial dependency of the exposure upon distance is due mainly to the geometrical spread of the radiation. Since there is significant shielding between post-closure fissile material in an underground geologic repository and the accessible environment, prompt exposures to humans, aboveground, are so small that they are not quantifiable. However, the regulatory compliance criteria for the proposed Yucca Mountain Repository remain uncertain; these criteria may be based entirely on release probabilities, risk to humans, or a combination of the two (Kastenberg, 1997).

Should the modeling results support this hypothesis, the NDCA will demonstrate that fuel-Doppler effects alone (which are inherent and prompt) greatly surpass those of Doppler plus the void-coefficent reactivity effects and will, therefore, bound a rapid power excursion. This phenomena is expected because Doppler effects (mostly fuel-Doppler supplemented by moderator-Doppler) are prompt and will act on a faster timescale than the void coefficient of reactivity, which requires a thermally-driven groundwater desaturation mechanism. Thus, it is expected that fuel-Doppler effects alone would result in the prompt shutdown of rapid power excursions prior to any geohydrology effects. An important aspect of the prompt shutdown is that even if the void coefficient gives a positive feedback (due to an over-moderated condition), shutdown would still occur promptly. Since uncoupled dynamics calculations do not model thermal-hydrology effects, they do not require significant computational time and the uncoupled dynamic model could be used extensively to investigate a multitude of conditions.

2.0 BACKGROUND INFORMATION

This chapter presents general information on nuclear criticality in a geologic repository. The discussion includes; 1) regulatory requirements concerning the criticality of fissile material in SNFs and HLWs disposed in a geologic repository, 2) interface of NDCA criticality analysis with repository performance assessment, and 3) limitations of the analysis presented in this report.

2.1 Regulations

This section presents discussion on criticality requirements and FEPs limits. Criticality requirements are in the 10 CFR 60 regulations. The FEPs limits will be in 40 CFR 197, which will be promulgated in the future. For this study the FEPs limits are assumed to be the same as that from 40 CFR 191.

2.1.1 Criticality Requirements in 10 CFR 60

For application to the Yucca Mountain Repository, criticality requirements are identified in 10 CFR 60. Unfortunately, the current requirements in 10 CFR 60 do not clearly specify whether the definition of "criticality" corresponds to "criticality safety" or "criticality consequences" (i.e., the results of a criticality excursion)[1]. The pertinent paragraph, 60.131(b)(7), states:

> "*Criticality control.* All systems for processing, transporting, handling, storage, retrieval, emplacement, and isolation of radioactive waste shall be designed to ensure that a nuclear criticality accident is not possible unless at least two unlikely, independent, and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety. Each system shall be designed for criticality safety under normal and accident conditions. The calculated effective multiplication factor (k_{eff}) must be sufficiently below unity to show at least a 5% margin, after allowance for the bias in the method of calculation and the uncertainty in the experiments used to validate the method of calculation."

As mentioned in Section 1.1.4, this report does not analyze criticality safety as can be implied form 10 CFR 60 regulations for post-closure conditions. Instead this study investigated criticality from a PA perspective with the intent to show that the risks associated by not requiring post-closure subcriticality limits are minimal. Thus, the criticality analysis results presented in this report correspond modeling of critical

[1] Discussion on criticality analysis can be found in: ANS 1983, Koponen 1982, Knief 1985, O'Dell 1974, Paxton 1972 & 1980, Smith 1981, and Thomas 1978.

assemblies (k_{eff} = 1.0) and not fissile mass assemblies requiring enhancements in order achieve the subcriticality limit: $k_{eff} \leq 0.95$ as suggested in 10 CFR 60 [2].

2.1.2 FEPS Limits in 40 CFR 191

The FEPs limits that will be applicable to the Yucca Mountain Repository will be in 40 CFR 197, which will be promulgated in the future. For this study the FEPs limits are assumed to be the same as that from 40 CFR 191 [3]. The Containment Requirements in 40 CFR 191 restrain the complementary cumulative distribution function (CCDF) at only two points, $m = 1.0$ and $m = 10.0$, is apparent (for detailed discussion, see Appendix B of this report). Despite this fact, the guidance-and-discussion sections of the Standard (EPA 1985, pp. 38070-38072) require that, if practical, the entire CCDF be constructed and exhibited as part of the formal assessment of compliance with Containment Requirements. The EPA recognizes that not all FEPs that may operate on or be present in a geologic waste disposal system need to be incorporated in the construction of the CCDF. The EPA offers specific guidance for determining the relevant agents to be included in the performance assessments:

> "The agency [EPA] assumes that such performance assessments need not consider categories of events or processes that are estimated to have less than one chance in 10,000 of occurring over 10,000 years. Furthermore, the performance assessments need not evaluate in detail the releases from all events and processes estimated to have a greater likelihood of occurrence. Some of these events and processes may be omitted from the performance assessments if there is a reasonable expectation that the remaining probability distribution cumulative releases would not be significantly changed by such omissions (EPA 1985, Appendix B)."

The above discussion identifies that the FEPs screening probability limit is 10^{-8} per year. If it can be shown that the probability frequency for postclosure criticalities is less than this limit, then the criticality FEPs screening arguments can be based on probability only. If the limit is exceeded then the screening arguments would need to be based on "risk" (consequences x probability, see Section 1.2).

2.2 NDCA Project Connection with INEEL Performance Assessment

The Nuclear Dynamics Consequences Analysis (NDCA) project is a component of the postclosure performance assessment of geologic repositories for the long-term containment of DOE-owned spent nuclear fuel (DSNF) packages. A performance

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2 Analyses of subcritical assemblies at k-effective ≤ 0.95 are currently being studied by DOE/RW analysts.

3 Previously 40 CFR 191 identified containment requirements for the YMS, but has since been remanded and will be replaced by 40 CFR 197. References ANS 1998, Clark 1998, and NRC 1995 have indicated that the FEPs probability screening limit for 40 CFR 197 is expected to be comparable to that of 40 CFR 191, namely that the probability limit for screening arguments is 10^{-8} per year.

assessment is a structured methodology to determine the long-term behavior of a geologic disposal system for nuclear waste. Formally, PA can be defined as a structured plan of investigation in which (1) features, events, and processes (FEPs) associated with the system are identified and ranked according to the degree that they affect system behavior, (2) the effects of significant FEPs on system performance are examined by means of mathematical models, taking into account all known uncertainties in model formulations and model parameters, and (3) the results of system performance, including the uncertainty of those results, are presented in probability distributions for system performance measures (EPA 1985, Rechard 1995a, Tierney 1995, Helton 1993; also see Appendix B).

A critical part of the PA methodology is called "FEP screening". FEP screening determines if each identified FEP plays an essential role in the performance of the system. The screening process proceeds by asking the following two questions for each FEP:

(1) Is the presence or occurrence of the FEP highly improbable?

(2) If the FEP is assumed to be present or may occur at some time during the period of performance of the system, would its presence or action cause only minor changes in normal system performance?

If the answer to either question is "yes," the FEP and its effects can be ignored in the PA model-building process (see Figure 1.2-1). The regulations also allow certain categories of FEPs to be eliminated (e.g., intentional intrusion into the repository).

The purpose of the analysis reported here is to provide a technical basis that can be used in FEPs screening arguments which are associated with a performance assessment for DOE-owned SNF in a geologic repository (Rechard 1998).

2.3 Caveats

A goal of this study was to identify generalized characteristics of postclosure criticalities, which is difficult because there are many variables. The results presented have a large number of significant caveats associated with them. Thus, this report serves strongly as a demonstration process. Many of the results clearly identify ranges of fissile mass and corresponding excursions that are important and because the computational results have corresponding quality assurance elements of transparency and traceability, they are acceptable for FEPs screening arguments.

The results presented in this report represent a parametric study in which a wide variation of input parameters were investigated. Thus, much of this parametric space may be null, lead to trivial solutions, or lead to results having a corresponding probability of occurrence that is not statistically significant. Because many of the supporting computations have a sizable amount of uncertainty associated with them, the user of this information must determine whether or not the present level of uncertainty is acceptable. Because of these and other major considerations, this section is presented to identify the concerns and limitations of data presented herein.

1. This report is intended for scientists and engineers with an elementary background in nuclear reactor physics. A scientist or engineer not familiar with elementary nuclear criticality should read references on criticality such as: ANS 1983, Koponen 1982, Knief 1985, O'Dell 1974, Paxton 1972 & 1980, Thomas 1979, and Smith 1981.

2. This report is not meant to be a "catchall" for nuclear criticality of DOE-owned SNFs in a geologic repository. This report is a "snapshot" of current parametric studies that were designed to identify the relative importance of key parameters of criticality. The calculations herein were designed to investigate a large parameter space. These parameter ranges are large enough to encompass nearly all combinations of interest for the disposal of DOE SNFs in a geologic repository located in a tuff host rock. Because the calculations presented in this report are automated in the RCS, additional computations can easily be performed by using the RCS setup. See Chapter 6 for discussion of RCS setup.

3. The quantitative uncertainties associated with the nuclear criticality of SNF in a repository are predominantly due to geoscience effects, not nuclear engineering features. For instance, if SNF package corrosion effects would never take place in a geologic repository, then nuclear criticality would be of no concern. This study does not integrate geoscience modeling/results into this report. The geoscience aspects of repository PA are the focus of a sister project (the INEEL 1997 PA, see Rechard 1997) that is being performed in parallel to this effort. The final results of the INEEL PA were not available for inclusion in this report (Rechard, 1998). It is strongly recommended that readers who intend to identify the overall risks from the nuclear criticality of DOE-owned SNFs in a geologic repository extract the net PA results (i.e., fissile mass, FM transport and reconcentration) and integrate them with consequence models from this study. For example, the maximum FM concentration could be conservatively compared with the FM/concentration limits identified in the "S-curves" within this report. The preferred method of analyzing the reconcentration of FM would be to use a sampling of criticality conditional scenarios of large complexity (i.e., conceptual models that have a significant coupling of geoscience physics), but this method requires a very detailed stochastic analysis approach. This approach will allow the identification of the probability and associated confidence level of attaining FM/concentration limits. Thus, the reader must not consider criticality from the point of view of identifying what aspects of criticality are "possible," but from the point of view of what is probable (with a weighting factor associated with the consequences of that scenario). More importantly, the reader should consider the comparison of criticality risks to other system risks (e.g., transportation, re-canisterization of SNFs, vitrification, etc.). This comparison needs

to be done in a framework using decision tools (i.e, using probabilistic cost/benefit analysis models).

4. In this report, the term *nuclear criticality* pertains to the consequences of nuclear excursions as attributed to risk in the long-term postclosure performance of a geologic repository containing SNFs. This report does not concentrate on *criticality safety* as it would apply to the operation of a nuclear facility. However, the computational methodologies for critical potential developed in this study can be applied to criticality safety (i.e., the 0.95 criticality safety limit).

5. This report does not address risk attributes that would apply to industry processes such as risk avoidance, risk transfer, risk reduction, and risk assumption. Risk, in this report, relates biological damage due to radionuclide doses to humans.

6. The Monte Carlo results (those obtained using the code MCNP) presented in this report were performed at an intermediate level of quality. In other words, they were obtained with minimal statistical accuracy, using 100,000 tallied neutron histories for each criticality calculation (typical standard deviations were on the order of +/- 0.001 to +/- 0.003 for typical 100,000 history runs). At present, it is suspected that the uncertainty associated with the 100,000 histories is small compared to data and modeling uncertainty. Typical high-fidelity calculations may exceed one million neutron histories for results with greater statistical accuracy, which may make the results more presentable to a regulatory agency. Since calculations in this report represent a parametric study, the 100,000-neutron-history level was used to allow an extra order of magnitude of variation in the parametric study. Thus, the results presented in this report could have an associated variance in the calculations could be significant. However, only limited sections of the calculations presented in this report would need to be reproduced at a high-fidelity for a regulator. Since the Monte Carlo calculations are automated within the RCS, performing high-fidelity calculations would not entail more set up time; only QA traceability would require any real level of effort by the analyst. It is strongly recommended that these final calculations be replicated through the RCS under a QA configuration management records system that insures the following QA goals: 1) traceability, 2) transparency, 3) technical reviews, 4) reproducibility, and 5) retrievability.

7. Significant computer resources may be required for static criticality calculations if detailed S-curves are to be generated as done for this study. As mentioned in "Caveat 6," the Monte Carlo (static) calculations were performed only at the 100,000 neutron history limit per individual eigenvalue calculation using the code MCNP. On a SUN Spark workstation, each of these calculations typically required 0.15 to 0.20 MB of disk space and from 20 to 120 minutes to run depending on CPU load. The CPU needs were significant. At various times during this study, the CPUs from 24 Digital Equipment Company (DEC) ALPHAs, 4 Sun WorkStations, 2 PCs, and a parallel CPU were used in combination to generate the data presented in this report. Each

criticality surface (3-D plot of the criticality eigenvalue as a function of FM and concentration) required from 300 to 1,000 computational runs. Figure ES-7 is an example of a typical plot. (Note that even though 300 to 1000 runs are batched for the criticality surfaces, not all of the data are significant or used in the plots.) In total, over thirty criticality surfaces were generated during the static criticality parametric study. This corresponded to more than 3 billion neutron histories; if all of the output files were to be saved, it would require disk storage on the order of approximately 5 GB. If only the net results, eigenvalues and associated uncertainties, are needed they could be post-processed with the RKeff code and the results table of results would require less than 1 MB. If future calculations need at a higher fidelity than that present here (at the FEPs screening arguments level) for QA or regulatory reasons, then only a small select set of eigenvalue calculations would be needed. These additional calculations would only be needed at the fissile concentrations at which minimum fissile mass is necessary for criticality. The results presented in this report identify theses regions of interest. More importantly, the results in this study identify that S-curves for near-field and far-field situations fall into major two groups: 1) those that have significant quantities of iron dispersed within them (such as rust/fissile slumps due to corroded waste packages) and 2) all other considered hostrock types. Also, during the development and trial calculations with the RKeff and MCNP codes several other hostrock materials were investigated (pure SiO_2, sandstone, saltrock, and other variations of tuff). The results indicated the following general trends:

1) Any materials that contain significant quantities of salt and iron will require very large fissile concentrations and mass quantities in order to achieve a critical geometry. These required fissile concentration values may not be possible due to natural causes and may be the basis for FEPs screening arguments.
2) The other media (SiO_2, sandstone, tuff, and concrete) required similar fissile concentrations, on the order of 10 kg/m^3 or greater in order to results in a critical assembly. Current conjecture is that the probability that concentration values of this magnitude occurring due to natural causes (geochemical precipitation) is unlikely, and even if they were to occur, the probability that a large geometrical zone (large enough to yield a critical assembly) is highly unlikely.

8. The computational results presented in this report were not performed in accordance with DOE/RW-0333P QA requirements. The results from this study were performed at a quality level necessary only for FEPs screening arguments. Thus, it was not necessary to save all of the code output listings generated from the static criticality (criticality potential) analyses. After the static criticality output was checked to determine if adequate statistical convergence (of the fundamental eigenvalue) was achieved, the output was postprocessed to extract the criticality eigenvalues and their estimated standard deviations. Output data was deleted if it did not yield any further usable information. However, computational "best practices" were used and enough

information is supplied for the reader to replicate the computational results or to use as a template for further analysis.

9. Proper scenario developments should be performed prior to the investigation of consequences of ad hoc criticality scenarios not presented in this study. This is important since it may be possible to generate a criticality scenario that results in significant consequences; however, it would not be realistic because it may be physically impossible to attain the initial conditions for that specific scenario.

10. The reader/user of the information in this study must recognize that the consequence results presented herein correspond to those necessary for PA consequence models and for the screening aspects of the Features, Events, and Processes (FEPs). These results are presented in a formalism used in 40 CFR 191. Even though 40 CFR 191 has been remanded for SNFs to be emplaced in a geologic repository, the requirements for such disposal (40 CFR 197, yet to be developed) do not currently exist, and it was deemed logical that 40 CFR 191 should be used as a template for generating FEPs and consequence results.

11. The static criticality analyses presented in this report used conservative geometries (spheres for far-field criticality and semi-hemispheres for near-field criticality). The amount of FM for other geometries using the same FM concentration can be computed by using the simple relationships for geometric buckling. Appendix L contains a discussion and an example of geometric buckling.

12. The static criticality analyses presented in this report used conservative FM compositions. For example, they do not take into account the neutron poisons in the fission yield products due to *burn up* of the spent nuclear fuels.

13. Overall prompt feedback coefficients were not calculated in this report. The procedure for determining these temperature-dependent coefficients would be to perform repetitive static criticality (eigenvalue) calculations using point-wise cross sections (for MCNP) processed at specific temperatures. The change in the eigenvalues as a function of temperature would yield the necessary coefficients. Thus, the nuclear dynamics presented in this report were performed as a parametric analysis with prompt feedback coefficients being varied over a large range. Since the vast majority of SNFs to be co-emplaced into a geologic repository have enrichments of less than 35 percent, the overall prompt feedback coefficient is guaranteed to be negative (Murray 1957 has indicated that for enrichments less than 35%, the Doppler coefficient is always negative.) The range chosen to be one order of magnitude larger than coefficients associated with commercial thermal reactors. The net results for excursions from this study clearly identified that the excursions result from a prompt reactivity insertion follow a simple scaling law in which the integrated number of fissions from small excursions directly related to three parameters (assembly mass, reactivity insertion, and prompt feedback coefficient). The results indicate that small

excursion consequences are expected over the range of parameters investigated and it is expected that for parameters outside of this current range the scaling law could be extrapolated since the scaling law is a simple power relationship.

14. The need for a detailed analysis of prompt feedback coefficients would only be necessary for very highly enriched SNFs. This would be the case for the disposal of excess weapons-grade plutonium (WGP) with approximately 94 percent enrichment. In such a case, the overall prompt feedback coefficient may initially be positive (indicating an autocatalytic power behavior) for small to medium temperature rises, after which it would become negative due to leakage from the system (indicating an auto-shutdown behavior). Because it has not been clearly identified at the present time that WGP would be disposed of in a geologic repository nor have these scenarios been generated to encompass the post-closure timeframe, neither the nuclear dynamics of WGP nor the identification of its prompt feedback coefficient is included in this study. Should the WGP scenarios be modeled, they would be expected to identify that the low solubility of ^{239}Pu and its decay to ^{235}U, with a short half-life, make it difficult to generate an assembly of ^{239}Pu when geological timeframes are necessary for corrosion, fissile movement, and reconcentration. Since the static criticality analysis is simple to analyze, criticality buckling searches ("S-curves") were generated for highly enriched plutonium for comparison purposes only.

15. The consequences results in this report were performed as a parametric study and did not specifically investigate very highly enriched fissile materials (enrichment on the order of 93 percent). Spent fuel elements with enrichments of this magnitude are complex to analyze because their prompt feedback coefficient is composed of three components: 1) thermal scattering (Doppler coefficient), 2) $S(\alpha, \beta)$ scattering kernel, and 3) non-leakage probability. The overall prompt feedback coefficient may be slightly positive (depending on reactor fuel/geometry design) until a limited temperature rise is experienced, after which the neutron from the system leakage (due to small changes in the fissile density and surface-to-volume ratio) increases sufficiently to shutdown the system. A concern for the disposal of highly enriched fissile material is the possibility for a large nuclear excursion. In order to experience such an excursion would require: 1) a significant quantity of relatively pure highly enriched fissile mass (essentially pure ^{235}U or ^{239}Pu in order to obtain a positive reactivity feedback due to Doppler), 2) rapid reactivity insertion rate, and 3) significant containment of the fissile material. Such a scenario has been postulated by Bowman 1995 & 1996, which analyzed weapons grade plutonium disposed in essentially pure SiO_2 and yielded explosion-type excursions. The model assumed conditions that highly unlikely since they assumed conditions that have not been proven to be possible in the YMS repository and thus they are not considered in this report. Fundamentally, the model is unlikely (or may not even be possible) due to the following reasons: 1) any HEU disposed in the YMS will be interspersed with LEU and HLW materials and commingled fissile material migrating from failed waste packages would result in significantly decreased enrichments (much lower than that

necessary to exhibit prompt positive Doppler feedback effects) than that used in the Bowman model, 2) disposed fissile in the YMS would not be subject to severe containment conditions which would be needed to prevent prompt negative leakage feedback effects, and 3) geologic events necessary to generate the assumed initial conditions may not be possible in the YMS.

16. There are two general classes of criticality scenarios involved with the SNFs: 1) the assembly of fissile material goes critical only due to the addition of water (moderator) and 2) a dry critical assembly. The analysis of the first class (a wet criticality) may also be influenced by delayed effects such as the void coefficient. One needs to remember that the void coefficient is a delayed effect, and prompt feedback effects would dominate the nuclear dynamics. Thus, a negative prompt feedback could be used to override a smaller positive (delayed) void feedback. For enrichments less than 35%, the prompt feedback is negative (Murray, 1957) and will prevent autocatalytic situations even in an over-moderated wet assembly. The analysis of the second class (a dry criticality) is complicated because of the geoscience modeling required as part of the scenario development. No references have been found to date that properly perform complete geoscience modeling that would lead to this conditional scenario. Thus, the dry critical assembly scenario is not addressed in this report. (Several references have postulated the possibility for a dry condition that may result from initiating wet critical events, but they have not yet a detailed analysis with geohydrology simulations modes/codes to prove this conjecture.) Also, over-moderated wet scenarios with large positive void coefficients are not addressed in this report because the scenario has not been properly developed.

3.0 CRITICALITY DEVELOPMENT

3.1 Overview of Criticality Development

This chapter presents a general discussion of effects on potential criticalities due to design engineered barrier system and anticipated degradation of these components over large time-scales. Figure 3.1-1 is a schematic showing waste packages placed in unsaturated tuff which is characteristic of the Yucca Mountain repository. The repository is located within unsaturated volcanic tuff (Topopah Springs Member). This location is approximately 350 m (1150 ft) below the surface and 230 m (755 ft) above saturated zone. Within the emplacement drifts will be a concrete liner and inverts (concrete) upon which the waste containers and their support systems are located (Figure 3.1-2). Typical waste containers (Figure 3.1-3) consist of two corrosion barriers; (1) an outer wall currently proposed to be constructed of corrosion allowance material (CAM, possibly carbon steel) and (2) an inner wall to be constructed of corrosion resistant material (CRM, possible a nickel based alloy such as Hastelloy C-22). Detailed information on the waste canisters and the geologic cross-section of the Yucca Mountain Repository can be found in Rechard 1997 and Rechard 1998.

It is expected that as water infiltrates the drift a series of four waste package degradation steps may occur. These degradation steps include the following:

Time 1: As the repository begins to cool down; water returns to host rock in the immediate vicinity. If present in sufficient quantity, the water may trickle down through the fractures in the host rock and drip on the waste container once the concrete liner begins to degrade.

Time 2: As the concrete liner continues to degrade the outer wall corrodes exposing the inner wall (CRM) to degradation.

Time 3: The inner wall (CRM) of the waste container corrodes and the fuel cladding (or canister) is breached. Water may then come into contact with the fuel assemblies and begin degradation of the fuel matrix.

Time 4: As the emplacement drift continues to collapse, two events may occur. The weight of the rock may crush the waste container and its fuel assemblies, exposing the fuel pellets directly to the near-field, and/or infiltration may impose further degradation of the cladding in which case the radionuclides in the fuel may be available for transport away from the immediate region.

The following three sections will discuss the various locations at which a critical assembly may occur. These locations correspond to: (1) internal, (2) near-field (within one tunnel diameter of the original waste container location), and (3) far-field (greater than one tunnel diameter away from the original waste container location).

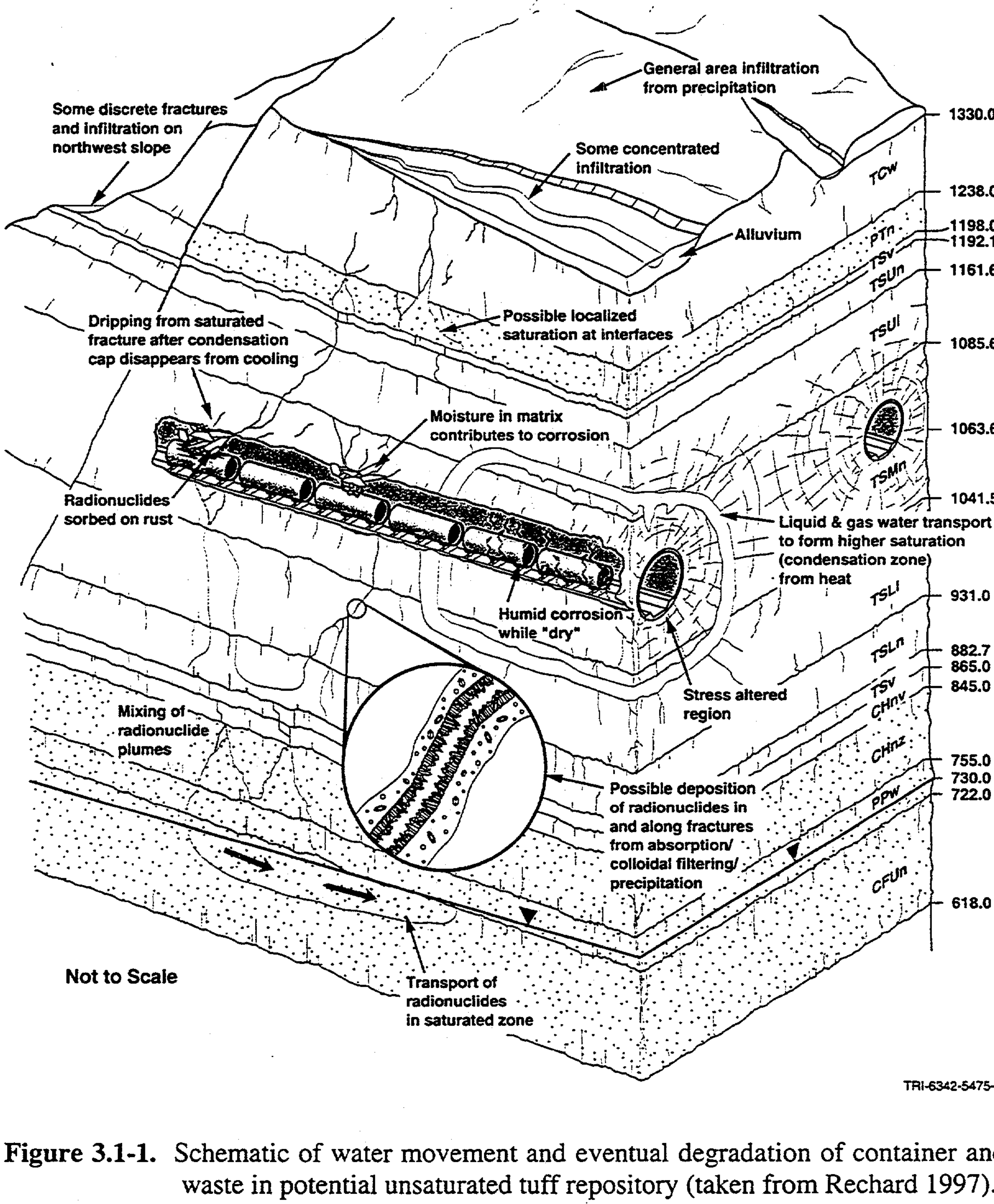


Figure 3.1-1. Schematic of water movement and eventual degradation of container and waste in potential unsaturated tuff repository (taken from Rechard 1997).

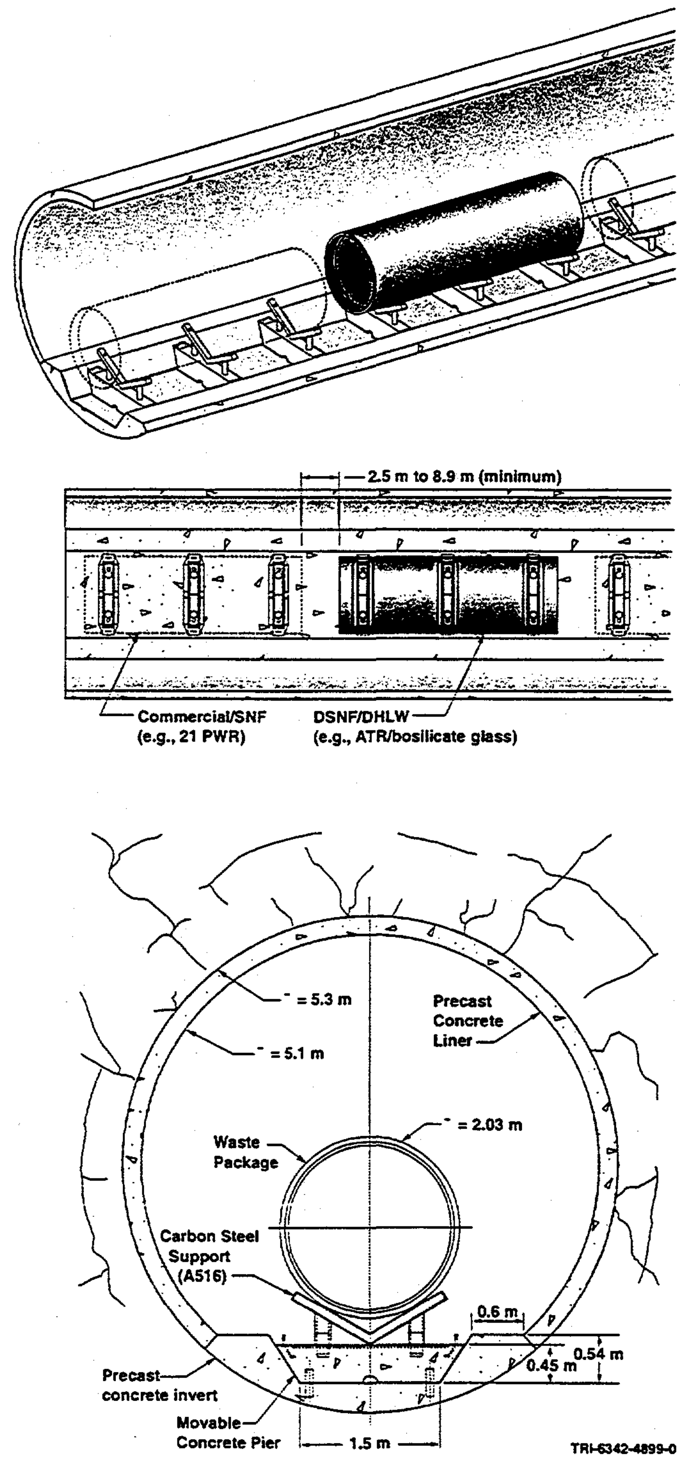


Figure 3.1-2. Orientation of waste packages (taken from Rechard 1997).

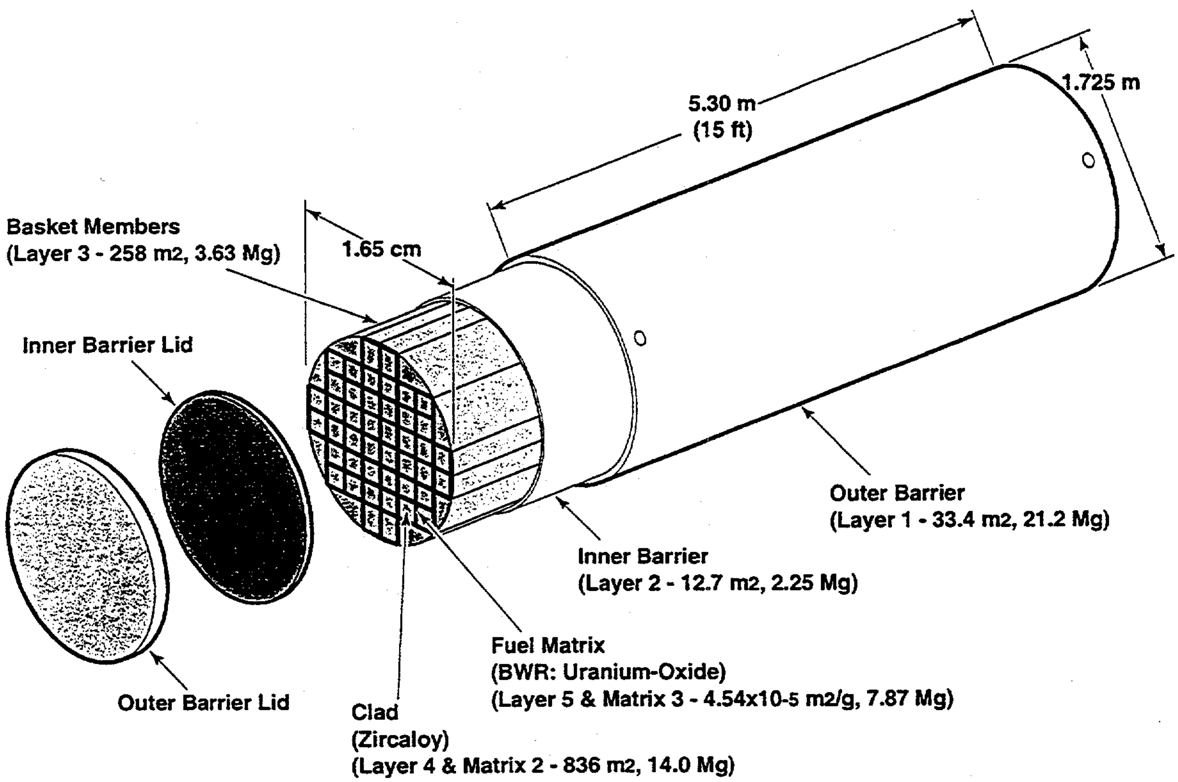


Figure 3.1-3. Category 15 spent fuel, represented by 44-BWR fuel assemblies, and disposal configuration (taken from Rechard 1997).

3.2 Introduction to the CX Model

The fundamental purpose of the Criticality Potential (CX) model is to identify the fissile material requirements needed in order to assemble a critical assembly. As can be seen in Figure 1.1.5-1, the CX model identifies the fissile mass and its corresponding fissile concentrations. These values are used by the UDX model, which identifies the number of fissions occurring in a critical excursion, and by the THX model, which identifies the frequency at which a critical assembly can repeat critical events.

3.2.1 Internal HLW/SNF Canister Criticality

Internal criticality was analyzed using existing criticality calculations that had been performed at INEEL. These criticality calculations will not consider groundwater intrusion rates (i.e., flooding of the underground waste repository as a result of inadvertent intrusion through exploratory drilling operations) or infiltration models driven by cyclic-type precipitation. The internal calculations only accounted for the case of sufficient water being present in the repository to corrode the waste packages. Probabilistic risk assessment (PRA) tools (see Chapter 6) were utilized with the internal model in an analysis to identify the probability frequencies for the initiation of a criticality. This PRA work is used along with the criticality consequences to identify the risks associated with criticality. It is postulated that corrosion of the waste packages could lead to two situations following package corrosion:

(1) Degraded: The SNF remains in roughly the same position as packaged, but sufficient neutron poison has been removed to allow criticality (e.g., neutrons 'cause' criticality, boron 'prevents' criticality). This model was studied with and without the grid structure spacers.

(2) Compressed: The structure of the internal package matrix is lost and the SNF collects together in the bottom of the container, either as intact elements or as a slurry, or distributed in a homogeneous, aqueous solution.

Since the nuclear dynamics (UDX) calculations were non-spatial (i.e., they correspond to a "point reactor model"), they are applicable to the *degraded* or *compressed* geometries.

3.2.2 Near-Field Criticality (Rust & Concrete Corrosion Slumps)

Near-field criticality occurs when the waste package has been breached by corrosion, and the fissile material is transported away from the original waste package region, but is in close vicinity to its original location. The fissile material is modeled in one of two geometries:

(1) Fissile material is intermixed with rust (the rust is representative of the corroded waste package).

(2) Fissile material has been dissolved, transported from its original location, and is deposited in the concrete inverts that comprised the floor of the repository.

The NDCA project considered only non-autocatalytic ("wet") critical systems for all the geometries studied. Under these circumstances the feedback mechanisms of the fissile materials exhibit a negative effect with increasing temperature. These thermal feedback mechanisms include: (1) Doppler temperature feedback and (2) non-leakage feedback due increasing the surface-to-volume ratio. Special calculations performed with the THX model (see Chapter 5) identified that post-closure repository criticality excursions would shutdown promptly due to thermal effects before any delayed moderator effects (negative or positive) could take place.

Autocatalytic criticalities are possible under very severe conditions of containment and concentration of fissile mass or possibly during over-moderated wet approaches to criticality. The term autocatalytic refers to using positive feedback mechanisms (hence, positive reactivity) to incur a continuous rapidly increasing power excursion that ultimately leads to an explosion. A non-autocatalytic system is associated with decreasing reactivity caused by physical changes such as: (1) the removal of the fissile material from the pore space of the host rock within the core region of the finite spherical model or (2) loss of moderation due to desaturation or moderator density decreases due to system heating in an under-moderated wet system. An autocatalytic criticality could be possible for weapons-grade materials. The direct disposal of weapons-grade plutonium (WGP) has been studied by others for geologic disposal and is a current option for the Yucca Mountain Repository, but is not considered in the NDCA. Thus, the NDCA calculations correspond only to non-autocatalytic situations. Also, since the thermal feedback effects occur prior to moderation changes (moderator void coefficient), the fissile assemblies modeled in this study would shutdown promptly for both over-moderated and under-moderated situations.

The "over-moderated" system defines a scenario wherein the neutron absorbing effect of the moderating material (e.g., water, heavy water, beryllium, etc.,) exceeds the material's moderating (slowing down of neutrons) contribution. In an over-moderated system, reactivity increases when the moderator material is removed from the pore space of the host rock within the core region of the finite model. Frequently over-moderated systems are termed as "wet systems" among hypothetical geological super criticality scenarios. Conversely, an "under-moderated" system corresponds to the case when the moderating effect exceeds the moderating material's neutron absorption capability. An under-moderated system is associated with increasing reactivity with the addition of the moderating material into the pore space of the host rock within the core region. Under-moderated systems are commonly denoted as dry systems in the literature.

The near-field geometries are modeled as hemispheres for rust/fissile scenarios and upside-down hemispheres for concrete/fissile scenarios. These scenarios are expected to assume a natural reactor environment which is a highly moderated, slow assembly.

3.2.3 *Far-Field Criticality (Precipitation in Volcanic Tuff Formations)*

Far-field criticality is the situation where the fissile material has been transported and collected in the silica-moderated tuff below the repository level. The geometry of the far-field nuclear dynamics consequence model is represented by a conservative paragon described as a spherical core surrounded by the reflector. Primary reasons for choosing a spherical model for the far-field NDCA calculations is that this geometry provides the "worst case" minimum critical mass. The fissile material physical geometry with the smallest ratio of surface area to volume will have the smallest critical mass (Glasstone, 1967: p.165). This spherical geometry adds significant conservatism to the far-field model NDCA calculations. The spherical geometry model is used to simulate a finite volume of leached radionuclides, or fissile materials (e.g., ^{233}U, ^{235}U, ^{239}Pu, ^{241}Pu, etc.) dissolved in water present in the fractures or pore space of the host rock. Therefore, four components will be modeled as the finite spherical system's core region: 1) fractures, 2) saturated host-rock, 3) water, and 4) fissile material.

The spherical core is modeled as a composite or mixture of host rock, water, and fissile material. The term "water" may also be substituted for moderator, since the water will moderate (or slow down) neutron activity. It should be noted that the presence of water in the repository is important for: (1) package failure, (2) moderation/reflection of fissile material and/or (3) dissolution/transport of fissile material. The reflector region is modeled as a concentric spherical shell encapsulating the host rock/moderator/fissile material core region. The reflector region consists of the host rock material alone and contains no fissile material. The reflector host rock material is assumed to be saturated at nominal saturation conditions (65 to 85%) and at ambient ground temperature conditions (GTC). Using the above described geometry, thermal-hydrology calculations were performed for selected nominal cases and analysis description and model results are presented in Chapter 5.

3.3 Description of Analysis (Codes: RKeff and MCNP™)

The CX model uses two major computational codes: RKeff (generated as part of the NDCA project) and MCNP (an existing industry standard code for neutral particle transport, Ref. Briesmeister 1988). The RKeff code was developed as a pre- and post-processor for eigenvalue (static criticality) calculations which identify the criticality potential of a fissile assembly. The code requires up to twelve input variables including: fissile mass, fissile concentration, model geometry shape, and saturation in the rock matrix. RKeff generates complete MCNP input files that are then used to identify whether an assembly of fissile material is subcritical, critical, or supercritical. Results are processed to identify critical fissile mass and concentration values necessary for given geologic conditions to result in a critical assembly. The critical mass and concentration values are then used in the THX, UDX, and DTHX models. The CX calculations were performed in a four-step process:

1) Perform k_{eff} Calculations

A 3-D MCNP model is generated for a baseline case study, which has a set of fixed parameters such as fissile material, enrichment, host rock type, and geologic quantities such as porosity and saturation. Then, for a fixed fissile concentration, a series of static criticality (eigenvalue) calculations were performed for various masses. These values can be plotted in a two dimensional curve termed a "criticality curve".

2) Generate Criticality Topomap

A new fissile concentration value is identified and the processes in Step 1 are repeated. This is performed for a multitude of concentration values and the results represent a two-dimensional parametric study of k-effective (k_{eff}) as a function of fissile mass and fissile concentration. The results can be plotted as three dimensional curves termed "criticality surfaces", which are accumulations of criticality curves. Typical results can be seen in Figure 3.3-1.

3) Perform Buckling Search and Generate Criticality S-Curve

Using results from Step 2, a criticality buckling search is performed. This corresponds to the identification of sets of minimum fissile mass and concentration values that are necessary to yield a critical assembly (i.e., k-effective = 1.0). Mathematically, the buckling search is performed by using Cubic Interpolating Splines (CIS) on computed data and finding the roots for $k_{eff} = 1.0$. The results can be plotted in a 2-D curve termed a "criticality S-curve". Typical results from this step can be seen in Figures 3.3-2 and 3.3-3.

4) Generate Criticality Saddle

A set of S-curves (from Step 3) can be obtained for a variation in a baseline parameter such as fissile enrichment. The results are plotted in a 3-D curve termed a "criticality saddle". Typical results can be seen in Figure 3.3-4.

From the above description it can be recognized that the development of criticality S-curves and saddles requires a large computational effort since each point on these curves corresponds to an eigenvalue search. In this study, key S-curves were generated for fissile material in near-fields consisting of rust and concrete host rock materials and also for far-fields consisting of Topopah Springs tuff host rock. These calculations are used to identify which fuels are capable of generating a criticality assembly. The masses for those situations that may yield a critical assembly are the basis for thermal hydrology and nuclear dynamic calculations.

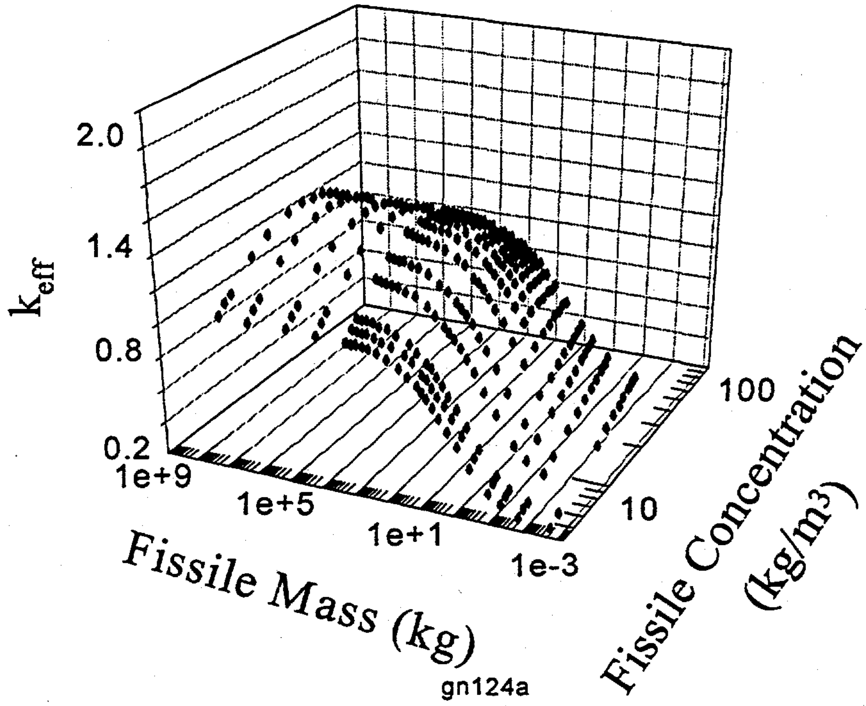


Figure 3.3-1. Typical far-field criticality surface for a selection of fissile concentrations. (data for 3% enriched uranium in Topopah Springs tuff at nominal geologic conditions).

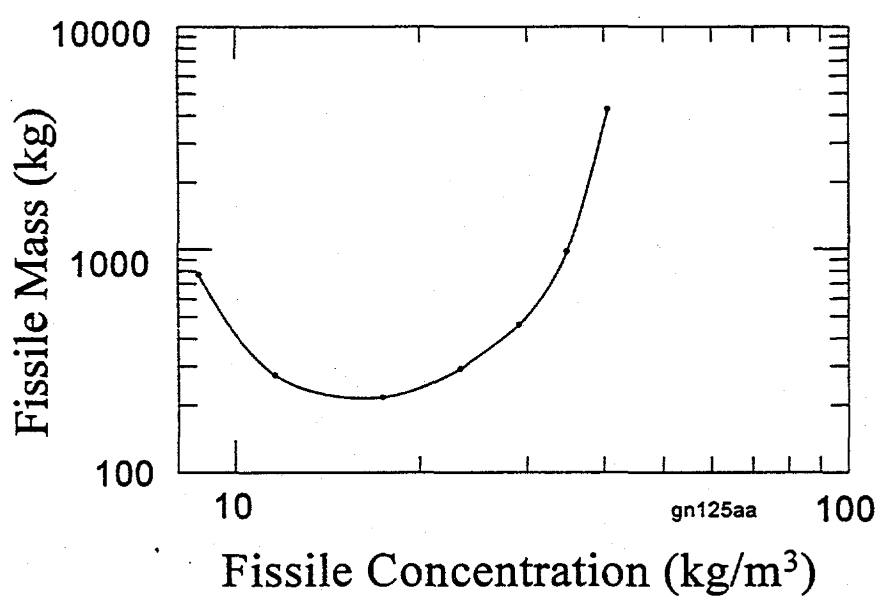


Figure 3.3-2. Typical far-field criticality S-curve (extracted from the criticality surface of Figure 3.3-1, data for 3% enriched uranium in Topopah Springs tuff at nominal geologic conditions).

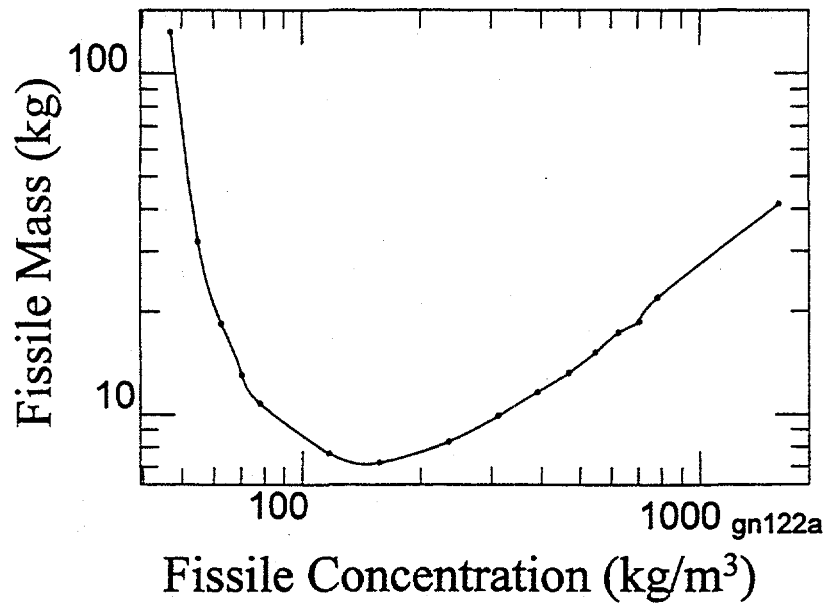


Figure 3.3-3. Typical near-field criticality S-curve (data for highly-enriched, ~80 %, uranium in rust at nominal conditions).

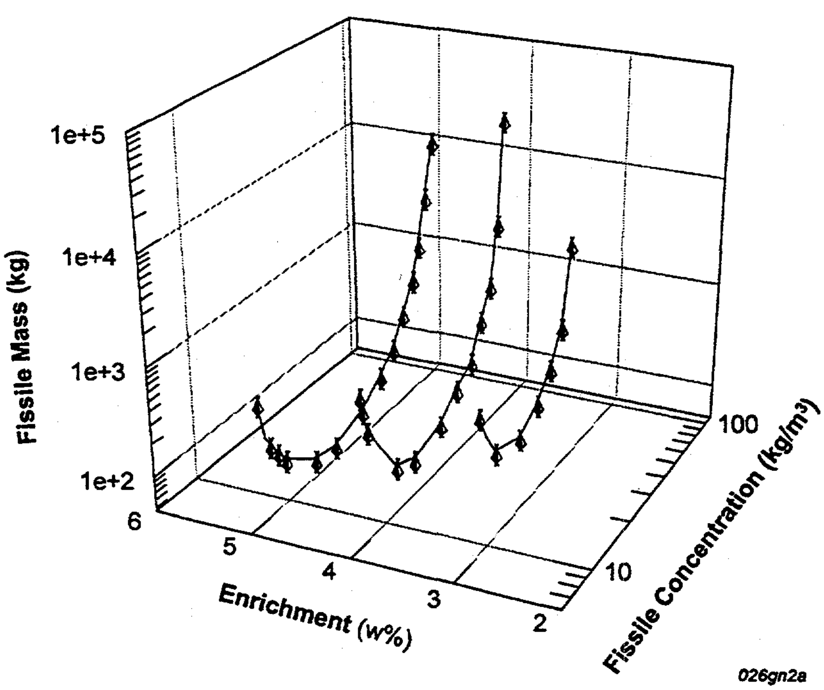


Figure 3.3-4. Typical criticality saddle generated from a series of criticality S-curves for various fissile enrichments (data for uranium in Topopah Springs tuff at nominal conditions).

Table 3.3-1 identifies the case studies selected for the criticality potential study of near-field and far-field criticality scenarios (internal scenarios were previously performed and net results are presented in Table 3.4-1). These baseline CX MCNP calculations were performed to identify fissile assembly masses and geometries which would result in a critical assembly (i.e., k_{eff} = 1.0) for expected groundwater saturation values (≈ 65 to 85%). Baseline CX calculations used nuclear cross-sections evaluated at ground temperature conditions to develop the "S-curve" for specific host-rock/fissile material/groundwater conditions. The S-curve which identify the relationship between the concentration of fissile mass (which is related to the moderator/fissile atom ratio) and the necessary total mass inventory required to yield a critical assembly. Each point on a "S-curve" corresponds to a "buckling search," where the first eigenvalue of the Boltzman transport equation (i.e., k_{eff}) is computed for a series of different masses from which the critical geometry can be estimated.

The far-field model baseline CX MCNP calculations used the geologic medium's standard saturation condition in the pore space of the "core" region (host rock-moderator-fissile material region). The critical mass and concentration corresponding to the far-field spherical radii of 0.5, 1.0, and 1.5 m for the "core" region.

There are an infinite combination of poison concentrations and semi-degraded SNF geometries that can yield a critical assembly in the near-field. Calculations will use two simple (and conservative) models to streamline the calculations in the near-field model baseline CX MCNP: (1) fissile material (less neutron poisons) in a slumped (hemispherical) geometry of rust and (2) fissile material (less neutron poisons) in a degraded concrete insert (modeled as upside down hemisphere). Calculations involving additional or other semi-degraded SNF geometries may be proposed in future work. Selected results obtained by using RKeff and MCNP are presented in Section 3.4.

Table 3.3-1. Criticality Scenarios and Fissile Materials Used for Parametric Static Criticality Calculations (a)

Run #	Fissile Assembly Characteristics						
	Host Rock				Fissile Material		
	Host Rock Type (Moderator Type)	Geometry	Reflector Type	Saturation (Porosity)	Source Type	Enrich-ment	Mineral Form
Near-Field Scenarios							
001	Rust (J-13 Well Water)	Hemisphere	TS Tuff	20% (20%)	Enriched U	5%	UO_2
002	"	"	"	"	"	10%	"
003	"	"	"	"	"	15%	"
004	"	"	"	"	"	20%	"
005	"	"	"	"	"	25%	"
006	"	"	"	40% (20%)	"	5%	"
007	"	"	"	"	"	10%	"
008	"	"	"	"	"	15%	"
009	"	"	"	"	"	20%	"
010	"	"	"	"	"	25%	"
011	"	"	"	60% (20%)	"	5%	"
012	"	"	"	"	"	10%	"
013	"	"	"	"	"	15%	"
014	"	"	"	"	"	20%	"
015	"	"	"	"	"	25%	"
016	"	"	"	80% (20%)	"	5%	"
017	"	"	"	"	"	10%	"
018	"	"	"	"	"	15%	"
019	"	"	"	"	"	20%	"
020	"	"	"	"	"	25%	"
021	"	"	"	100% (20%)	"	5%	"
022	"	"	"	"	"	10%	"
023	"	"	"	"	"	15%	"
024	"	"	"	"	"	20%	"
025	"	"	"	"	"	25%	"
026	"	"	"	"	"	80%	"
027	Concrete (J-13 Well Water)	Hemisphere	TS Tuff	100% (10%)	Enriched U	80%	UO_2
041	"	"	"	20%	"	5%	"
042	"	"	"	"	"	10%	"

Run #	Fissile Assembly Characteristics						
	Host Rock				Fissile Material		
	Host Rock Type (Moderator Type)	Geometry	Reflector Type	Saturation (Porosity)	Source Type	Enrich-ment	Mineral Form
Near-Field Scenarios							
043	"	"	"	"	"	15%	"
044	"	"	"	"	"	20%	"
045	"	"	"	"	"	25%	"
046	"	"	"	40%	"	5%	"
047	"	"	"	"	"	10%	"
048	"	"	"	"	"	15%	"
049	"	"	"	"	"	20%	"
050	"	"	"	"	"	25%	"
051	"	"	"	60%	"	5%	"
052	"	"	"	"	"	10%	"
053	"	"	"	"	"	15%	"
054	"	"	"	"	"	20%	"
055	"	"	"	"	"	25%	"
056	"	"	"	80%	"	5%	"
057	"	"	"	"	"	10%	"
058	"	"	"	"	"	15%	"
059	"	"	"	"	"	20%	"
060	"	"	"	"	"	25%	"
Far-Field Scenarios							
028	Topopah Springs Tuff (J-13 Well Water)	Sphere	TS Tuff	65% (13.9%)	Enriched U	0.8%	Uo_2
029	"	"	"	"	"	80%	"
030	"	"	"	"	"	1%	"
031	"	"	"	"	"	2%	"
032	"	"	"	"	"	3%	"
033	"	"	"	"	"	4%	"
034	"	"	"	"	"	5%	"
035	"	"	"	"	"	10%	"
036	"	"	"	"	"	15%	"
037	"	"	"	"	"	20%	"
038	"	"	"	"	"	25%	"
039	"	"	"	"	"	80%	"
040	"	"	"	"	"	100%	"

Table 3.3-1. Criticality Scenarios and Fissile Materials Used for Parametric Static Criticality Calculations (Continued)

Table 3.3-1. Criticality Scenarios and Fissile Materials Used for Parametric Static Criticality Calculations (Continued)

Run #	Fissile Assembly Characteristics						
	Host Rock				Fissile Material		
	Host Rock Type (Moderator Type)	Geometry	Reflector Type	Saturation (Porosity)	Source Type	Enrich-ment	Mineral Form
Benchmarks							
X1	Pure Water (Pure Water)	Sphere	Water	100% (100%)	Enriched U	100%	U
X2	"	"	None	"	"	"	"
X3	"	"	Water	"	Enriched Pu	100%	Pu

(a) See Appendix E for figures corresponding to these static criticality runs.

3.4 Results of CX Model

The results of the CX model are used for the identification of fissile masses, concentrations, and geometrical sizes which achieve criticality for a given input of repository and DSNF conditions (see Figure 1.1.5-1). Three criticality types were studied in this NDCA report each involving a different host matrix indicative to the Yucca Mountain geologic repository. The host rock materials studied were; (1) Topopah Springs Tuff, (2) rust (from the corrosion of the confinement canisters), and (3) concrete (from the floor of the repository). Each case was examined for a variety of water saturation values (J-13 well water) and for a variety of DSNF fissile uranium enrichments (wt% ^{235}U). Table 3.3-1 lists the scenarios investigated in this report by case number (CX number) and gives a brief description of key parameters and results for each scenario (further information on the static criticality calculations can be found in Appendix E). Figures 3.3-1 through 3.3-3 are typical examples of the resulting criticality surfaces and S-curves. A complete set of figures, for assemblies that could achieve criticality, can be found in Appendix E. A very important set of fissile mass and concentration values are obtained from the minima of each S-curve. These minima correspond to the minimum amount of fissile mass necessary to achieve criticality. Table 3.4-1 lists the approximate minima of the S-curves for each scenario by case number. Fissile mass and concentration values are also included in Table 3.4-1, which correspond to an over-moderated situation where the fissile concentration is roughly half of the value at the minimum. It is important to note that as the fissile concentration decreases from the minima, the fissile mass necessary for criticality increases dramatically. This information is valuable for future work to identify the probability of over-moderated scenarios.

The most important feature of the S-curves shown in Appendix E and values listed in Table 3.4-1 is that there are two general classes of fissile concentrations; (1) near-field assemblies with rust material and (2) all other near-field and far-field cases. Since the iron in rust has significant neutron absorption properties, the rust/near-field case require very large concentrations of fissile material (usually greater than 60 kg/m^3 or greater, see S-curves in Appendix E). These cases also require substantial fissile masses in order to achieve criticality, from as low as 7 kg (for HEU fuels) to several hundred kg (for LEU fuels). Even though the S-curves in Appendix E indicate that a critical assembly can be achieved with as low as 7 kg of fissile mass, it is very important for the reader to remember that this at absolute worst case conditions. This would require a homogeneous hemi-spherical geometry with optimal moderation and a very large fissile concentration. It could be possible to avoid these conditions by a multitude of methods (i.e., dilution of the HEU by co-disposal with non-HEU in a waste package, limitation of waste package design to ensure that the radius of degraded package slump does not approach the necessary size to achieve criticality, etc.,). The second general class of fissile concentration corresponds to concrete/near-field and tuff/far-field cases. For these cases, the concentration of fissile material necessary to generate a critical assembly is 6 kg/m^3 or greater. Even though this is an order of magnitude less that the rust/near-field case, it is very difficult to generate concentrations on this order of magnitude by natural causes (a concentration of 6 kg/m^3 is extremely large in natural analogs). The mechanisms (groundwater transport, dissolution, precipitation, etc.,) necessary to generate an ore body formation, of fissile material, are highly unlikely to occur at the Yucca Mountain Site (DOE-RW, 1998). Even if there was a non-trivial probability that the required concentration of fissile material could occur due to natural causes, there is an extra dimension to the problem. This other important factor is the associated probability for the size for a localized ore body formation (quantities of fissile masses from 20 kg to multi-hundreds of kgs, would also be needed in these cases). Thus, if a large concentration approaching the large values needed for far-field criticality could some how occur at the YMS, it would be very unlikely that a significant volume could be formed. Undocumented static criticality calculations for host rocks of sandstone and limestone generated S-curves nearly identical to those for concrete/near-field and tuff/far-field. These finding indicate the following general trend: Unless the host rock material contains significant neutron poisons, they will yield S-curves similar to those identified for concrete/near-field and tuff/far-field. This important finding can be part of the basis for FEPs criticality screening arguments. If the screening arguments for near-field and far-field criticality are based solely on fissile concentration, then the worst case concentrations would be these non-rust cases and further investigation of other host rock types are not necessary.

Run # (b)	Fissile Assembly Characteristics						
	Optimal Moderation (approximate) (c)					Over-Moderated (conc=½optimal) (c)	
	Host Rock Type (Moderator Type)	Enrich-ment [w %]	Mass [kg]	Concen-tration [kg/m^3]	Radius [cm]	Mass [kg]	Concen-tration [kg/m^3]
Near-Field Scenarios							
002	Rust (J-13 Well Water)	10 %	96.6	210.	47.8	103.	105.0
003	"	15 %	56.9	142.	45.8	187.	71.0
004	"	20 %	48.8	168.	41.1	69.0	84.0
005	"	25 %	43.3	158.	40.3	67.0	79.0
007	"	10 %	81.6	105.	57.2	>1000.	52.5
008	"	15 %	49.6	142.	43.8	153.	71.0
009	"	20 %	41.2	126.	42.8	134.	63.0
010	"	25 %	35.5	131.	40.1	271.	65.5
012	"	10 %	79.2	105.	56.6	>1000.	52.5
013	"	15 %	44.0	126.	43.6	167.	63.0
014	"	20 %	35.5	147.	38.6	88.	73.5
015	"	25 %	30.6	131.	38.2	158.	79.0
017	"	10 %	72.1	105.	54.8	~1000.	52.5
018	"	15 %	38.4	126.	41.7	171.	63.0
019	"	20 %	31.3	147.	37.0	68.	73.5
020	"	25 %	26.9	158.	34.4	39.	79.0
022	"	10 %	63.5	105.	52.5	>500.	52.5
023	"	15 %	34.7	142.	38.8	~90.	71.1
024	"	20 %	27.3	147.	35.4	52.	73.5
025	"	25 %	23.5	131.	34.9	75.	65.5
Far-Field Scenarios							
032	Topopah Springs Tuff (J-13)	3 %	216.	17.4	143.	767.	8.7
033	"	4 %	95.4	15.5	114.	431.	7.75
034	"	5 %	63.1	19.4	91.9	113.	9.7

Table 3.4-1. Select Results Derived From Parametric Static Criticality Calculations (a)

Table 3.4-1. Select Results Derived From Parametric Static Criticality Calculations (Continued)

Run # (b)	Fissile Assembly Characteristics						
	Optimal Moderation (approximate) (c)					Over-Moderated (conc=½optimal) (c)	
	Host Rock Type (Moderator Type)	Enrich-ment [w %]	Mass [kg]	Concen-tration [kg/m^3]	Radius [cm]	Mass [kg]	Concen-tration [kg/m^3]
035	"	10 %	31.5	15.2	79.0	79.	7.6
036	"	15 %	24.3	20.0	66.2	32.	10.0
037	"	20 %	21.3	22.9	60.6	26.	11.45
038	"	25 %	21.3	22.9	60.6	26.	11.45
Near-Field Scenarios							
041	Concrete (J-13 Well Water)	5%	53.	20.	109.	215.	10.
042	"	10 %	43.	21.	79.	77.	10.5
043	"	15 %	33.	24.	70	47.	12.
044	"	20 %	29.	19.	72	32.	14.5
045	"	25 %	26.	21.	67	31.	13.
046	"	5 %	47.	25.	97	120.	12.5
047	"	10 %	37.	21.	75	68.	10.5
048	"	15 %	29.	24.	67	41.	12.
048	"	20 %	25.	21.	65	43.	10.5
050	"	25 %	22.	24.	61	32.	12.
051	"	5 %	35.	20.	95	159.	10.
052	"	10 %	33.	21.	72	68.	10.5
053	"	15 %	25.	24.	63	37.	12.
054	"	20 %	21.	21.	62	40.	10.5
055	"	25 %	20.	26.	56	25.	13.
056	"	5 %	32.	20.	92	149.	10.
057	"	10 %	28.	21.	69	61.	10.5
058	"	15 %	21.	24.	60	34.	12.
059	"	20 %	19.	21.	60	38.	10.5
060	"	25 %	17.	26.	54	24.	13.

(a) See Appendix E for figures corresponding to these static criticality runs.

(b) NOTE, results for several runs are not reported because they did not achieve criticality. Those runs corresponded to enrichments that are not sufficient to yield a critical assembly.

(c) All values in this table were obtained visually and have an estimated uncertainty of +/- 15%.

4.0 NUCLEAR DYNAMICS (UDX/DTHX) MODELS

4.1 Introduction to UDX and DTHX Models

The fundamental purpose of the Nuclear Dynamics (UDX and DTHX) models was to identify the additional fissions resulting from criticality excursions in geologic media. As can be seen in Figure 1.1.5-1, the UDX and DTHX models use the fissile mass and its corresponding fissile concentrations determined from the CX model. Of the two dynamics models, only the DTHX model is fully-coupled to the thermal hydrology of the geologic media. This model uses the DINO code; a computationally expensive code. The DINO code was used only for three calculations, which were designed so the DTHX model could be directly compared to the UDX model, which requires much less computational effort. The calculations are intended to identify that the uncoupled nuclear dynamics model (UDX) is conservative and bounds the results from DTHX for nominal scenarios. Thus, the UDX model could be used for large sets of calculations. After the models were compared together, a multi-dimensional sensitivity (MDS) analysis was performed using the NARK code to characterize the influence of several input parameters and their importance in limiting a criticality event (or a rapid power excursion).

Transient analyses of nuclear excursions were performed for fissile material comprised of 100% ^{239}Pu and 100% ^{235}U. The calculations were performed for various combinations of fissile mass, initial system reactivity, initial power, fuel Doppler-temperature coefficient, and effective thermal neutron lifetime. Since these calculations are transient, the analyses correspond to a six-dimensional solution space with time being the sixth dimension. Selected results of the sensitivity can be found in Section 4.3 and Appendix E.

It is expected that nuclear excursions should shut-down due to negative prompt effects before delayed effects occur. Furthermore, even if the delayed effects are positive (but not greater in magnitude than the prompt effects) they would not significantly impact the excursion time coherence. If this conjecture is true, then the excursion results from the UDX model (prompt effects only) will give slightly conservative estimates for excursion results. Thus, the results from the UDX model give an upper bound estimate for the excursion consequences (for cases that have delayed negative feedback effects).

This phenomena is expected because prompt effects (mostly changes in the non-leakage probability and fuel-Doppler supplemented by moderator-Doppler) will act on a faster timescale than delayed effects (e.g. void coefficient of reactivity, which requires a thermally-driven groundwater desaturation mechanism). Thus, it is expected that prompt effects alone would result in the shutdown of rapid power excursions prior to any geohydrology effects. An important aspect of the prompt shutdown is that even if the void coefficient gives a positive feedback due to an over-moderated conditions, shutdown would still occur promptly. Since uncoupled dynamics calculations do not model thermal hydrology effects, they do not require significant computational time and the uncoupled dynamic model could be used extensively to investigate a multitude of conditions.

A short description of each of the nuclear dynamics models is shown below.

4.1.1 UDX Model (Uncoupled Nuclear Dynamics Model)

The UDX model uses the computational code NARK, which was generated as part of the NDCA project. This code was developed to determine the transient behavior (nuclear dynamics) of the neutron population in a critical assembly (uncoupled from groundwater effects) by using the "point-reactor" model (detailed discussion the point reactor kinetics model and it incorporation into the NARK code can be found in Chapter 10 of Rechard 1997b). Output from NARK is used to identify the power history of a nuclear excursion, total number of fissions from the excursion, and the duration of a single excursion. NARK uses modern self-adaptive and self-diagnostic numerical algorithms to solve sets of ordinary differential equations (ODEs). Input parameters include: fissile material type, delayed neutron lifetimes, half-lives of delayed neutron groups, initial conditions (power, reactivity, and select output from the RKeff code (e.g., fissile mass).

4.1.2 DTHX Model (Fully-Coupled Nuclear Dynamics Model)

The DTHX model is comprised of the THX and UDX models coupled together resulting in the code DINO. This computational code was generated from the NARK and BRAGFLO_T codes. It models fully-coupled (neutronics and repository response) far-field nuclear dynamics excursions. Since this computational code is large and is computationally intensive, it was only used for a small set of analysis runs. The output was compared to results from the UDX model and identified that the UDX results give conservative estimates of the transient behavior of the neutron population during an excursion. Thus, large parametric studies for excursion consequences could be obtained from the UDX model.

Calculations performed with the above models are not dependent upon the enrichment of the fissile material. However, it is known that the prompt feedback coefficient is always negative for enrichments less than 35% (Murry, 1957). Fissile material with enrichment above this value need to be investigated on a case-by-case basis. (Note, there currently exist experimental pulse reactors with enrichments greater than 90% that have an overall negative prompt feedback coefficients. Their fuel-Doppler may be positive, but their prompt leakage effects are strongly negative. The only way to limit the magnitude of the leakage effects would require strong containment or implosion boundary conditions.)

4.2 Description of Analyses

The nucleonics modeled in the NARK code (uncoupled to geologic responses) and the DINO code (coupled to geologic responses) was the simple "point reactor kinetics model." This model included one group corresponding to prompt neutrons and six groups for the delayed neutron precursors. The model also included eleven groups for the decay heat precursors (detailed discussion can be found in Chapter 10 of Rechard 1995b). The number of groups for either model could be changed to arbitrary group structures. For the NARK code, the thermal response was modeled as being an adiabatic process. This model uses only ordinary differential equations, which are easy to solve with self-adaptive numerical algorithms. It is expected that the uncoupled model would yield slightly conservative results compared to that expected from a fully-coupled model for under-moderated wet systems (this is also true for over-moderated wet systems if the delayed positive void coefficient is of less magnitude than that from the prompt negative coefficient). Thus three test problems were generated for use in comparing the two models. In total three selected test cases are present here as a quality check on the dynamics models. The first two are used to verify that "point reactor" model behaved appropriately for large and small reactivity insertions. The third test case is used to directly compare the UDX model with the DTHX model. The test cases are referred to as: 1) Nordheim-Fuchs Approximation, 2) small reactivity excursion, and 3) fully-coupled dynamics demonstration test cases.

The uncoupled nuclear dynamics multi-dimensional sensitivity (MDS) analysis was divided into two sets, ^{239}Pu and ^{235}U, and the NARK calculation sets were called "INEEL MDS SET ID N49" and "INEEL MDS SET ID N25". NARK input sensitivity parameter values for both the N49 and N25 MDS analyses are listed in Table 4.2-1.

Table 4.2-1. NARK Input Sensitivity Parameter Values for N49 and N25 MDS Analyses.

Sensitivity Parameter	Variable Name	Units	Values
Initial Power	N_e	W	1, $1x10^3$, $1x10^5$
Initial Reactivity	ρ_0	$	$1x10^{-4}$, $5x10^{-3}$, $1x10^{-3}$, 5 x 10^{-2}, $1x10^{-2}$
TFM Mass	M_{TFM}	Kg	10, $1x10^2$, $1x10^3$, 1 x 10^4, $1x10^5$
Doppler-temperature Coefficient	α_D	$\Delta k_{eff}/k_{eff}/K$	$-5x10^{-6}$, $-1x10^{-5}$, $-5x10^{-5}$, $-1x10^{-4}$, $-5x10^{-4}$
Effective thermal neutron Lifetime	l	Sec	$1x10^{-4}$, $2,5x10^{-4}$, $7.5x10^{-3}$, $1x10^{-3}$

As previously discussed, the "core" region is a composite or mixture containing fissile material, water, and the tuff host rock (for far-field media). Since the analysis corresponds to a "point reactor model", the results obtained for far-field geometries can also be used to estimate the expected behavior for internal and near-field geometries that have similar fissile quantities. For the MDS analysis, a fissile material volume fraction of the spherical geometry was chosen as a constant value of 0.35, and is similar to other thermal fissile material criticality calculations (see Table 4.2-2).

Assuming a fissile material density (TFM=^{239}Pu) ρ_{TFM} =19.70 x 10^3 kg/m^3, the fissile volume fractions (TFMVFR, ϕ_{TFM}) can be computed using the mixture radius, r_{mix}, and fissile mass, M_{TFM}, as:

$$\phi_{TFM} = \frac{3 \cdot M_{TFM}}{4 \cdot \pi \cdot \rho_{TFM} \cdot r^3_{mix}} \qquad (4.2\text{-}1)$$

Upon substitution of the Kastenberg 1996 ^{239}Pu loadings for various heterogeneous spherical core radii, the corresponding fissile volume fractions (TFMVFR, ϕ_{TFM}) were computed (see Table 4.2-2).

Table 4.2-2. The ^{239}Pu Loadings Used in the Kastenberg 1996 Thermal Fissile Material Criticality Calculations for Tuff Host-Rock (Rock Density = 2200 kg/m^3).

No.	Mixture Radius r_{mix} (cm)	TFM mass (kg)	TFMVFR	TFMMFR
1.	100.0	36.7	0.4438	0.7903
2.	200.0	254	0.3840	0.8481
3.	300.0	794	0.3556	0.8317
4.	400.0	1841	0.3489	0.8275

In a similar fashion, the corresponding fissile mass fractions (TFMMFR, ϕ'_{TFM}) for the various Kastenberg 1996 ^{239}Pu loadings (according to fissile volume fraction, mixture radius, and mass) were derived using the following equation:

$$\phi'_{TFM} = \frac{\rho_{TFM} \cdot \phi_{TFM}}{(1-\phi_{TFM}) \cdot \rho_{hostrock} + \rho_{TFM} \cdot \phi_{TFM}} \tag{4.2-2}$$

Since the NARK MDS calculations used a constant value of ϕ_{TFM}=0.35, and the input sensitivity parameter, M_{TFM} (fissile mass) was varied for each run, a unique mixture radius was computed from the formula:

$$r_{mix} = \left(\frac{3 \cdot M_{TFM}}{4 \cdot \pi \cdot \rho_{TFM} \cdot \phi_{TFM}} \right)^{1/3} \tag{4.2-3}$$

Discussion and quantification of the difference between fissile volume and fissile mass fractions (ϕ_{TFM}, and ϕ'_{TFM}) is necessary because the adiabatic heat loss model of the NARK code incorporates a mixture (or composite) of specific heat capacitance, $c_{p,mix}$. The mixture radius for a given composition (M_{TFM}, ρ_{TFM}, and ϕ_{TFM}) is "volumetric averaged" and can be computed by using Equation 4.2-3. In addition, the mixture density, ρ_{mix}, is also "volumetric" dependent and can be derived from the TFM volume fraction as

$$\rho_{mix} = \rho_{hostrock} \cdot (1-\phi_{TFM}) + \rho_{TFM} \cdot \phi_{TFM} \tag{4.2-4}$$

In the NARK MDS calculations, both the rock (tuff for far-field criticality analysis) and water content volumetric compositions were combined into the term, $\rho_{hostrock}$ to simplify the NARK input files. The value of $\rho_{hostrock}$ = 2273 kg/m^3 was held constant throughout the calculations, and is representative of the Topopah Springs Tuff composition of a fully saturated medium with 13.9 % porosity (void volume) $\left[\rho_{hostorck} = \rho_{tuff} \cdot (1-\phi) + \rho_{water} \cdot \phi\right]$ (Rechard, 1995b). In a similar fashion, the value of $c_{p,hostrock}$=1325 J/kg/K was also held constant throughout the NARK runs and was computed using the same volumetric composition averaging used in the host-rock density formula $\left[c_{p,hostorck} = c_{p,tuff} \cdot (1-\phi) + c_{p,water} \cdot \phi\right]$ (Rechard, 1995b). It should be noted that the "volumetric" averaging used to compute the combined rock + water specific heat capacitance is slightly incorrect, since it should have been "mass" averaged. However, since the reference was lacking any information regarding total mass, this value of $c_{p,hostrock}$ = 1325 J/kg/K, was determined as the best available.

The mixture specific heat capacitance, $c_{p,mix}$, is "mass dependent" and is dependent on the fissile mass fraction, ϕ'_{TFM}. This is a reasonable assumption since the essence of the point kinetics (or dynamics) model involves a zero-dimensional spatial regime and incorporates "lumped parameters". Therefore, a rigorous and correct mixture heat capacitance value used in all NARK MDS calculations, was computed from the equation:

$$c_{p,mix} = c_{p,hostrock} \cdot (1-\phi'_{TFM}) + c_{p,TFM} \cdot \phi'_{TFM} \qquad (4.2\text{-}5)$$

The total number of NARK MDS runs, for each of the N49 and N25 configurations, resulted in 1875 unique NARK calculations (NRUNS) for each configuration:

NRUN1 = number of unique initial power values (4.2-6)

NRUN2 = number of unique initial reactivity values

NRUN3 = number of unique TFM mass values

NRUN4 = number of unique Doppler-temperature coefficient values

NRUN5 = number of unique effective neutron thermal lifetime values

NRUNS = NRUN1 * NRUN2 * NRUN3 *NRUN4 * NRUN5

NRUNS = (3) * (5) * (5) * (5) * (5)

NRUNS = 1875

4.3 Fully-Coupled Nuclear Dynamics (DTHX) Demonstration Calculations (Comparison to Uncoupled Nuclear Dynamics)

Three fully-coupled nuclear dynamics calculations were performed using the code DTHX for comparison with an uncoupled nuclear dynamics calculation. The coupling mechanism involved linking the thermal-hydrology model (i.e. BRAGFLO_T/X-1.0) with the nuclear dynamics model (i.e. NARK). This coupling mechanism was incorporated into the DTHX code using two methods. The first method simply used temperature and saturation values (calculated from BRAGFLO_T/X-1.0) to dynamically alter the spherical heat generation zone material properties (e.g., composite density, composite specific heat capacitance, etc.). These composite material properties of the spherical heat generation zone (region where the nuclear criticality was modeled) were updated for each thermal hydrology calculation time step and then used in the temperature ordinary differential equations (ODEs) of the nuclear dynamics model (NARK). Since the Doppler feedback mechanism is temperature dependent, and the temperature ODE of the nuclear dynamics model uses a composite specific heat capacity (mixture of host rock, fissile material, and water), the thermal hydrology was coupled into the nuclear dynamics model. The second method (currently not implemented in the DTHX code) adds the void coefficient of reactivity effects resulting from the transient saturation behavior. Within the second method, the void coefficient of reactivity effects typically result in positive contributions to nuclear dynamics feedback mechanisms. Method one was used for this comparison and demonstration calculation. This was a reasonable approach since all the uncoupled nuclear dynamics calculations showed that the Doppler contribution to the nuclear dynamics feedback mechanism were prompt. The uncoupled nuclear dynamics (UDX) calculations revealed that the nuclear excursion time period was relatively short (less than 4 days). Thus, the saturation effects (i.e. void coefficient of reactivity) would not have time to contribute to the power excursion. This prediction was verified from the uncoupled thermal hydrology (THX) calculations. These THX calculations showed that the temperature "recycle" times were substantially less than the saturation "recycle" times.

For the three demonstration DTHX calculations, the thermal-hydrology model input parameters were identical to those used in the uncoupled nuclear dynamics calculations wherever possible. Initial saturations (S_0) of 100%, 85%, and 65% were used in the DTHX calculations and a initial saturation of 100% was used in the single NARK calculation. For all the demonstration calculations the host rock porosity (ϕ) of 13.9% was used. In addition, a thermal fissile material (TFM) mass of 50 kg within the heat generation zone was also constant throughout the calculations. The heat generation zone was modeled as a sphere and contains a mixture of fissile mass, host rock, and water. From knowledge of the expected fissile mass, and heat generation zone radius, the concentration (c) of the fissile mass in the heat generation zone (i.e., a sphere of radius equal to 1.0m) was computed as 4.188. Both the NARK and DTHX codes use a common definition of concentration equal to the fissile mass divided by the volume of the mixture of fissile mass, host rock, and water. The fissile material volume fraction (ϕ_{TFM}) of 2.197 x 10^{-4} was then computed from the relation $\phi_{TFM}=c/\rho_{TFM}$, where ρ_{TFM} is the constant fissile density (TFM= ^{235}U and ρ_{TFM} = 1.907 x 10^4 kg/m3). From the initial saturation (S_0) and host rock porosity (ϕ), the mixture density (ρ_{mix}) and mixture specific heat capacitance ($c_{p,mix}$) values for the heat generation zone were computed from the following relations:

$$P_{mix} = S_0 \phi \rho_{H_2O} + (1-\phi)\rho_{hostrock} \tag{4.3-1}$$
$$c_{p,mix} = S_0 \phi c_{p,H_2O} + (1-\phi)c_{p,hostrock} \tag{4.3-2}$$

The host rock density ($\rho_{hostrock}$), host rock specific heat capacitance ($c_{p,hostrock}$), water density (ρ_{H2O}), and water specific heat capacitance ($c_{p,H2O}$) used in all demonstration calculations were 2485.0 kg/m^3, 958.4 J/kg/K, 4217.0 kg/m^3, and 858 J/kg/K respectively (Rechard, 1996: pg. 24). The computed initial mixture density and specific heat capacitance values used in the demonstration calculations are property values are listed in Table 4.3-1. The nuclear dynamics model input parameters for the demonstration calculations are shown in Table 4.3-2.

Table 4.3-1 Initial Mixture Density and Heat Capacitance Values Used in DTHX Calculations

Calculation Type	Code	Initial Saturation (%)	ρ_{mix} (kg/m^3)	$c_{p,mix}$ (J/kg/K)
Uncoupled Nuclear Dynamics	NARK	100	2272.803	1324.901
Fully Coupled Nuclear Dynamics	DTHX	100	2272.803	1324.901
Fully Coupled Nuclear Dynamics	DTHX	85	2252.82	1236.977
Fully Coupled Nuclear Dynamics	DTHX	65	2226.176	1119.744

Table 4.3-2 Nuclear Dynamics Model Input Parameters

Description	Units	Value
TFM mass	kg	50.0
TFM volume fraction	dimensionless	2.196534x10^{-6}
Effective neutron lifetime, l	s	5.0 x 10^{-5}
Excess reactivity insertion, ρ_0(¢)	¢	10.0
Initial Power, N_0	w	1.0
Fuel-Doppler temperature Coefficient, α_T^F	k_{eff}/k_{eff}/K	-5 x 10^{-5}

The results of the demonstration calculations are presented as power histories and integrated energy histories in Figures 4.3-1 and 4.3-2. In addition, an expanded linear scale version of both the power and integrated energy release histories are *shown in* Figures 4.3-3 and 4.3-4. As seen from the power histories, the fully coupled nuclear dynamics model (DTHX) peak power response for all initial saturation values, is less than the peak power found from the uncoupled nuclear dynamics model (NARK). In addition, the integrated energy released history figures also reveal that the total energy released (in units of fissions) from all three fully coupled nuclear dynamics calculations is bounded by the uncoupled nuclear dynamics (NARK) model.

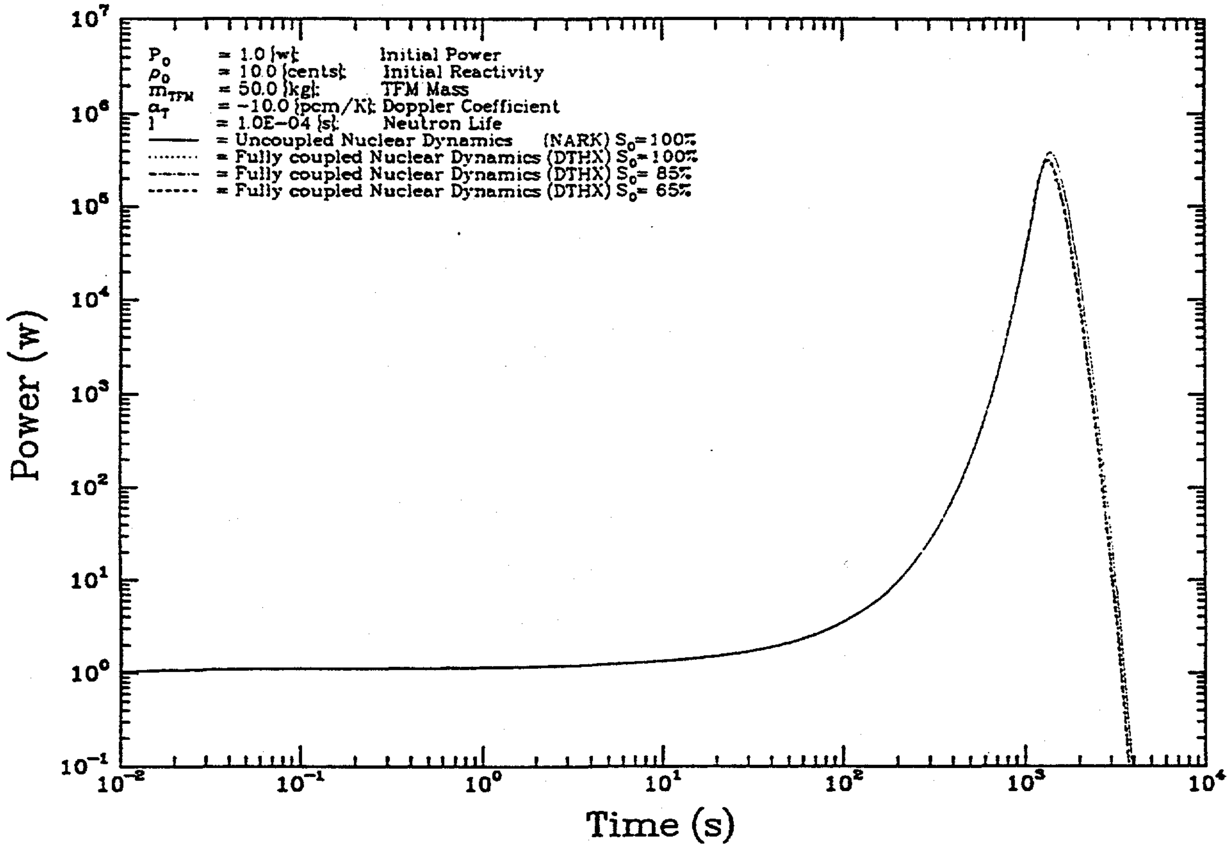


Figure 4.3-1. Fully-Coupled and Uncoupled Nuclear Dynamics Power Histories

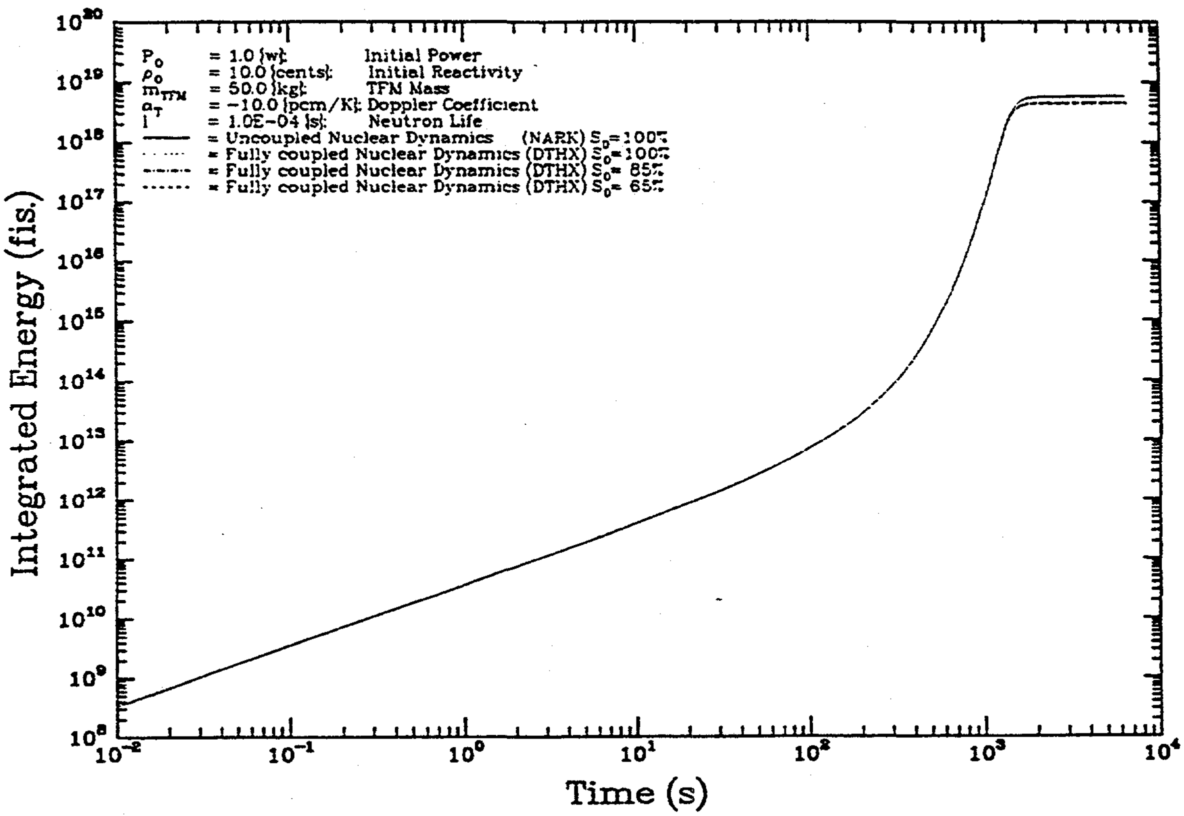


Figure 4.3-2. Fully-Coupled and Uncoupled Nuclear Dynamics Energy Histories

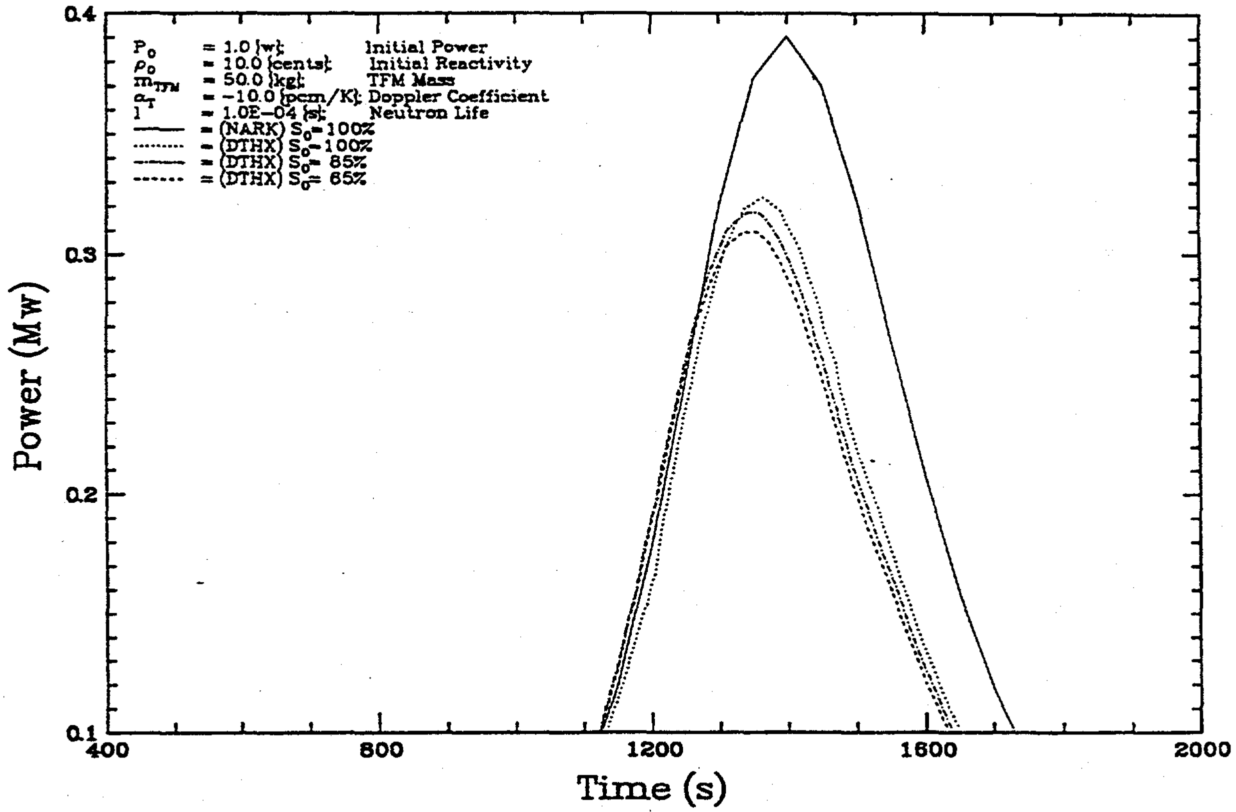


Figure 4.3-3. Fully-Coupled and Uncoupled Nuclear Dynamics Power Histories

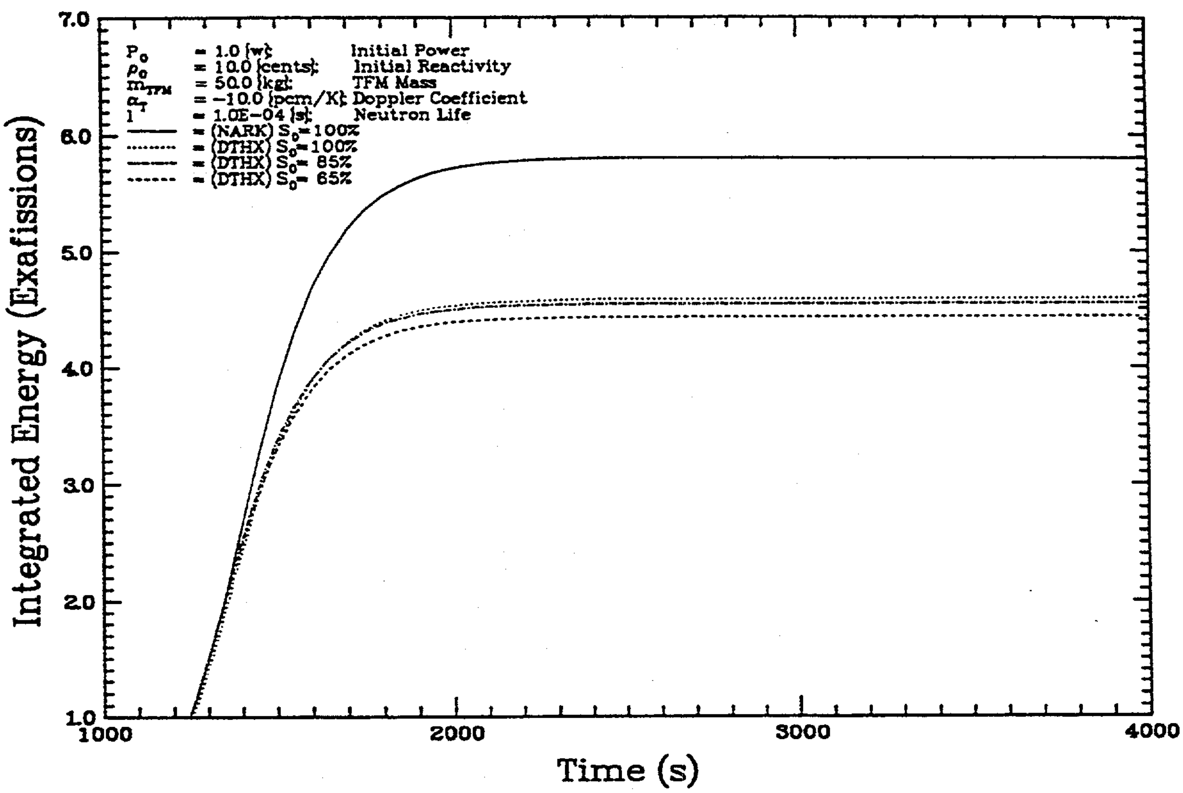


Figure 4.3-4. Fully-Coupled and Uncoupled Nuclear Dynamics Energy Histories

4.4 Results of the UDX Model (NARK Code)

Fuel-Doppler Temperature Effects on Reactivity [NARK]

A large number (3,750) of uncoupled nuclear dynamics calculations (UDX) were performed using the code NARK (see Equation 4.2-6 and Table 4.2-1) for both ^{239}PU and ^{235}U. This large number of calculations was easy to accomplish since the NARK uses self-adaptive ODE solvers. (NARK is a NucleAR Kinetics and dynamics code (see Appendix F) that uses modern ordinary differential equation (ODE, Gear 1971) solution algorithms to solve sets of "stiff" coupled ODEs that make the standard "point reactor kinetic" model (Keepin, 1965; Hetrick, 1971) that are common with nuclear dynamics models.) These calculations were all computed in a short time frame, approximately one day. As mentioned previously, these calculations corresponded to a full sensitivity analysis for the range of parameters identified in Table 4.2-1. However, most of the calculations yielded only trivial results, which had an integrated number of fissions less than 10^{17} (analysis performed by the THX model indicated that values less than ~10^{18} do not produced calculable temperature rises). Thus for simplicity, a single parameter sensitivity (SPS) analysis was also performed corresponding to only 162 calculations. Select results for the first block of sensitivity calculations are shown in Figure 4.4-1. This figure indicates that significant conditions (mainly fissile mass) are necessary to produce peak powers on the order of 100 watts. The key parameter used as input for the NARK model is the feedback coefficient. Table 4.4-1 identifies various fuel-Doppler temperature coefficients, α_T^F, that are typical of small experimental nuclear reactors and Table 4.4-2 lists the limited parameters used for the single parameter sensitivity analysis (see Appendix F for tabulated results for all 162 calculations). Comparison of the feedback values, for water moderated reactors, indicates that the range of coefficients listed in Table 4.2-2 should allow a good investigation of the dependence of excursion fissions upon the feedback coefficient. Even though this table identifies the feedback as being only due to the fuel-Doppler (the range of values for fuel-Doppler temperature coefficients: $-7.5 \times 10^{-5} \leq \alpha_T^F \leq -2.5 \times 10^{-4}\ \Delta k_{eff}/k_{eff}/K$), the NARK code uses this input parameter as an overall prompt feedback. Thus, if additional feedback effects (e.g. moderator-Doppler, non-leakage, etc.) were included, the overall feedback would be expected to a much larger negative effect. An important annotation needs to be made here; even if a fissile type were to have a positive fuel-Doppler (such as highly enriched uranium), the overall feedback coefficient would in most cases be negative. There are very stringent requirements necessary to yield a positive feedback effect (these are beyond the scope of this project). The most pronounced being containment, where in an underground repository this would require fissile material to somehow be transported into fractures or vugs and be deposited at extremely large densities. Only under these conditions could some containment characteristics be generated due to the overburden pressure and the disassembly equation of state of the host rock. Only in this incredibly unlikely event could increased excursion yields be generated. However, the probability for these occurrences is highly unlikely, resulting in net risks that would be expected to be less than nominal scenarios. Hypothetical autocatalytic scenarios have been studied and subsequently rejected in the open literature (within Section 9 there are a several citations on this scenario, which is not a subject of this study).

As previously mentioned in Section 4.3, the UDX (uncoupled nuclear dynamics) calculations yielded power excursions (rise and fall of power above initial power conditions), which yielded a range of output energies from 10^{17} to 10^{20} fissions. These results are similar to those input energy conditions used in the THX computations and are in agreement to open literature values for criticality accidents that occurred in processing plants and listed in Tables B.2-1 and B.2-2. The goal of the UDX model was determine post-closure repository criticality excursion energies (expressed in units of fissions) and compare them to the values in these tables, which can be identified to be in agreement.

From the k_{eff} vs. concentration curves for Topopah Spring tuff it was identified that a critical state could be achieved at a concentration of 5 kg/m³. Thus, three values of corresponding thermal fissile mass (TFM) were used to bound the UDX calculations: 25, 50, and 100 kg. Since the TFM volume fraction, ϕ_{TFM}, (ϕ_{TFM} = TFM volume/mixture volume) is related to the concentration, c, and the TFM density, ρ_{TFM}, a constant value of TFM volume fraction of 262.155 x 10^{-6} was computed from relation $\phi_{TFM} = c/\rho_{TFM}$. Using ^{235}U as the TFM (ρ_{TFM} = 19.070 x 10^3 kg/m³), constant values of ϕ_{TFM} were used throughout all UDX calculations. Since it was desirable to have a range on the sensitive input parameter, TFM mass (m_{TFM}), then a relation of the mixture radius (mixture of the host rock + water + TFM) can be found as

$$r_{mix} = \left[\frac{3m_{TFM}}{4\pi c}\right]^{\frac{1}{3}}. \qquad (4.4\text{-}1)$$

Thus, the mixture radii were computed as 1.0607, 1.3365, and 1.6839 m, which correspond to the TFM mass values of 25, 50, and 100 kg, respectively. The concentration, c, mixture radius, r_{mix}, and TFM volume fraction, ϕ_{TFM}, relations are displayed visually in Figures 4.4-1 (mixture radii, r_{mix} vs. ^{235}U concentration) and 4.4-2 (ϕ_{TFM} vs. ^{235}U concentration).

The host rock and water properties of the mixture used in the UDX/fuel computations were the same as those used in the MDS dynamics calculations: the density of host rock (Tuff) + water = 2273.0 kg/m³ (incorporates100% saturation of pore space with water); host rock (Tuff) porosity = 13.9%; and the specific heat capacitance of the host rock (Tuff) + water = 1325.0 J/kg (Rechard, 1995b: pg. 24).

Using all the sensitivity input parameters, a total of 162 (162 = 3·2·3·3·3) NARK calculations were run. Each UDX calculation was assigned as run ID as dxf0001 through dxf00162. Table F.2-2 lists the NARK run ID dxf0001 through dxf0162 sensitivity input parameters. Other key input parameters that were held constant or fixed (fixed input parameters) used in all the UDX calculations are listed in Table F.2-3. Table F.2-4 displays the maximum amount of integrated fissions (energy released) and the peak power achieved for each UDX/fuel run. Figure 4.4-1 corresponds to the first several runs identified in Tables F.2-2 and F.2-4 and displays the relationship between fissile mass, excursion power and the thermal mass. The output from the UDX calculations reveal how fast the power excursion is "shut down" due to fuel-Doppler effects alone. As seen in Table F.2-4, the maximum number of integrated fissions during an excursion ranges from 1.30×10^{16} to 5.54×10^{19}. Also, this table indicates that the maximum power achieved ranges from 7.64 to 3.62×10^{6} W and that the excursion times ranges from 3.17×10^{3} to 3.46×10^{5} s.

Regression analysis of the excursion energy values identified that the excursion energies are significantly dependent upon the initial power, assuming that excursions start from near zero power densities, and effective thermal neutron lifetime. Ranking analysis yielded scatter plots, of which Figure 4.4-4 is a typical example. Pattern recognition techniques ultimately resulted in Figure 4.4-5, which identified a simple relationship which yields the maximum integrated number of fissions. Thus it can be identified that there is a simple scaling law for excursions as linear function, in log-log space, of fissile mass, reactivity insertion, and feedback coefficient. The integrated fissions from an excursion is dependent on a single "quantity" of units: (cents-kg/pcm) which depends only on the three parameters. Because of the strong correlation between these parameters, parameter spaces slightly larger than that used to generate Figure 4.4-5 could simply be extrapolated. Thus, Figure 4.4-5 will allow future repository criticality investigators to avoid performing nuclear dynamic calulations.

Table 4.4-1. Doppler-Temperature Reactivity Coefficients

Reactor	**Effect**	**Reactivity Coefficient** *(dk/k/dT)*
CP-2[1]	Temperature	-1.0×10^{-4} /K
Brookhaven (graphite moderated)[1]	Overall Temperature	-4.0×10^{-5} /K
Brookhaven (graphite moderated)[2]	Fuel Temperature	-2.0×10^{-5} /K
Argonne CP-5[1]	D_2O Temperature	-4.0×10^{-4} /K
JEEP[1]	D_2O Temperature	-2.0×10^{-4} /K
PWR[1]	H_2O Temperature	-3.6×10^{-4} /K
Russian Light H_2O Research[1]	H_2O Temperature	-3.2×10^{-5} /K
SRE (sodium-graphite)[2]	Overall Temperature	$+1.2 \times 10^{-5}$ /K
SRE (sodium-graphite)[2]	Fuel Temperature	-1.4×10^{-5} /K
Calder Hall (graphite, gas-cooled)[2]	Temperature	-6.0×10^{-5} /K
MORE (organic moderated and cooled)[2]	Temperature	$+3.5 \times 10^{-4}$ /K
Shippingport (PWR)[2]	Temperature	-5.5×10^{-4} /K
Water Boiler (homogeneous)[2]	Temperature	-3.0×10^{-4} /K
EBR-I (fast)[2]	Temperature	-3.5×10^{-5} /K
Enrico Fermi (fast)[2]	Temperature	-1.8×10^{-5} /K
PWR (average)[3]	Temperature	-1.0×10^{-4} /K
LMFBR (average)[3]	Temperature	-1.0×10^{-5} /K
AGN 201-M[4]	Temperature	-3.6×10^{-4} /K
University of Wisconsin (TRIGA-FLIP)[5]	Fuel Temperature	-1.26×10^{-4}/K
Michigan Memorial Phoenix Project (Ford Nuclear Reactor)[7]	Temperature	-9.9×10^{-5}/K
Reactor	**Effect**	**A=Doppler Constant**† *(A = +T dk/dT)*
PHENIX (270 MW)[7]	Average Core Temperature	-3.6×10^{-3}
SUPERPHENIX[7]	Temperature	-8.0×10^{-3}
CRBR (350 MW)[7]	Temperature	-5.0×10^{-3}

† Doppler constant (A) is insensitive to temperature change, yet the effect is that the Doppler coefficient (*dk/dT*) will decrease as temperature changes increase.

[1]Stephenson, R., 1958. *Introduction to Nuclear Engineering* Second Edition. McGraw-Hill. New York. P. 328, Table 8-2; Experimental Values of Reactor Coefficients.

[2]Glasstone S. and A. Sesonske, 1967. *Nuclear Reactor Engineering*. Van Nostrand Renhold. New York. P. 257, Table 5.4; Reactor Temperature Coefficients.

[3]Profio, A. Edward, 1976. *Experimental Reactor Physics.* John Wiley & Sons, Inc. New York. Page 728.

[4]Biehl A.T., R.P. Geckler, S. Kahn, and R. Mainhardt, Editors. 1957. "Elementary Reactor Experimentation," *Aerojet-Nuclear Nucleonics*, University of California: Department of Nuclear Engineering, Berkely , California. Page 129.

[5](http://www.engr.wisc.edu/groups/rxtr.lab/UWNR.desc.html)

[6](http://www.umich.edu/~mmpp/fnr/power.html)

[7]Wilson, R., 1977. "Physics of liquid metal fast breeder reactor safety". *Reviews of Modern Physics*, Vol. 49, No. 4, October 1977. P. 898.

Table 4.4-2. NARK UDX Single Parameter Sensitivity Input Values

NARK Sensitivity Input Parameter	Units	Number of Sensitivity Input Parameters	Values of Sensitivity Input Parameters
TFM mass	Kg	3	25.0, 50.0, 100.0
TFM volume fraction	Dimensionless	1	262.155×10^{-6}
Effective neutron lifetime, l	S	2	1.0×10^{-4}, 5.0×10^{-4}
Excess reactivity insertion, $\rho_0(¢)$	¢	3	0.1, 1.0, 10.0
Initial Power, N_0	W	3	0.001, 0.1, 1.0
Fuel-Doppler temperature coefficient, α_T^F	$k_{eff}/k_{eff}/\mathrm{K}$	3	-7.5×10^{-5}, 10^{-4}, -2.5×10^{-4}

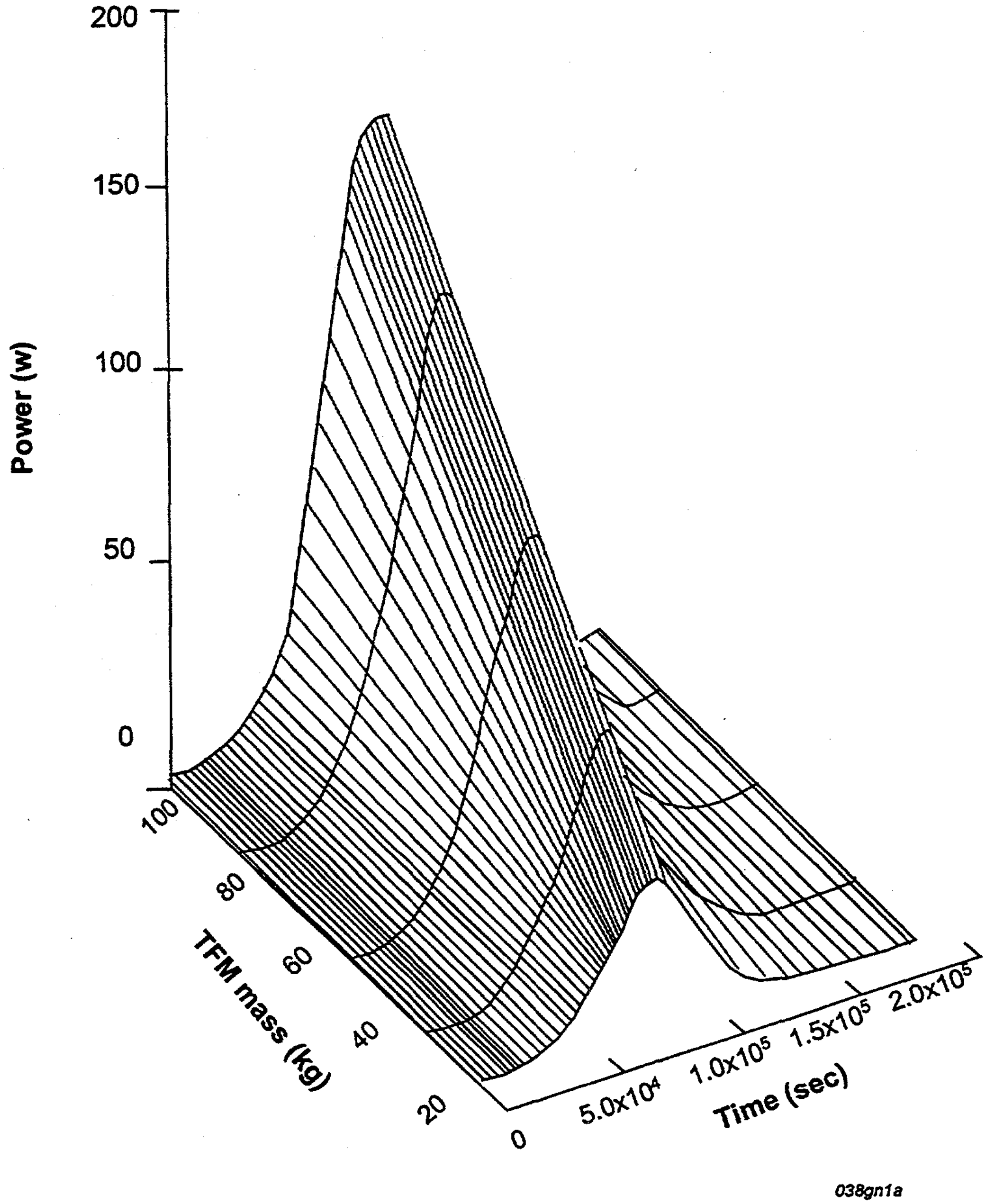


Figure 4.4-1. Select NARK results from computational runs dfx0001 through dfx0009 (see Appendix F for tabulated data).

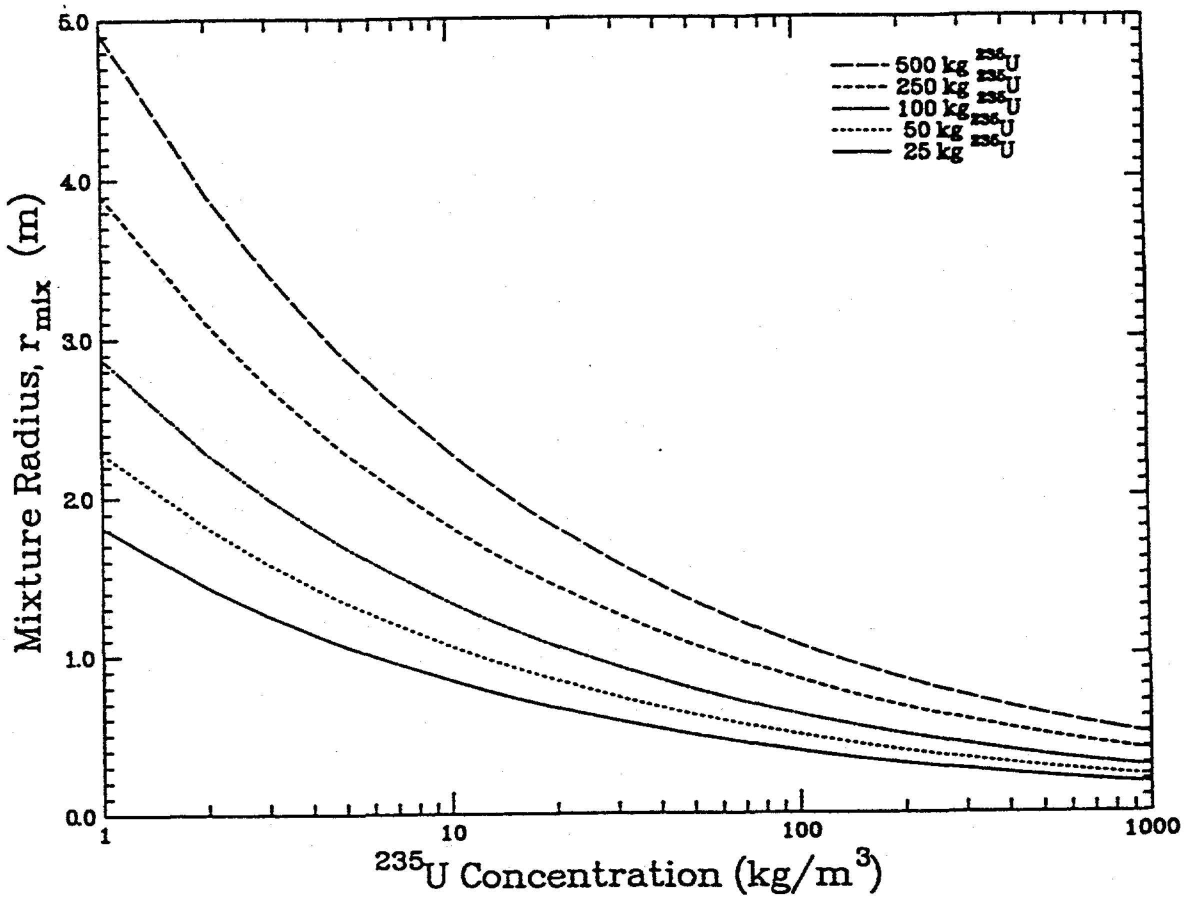


Figure 4.4-2. Mixture radii as a function of fissile concentration.

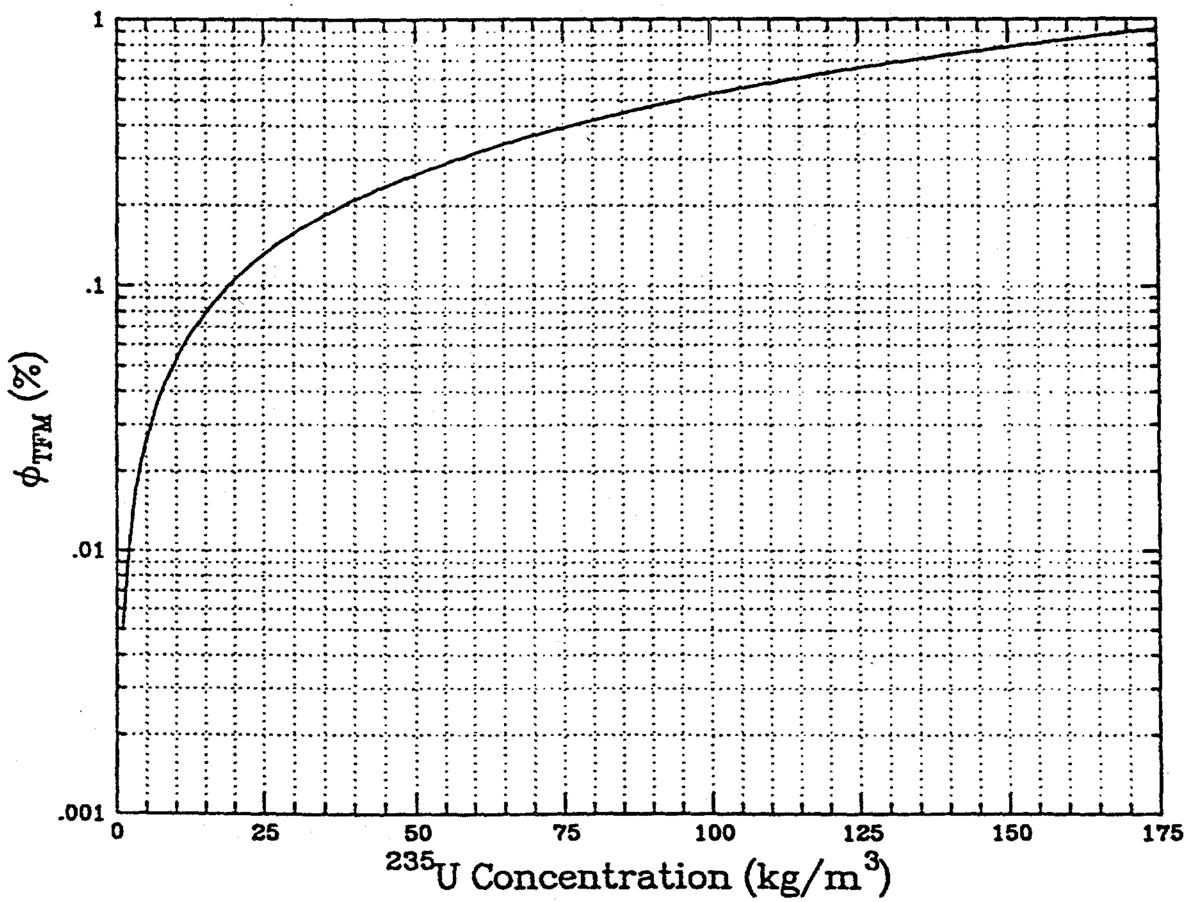


Figure 4.4-3. Fissile volume fraction as a function of fissile concentration.

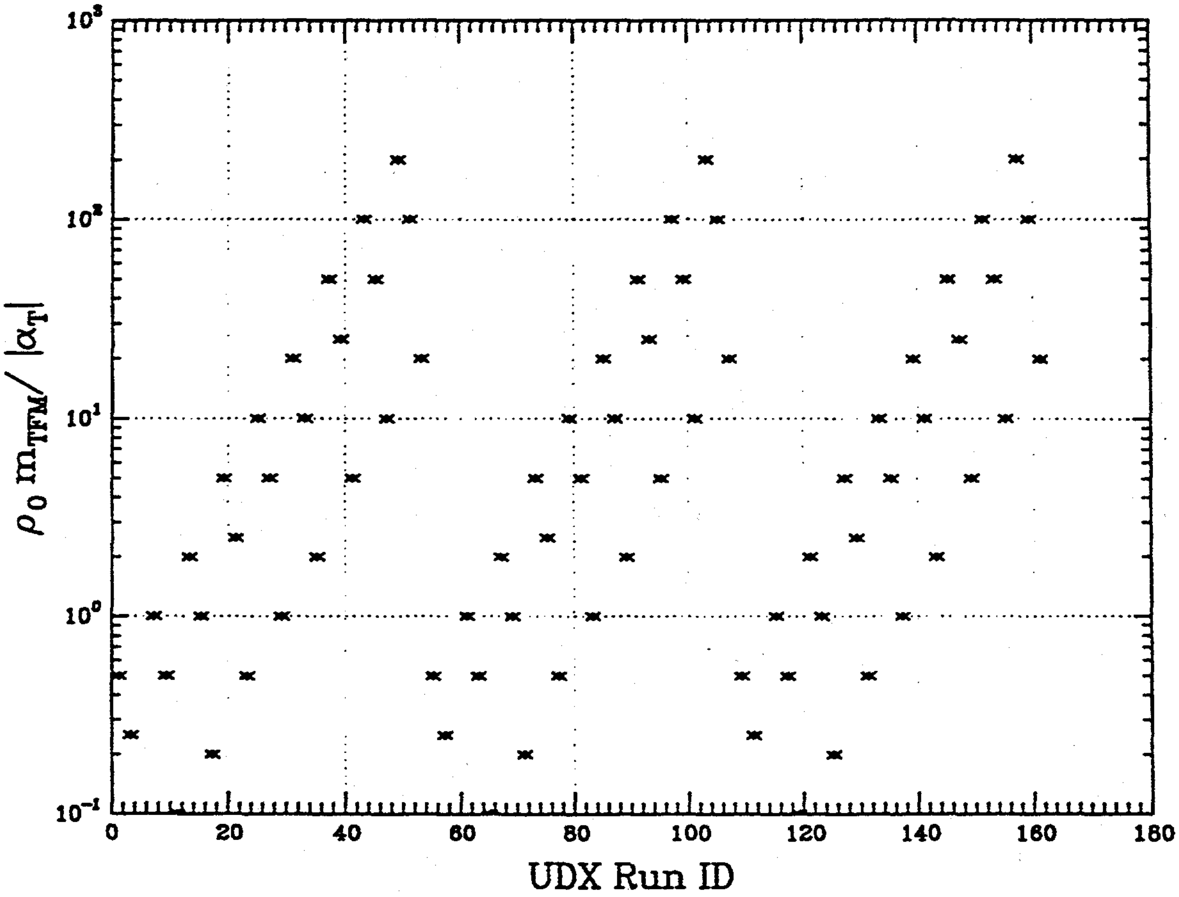


Figure 4.4-4. Example of a ranking scatter plot for UDX results.

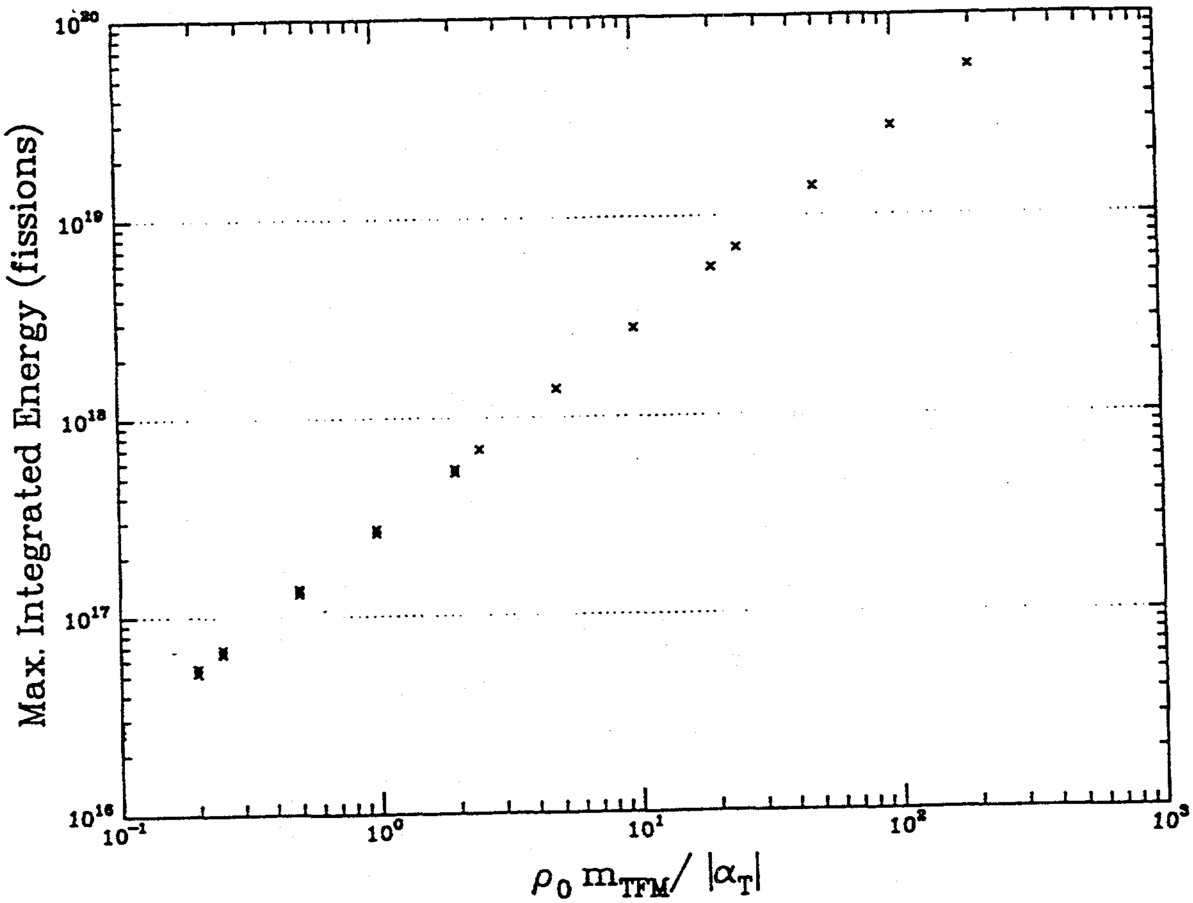


Figure 4.4-5. Relationship between excursion fissions and key nuclear dynamic input parameters (ρ_o = initial reactivity insertion [c], m_{TFM} = fissile mass [kg], and α_t = prompt feedback coefficient [pcm/K]).

5.0 THERMAL HYDROLOGY (THX) MODEL

5.1 Introduction to the THX Model

The fundamental purpose of the Thermal Hydrology (THX) model is to estimate the maximum frequency (cycle rate) for continuous criticality in a far-field scenario (which should be similar to that for a near-field case). This cycle rate corresponds to subsequently criticalities occurring only after an initial criticality has taken place. As can be seen from Figure 1.1.5-1, the THX model uses the fissile mass and its corresponding fissile concentrations determined from the CX model and the energy released from an individual excursion (expressed in units of fissions) from the UDX model. The THX model used an existing code (BRAGFLO_T, Rechard 1995b) that is used for two-phase groundwater flow analysis in geologic repositories. This model is complex to setup and run using the BRAGFLO_T code, hence, it was used only for 45 calculations. These calculations were designed so that the dependence of cycle time upon a wide range of excursion parameters could be investigated. The parameters used for these 45 runs and key results are presented in Section 5.3. These results are presented for a mixture of geologic media, moderator (water) and the fissile mass in the core region of a critical assembly. The larger of the two recovery times, to return to the initial temperature or saturation conditions, will determine the maximum frequency ("recycle time") for occurrence of continuous post-closure nuclear criticalities.

Limited discussion on the THX model and its results are given in this section, further discussion can be found in Ref. Rechard 1997 and Appendix G.

5.2 Description of Analysis

The NDCA study used the THX model to predict the geologic response (i.e., the temperature and saturation effects of a repository) resulting from a post-closure nuclear criticality. The criticality feature of concern here is the thermal pulse due to a rapid excursion. The THX model used a geometry corresponding to a far-field location where a heat generation zone (containing groundwater, volcanic tuff and fissile material) is at nominal conditions for porosity, saturation, permeability, etc. Results from the model are obtained for various excursion profiles, total energy releases, and zone dimensions. The code used in the THX model was BRAGFLO_T, which is a transient multi-phase (water and vapor) fluid and energy simulator. It has been used in repository performance assessments in its current form (Rechard, 1995b) and its isothermal form (WIPP, 1992a). The enhancements include the addition of the energy balance equation and the incorporation of thermal effects on both fluid and rock properties. The code also contains submodels that predict gas and water consumption/production as a result of waste package corrosion, and a submodel that predicts the energy released as the result of radioactive decay of the waste. BRAGFLO_T includes many features and solution techniques used in TOUGH2 (Pruess, 1991), such as effective continuum approximation for modeling fractured porous media, vapor pressure lowering due to capillary pressure and diffusive mass flux in the gas phase.

5.3 Results of the THX Model

The 45 THX calculations show that the temperature recycle time is much less than the saturation recycle time (see Figure 5.3.1 for an example set of results). This relationship between the two different recycle times indicate that prompt nuclear dynamics feedback mechanisms (such as Doppler broadening of neutron absorption resonance cross sections), due to the sudden increase in temperature, limit the duration of a criticality event. The quick shut down of a criticality event due to prompt feedback mechanisms mean that it is highly unlikely that positive delayed feedback mechanisms, such as positive voiding, could lead to a runaway (autocatalytic) criticality. Calculations of nuclear dynamics responses to temperature effects from the UDX model also indicate this effect. Comparison of UDX results for excursions times indicated that the time scale for criticality events are far smaller than the recycle times for saturation and also less than the temperature recycle times. THX results yielded temperature recovery times ranging from a minimum of 12.3 days to a maximum of 116.1 days, and saturation recovery times ranging from 129 days to 7978 days (see Table 5.3.1). These temperature and saturation recovery times can be used to determine a frequency for criticality events in a geologic repository. Naturally, a repeat of a criticality event after an initial criticality will not occur until both the temperature and saturation have returned to a condition where criticality is possible, in this case the period of criticality is the saturation recycle time. (However, for conservative bounding calculations, the temperature recovery time may be used as the criticality period.) One of the key finding, from the model was that for integrated excursion fissions less than 10^{18} fissions, the THX model yielded undetectable thermal results

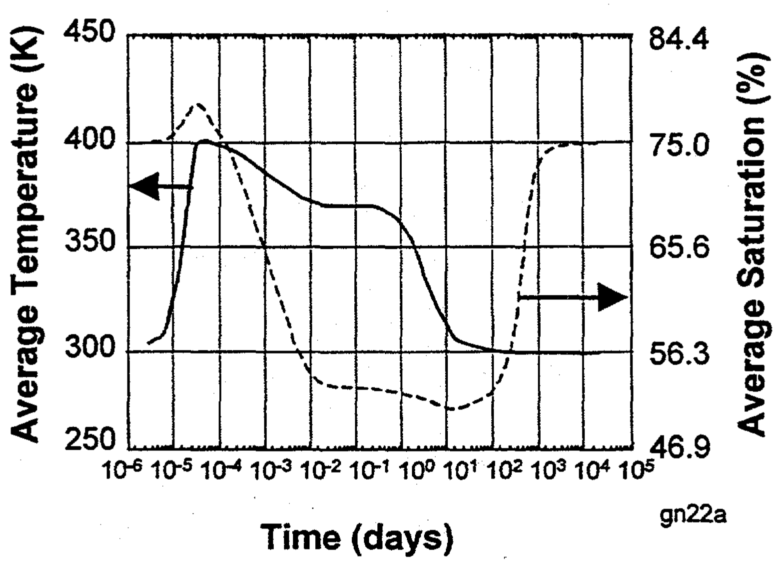


Figure 5.3-1. Typical thermal hydrology / groundwater transport computational results. (Data for uranium in Topopah Springs tuff at nominal geologic conditions.)

For purposes of estimating the nominal risks associated with criticality, the maximum criticality recycle frequency was set at 15 criticalities per year. The frequency value was given this large value in order to factor-in some of the uncertainty in the model. Much of this uncertainty resulted because the analysis performed with the THX model corresponded to an idealistic far-field geometry, corresponding to a spherical mixture of fissile mass, volcanic media and groundwater, which may result in an slight underestimation of the recovery times. Since it is conceivable that fractures may exist in the vicinity, they may accelerate the recovery of groundwater to initial saturation conditions after a criticality. Thus, the recycle frequency was increased to allow partial credit for effects due to fractures. (The probabilistic analysis of the influence of fracturing is complicated and beyond the scope of work for this project.)

The criticality recycle frequency was not identified for *in situ* or near-field-field geometries because not enough information was available during the development of the THX model to properly model these scenarios. For the purposes of the NDCA project, it was assumed that they would have recycle frequencies that are on the same order of magnitude as that for the far-field.

Table 5.3-1. Average Saturation and Temperature Recycle Times from THX Model

THX RUN ID	Initial Saturation (%)	Heat Generation Zone Radius (m)	Input Energy (fissions)	Space Power Density Function	Saturation Recovery Time {days}	Temperature Recovery Time {days}
THX001	65	0.5	2.0×10^{18}	Heaviside	2374.005	14.204
THX002	65	0.5	3.0×10^{18}	Heaviside	1115.635	13.413
THX003	65	0.5	4.0×10^{18}	Heaviside	2213.275	13.611
THX004	65	0.5	2.0×10^{18}	SIN()	2850.914	16.660
THX005	65	0.5	3.0×10^{18}	SIN()	919.392	14.279
THX006	65	1.0	2.0×10^{19}	Heaviside	1607.431	44.127
THX007	65	1.0	3.0×10^{19}	Heaviside	4013.646	45.480
THX008	65	1.0	2.0×10^{19}	SIN()	1618.611	47.930
THX009	65	1.0	3.0×10^{19}	SIN()	3895.995	45.865
THX010	65	1.5	8.0×10^{19}	Heaviside	5081.296	111.634
THX011	65	1.5	9.0×10^{19}	Heaviside	6933.507	94.204
THX012	65	1.5	1.0×10^{20}	Heaviside	7273.796	107.489
THX013	65	1.5	8.0×10^{19}	SIN()	5004.502	116.144
THX014	65	1.5	9.0×10^{19}	SIN()	6712.269	99.217
THX015	65	1.5	1.0×10^{20}	SIN()	7997.743	86.942
THX016	75	0.5	2.0×10^{18}	Heaviside	149.513	15.821
THX017	75	0.5	3.0×10^{18}	Heaviside	404.256	12.304
THX018	75	0.5	4.0×10^{18}	Heaviside	820.417	12.894
THX019	75	0.5	2.0×10^{18}	SIN()	188.209	15.745
THX020	75	0.5	3.0×10^{18}	SIN()	525.198	13.267
THX021	75	1.0	2.0×10^{19}	Heaviside	772.997	51.369
THX022	75	1.0	3.0×10^{19}	Heaviside	1918.715	42.781
THX023	75	1.0	2.0×10^{19}	SIN()	873.524	44.296
THX024	75	1.0	3.0×10^{19}	SIN()	1997.118	45.711
THX025	75	1.5	8.0×10^{19}	Heaviside	2565.012	104.124
THX026	75	1.5	9.0×10^{19}	Heaviside	3416.516	93.494
THX027	75	1.5	1.0×10^{20}	Heaviside	3843.009	104.000
THX028	75	1.5	8.0×10^{19}	SIN()	3335.428	105.360
THX029	75	1.5	9.0×10^{19}	SIN()	3673.391	96.771
THX030	75	1.5	1.0×10^{20}	SIN()	3746.042	109.385
THX031	85	0.5	2.0×10^{18}	Heaviside	143.065	12.438
THX032	85	0.5	3.0×10^{18}	Heaviside	207.259	14.994
THX033	85	0.5	4.0×10^{18}	Heaviside	285.475	12.518
THX034	85	0.5	2.0×10^{18}	SIN()	128.725	13.919
THX035	85	0.5	3.0×10^{18}	SIN()	207.758	15.778
THX036	85	1.0	2.0×10^{19}	Heaviside	510.316	46.315
THX037	85	1.0	3.0×10^{19}	Heaviside	1063.277	41.191
THX038	85	1.0	2.0×10^{19}	SIN()	559.147	50.027
THX039	85	1.0	3.0×10^{19}	SIN()	874.119	43.526
THX040	85	1.5	8.0×10^{19}	Heaviside	1373.831	94.379
THX041	85	1.5	9.0×10^{19}	Heaviside	1426.597	111.408
THX042	85	1.5	1.0×10^{20}	Heaviside	1633.287	99.411
THX043	85	1.5	8.0×10^{19}	SIN()	1321.771	98.666
THX044	85	1.5	9.0×10^{19}	SIN()	1416.979	91.375
THX045	85	1.5	1.0×10^{20}	SIN()	1798.900	102.680

6.0 PROBABILISTIC (PRA) MODEL

6.1 Introduction to PRA Model (SLAM & Event Trees)

This chapter presents net findings from a preliminary probabilistic risk assessment (PRA) used to estimate rough order of magnitude (ROM) values for the probabilities of nuclear criticality for DOE-owned spent nuclear fuel (DSNF) at Yucca Mountain. At the present time, the modeling of the probability for criticality scenarios within the Yucca Mountain repository have not reached a high level of maturity. The set of system submodels important to nuclear criticality (corrosion allowance material – outer canister material, corrosion resistant material – inner low corrosion rate canister material, fuel cladding, etc.,) have not all been adequately modeled to the extent that probabilities for criticality can be determined accurately. Although there is a good confidence in the existing PRA methodology, there is not enough resolution in current PA models, especially corrosion, to adequately determine waste package degradation probabilities that could lead to a criticality.

The PRA calculations presented in this section were generated the computational code: SLAM. This computational tool is currently being replaced with the computational code SAPHIRE (NUREG 1994) along with the use of newer climate models (which were not available when the SLAM calculations were performed). Since all the PRA model results form the SLAM code will be discarded in the near future, only limit discussion will be presented in this report. This section will only present net results from the PRA/SLAM modeling effort and Appendix H will present an abbreviated discussion of key findings from the PRA/SLAM calculations. The PRA results presented in this report should be considered to be "place saver" values until updated results are presented in the near future. Even though these PRA results are only ROM values, they are vital for estimating risks. As will be identified in Section 7, the computed risks values, even though they only first-order estimates, clearly indicate that the risks due to post-closure criticality are not significant.

The present PRA/SLAM results, using assumed upper limit probabilities for modeling parameters, identify that criticality may occur in the *in situ* or the near-field over a 100,000-year period (only under high water infiltration rates) and is very unlikely in the far-field. Far-field criticalities are very difficult to generate since reconcentration of transported fissile material would require very exceptional conditions to occur. The preliminary PRA presented a rough estimate of approximately two *in situ* or near-field criticalities occurring per 100,000-year period when experiencing high water infiltration periods (i.e. glacial conditions). These criticalities are not of major concern because they would result in only a very small increase in the fission yield products. The quantity (magnitude) of these additional fission yield products is so small that when these values are integrated into the source term radionuclide inventory, their contribution would be orders of magnitude less than source term inventory values at time of repository closure. Thus, their contribution would be lost in the round-off. As mentioned in Chapter 1, since the initial source term for the radionuclide source may only be accurate to only two significant decimal digits, it was deemed logical for this study that nuclear criticality FEP consequences could be screened out at the 1% (of the initial source term) level (see

Figure 1.1.3-2). Furthermore, the additional fissions are so small that it may not be possible to identify their dose or risk impacts to the overall system. Within Appendix H, event trees (special case of fault trees) are presented for "short- term" and "long-term" infiltration that may result in a criticality event.

In Appendix H key results can be found in Tables H.1-1 and H.1-2 and H.1-3. Table H.1-1 identifies subcritical mass limits for the major DOE fuel types. In this table, criticality is credible only if more than 97% of the chromium boride is in the borated stainless steel matrix is removed. This would occur if the chromium boride is removed from between fuel elements or if borated plates are not installed, see Appendix H. Table H.1-2 identifies the fraction of DOE packages (column #4) that may potentially lead to a criticality for non fissile-mass packing limits of 14.4 kg (HEU), 42 kg (MEU) and 200 kg (LEU) based on packaging constraints and slurry criticality calculations with major loss of boron - - neutron poisons. A synopsis of probability frequencies determined with the PRA/SLAM model are listed in Table 6.1-1.

It is important for the reader to understand that even though preliminary criticality analysis results (probabilities) are presented in this chapter and Appendix H in event tree/fault tree format, the results were obtained by using a simulation code. In general, event tree/fault tree PRA methodology are not capable of modeling the detailed performance of geologic repository and predict probabilities for conditional scenarios leading to criticality. The reason is that many of the event probability distributions are a function of time and have conditionally dependent event-timing. However time-dependent conditional scenarios can be modeled in Monte-Carlo simulation codes (in the time domain). The calculation of the distribution for the time-to-failure values of the waste packages were done with "SLAM" which is a simulation code. In total 313,100 trials (100 per DOE package) were run in the Monte-Carlo simulations. Post-processing of these simulations was then conducted to estimate generalized probabilities for key events. The best logical method to display these events is the event tree/fault tree format. For simplicity, these results are displayed and discussed in Appendix H in terms of event trees. The criticality probabilities determined in the PRA analysis are considered to be rough order of magnitude (ROM) values. Consequences would then be less than the round-off error of the radionuclide source term values. Thus it is expected that criticality consequences are expected to be technically insignificant.

Table 6.1-1. Key Results Obtained from Preliminary Probabilistic Risk Assessment of Criticality Scenarios for Spent Nuclear Fuels in the Yucca Mountain Site		
Item	**Description**	**Numerical Value (if applicable)**
1a 1b	Expected number of criticalities under "present conditions" (i.e., short term infiltration rates comparable to predicted values over the next 300 to 500 years). (Probabilities assumed to be uniform between the first year and 100,000 year). Probability of short-term criticalities on a per annual basis.	$7.\text{x}10^{-2}$ casks 7.10^{-7}/yr
2a 2b	Expected number of calculations under "glacial conditions" (i.e., long term infiltrations). Probability of long-term criticalities on a per annual basis.	2.2 casks $2.2\text{x}10^{-5}$/yr
3	In order for criticality to occur, these conditions are needed: (1) significant amounts of water must be present, (2) more than 97% of the boron used for criticality control would need to be removed (note, the probability that water ingress from the surface and into the package, and removed of all the borated stainless steel is very unlikely to occur within the first 10,000 years after emplacement), (3) the fuel type must be one of the following: (A) ATR-Aluminum, (B) N-Reactor, or (C) Triga Flip.	
4	For in situ geometries, it is not possible to achieve criticality for the following in situ configurations: (1) unpoisoned structure (loss of boron but iron oxide supports fuel elements). (2) collapsed fuel rods (borated stainless steel supports corroded and collapsed, fuel rods still intact). (3) Slurry (all components have lost integrity and structure) – if all the boron (neutron poison) is somehow contained in the slurry with concentration > 3% of initial inventory.	

6.2 Results of PRA Study

Due to their size and complexity, and the fact that are currently being updated and will soon be out of date, the fault trees used as input for the PRA/SLAM model are not presented in this report. The net results of the PRA study using those fault trees are: (1) the maximum expected probability for criticality is $2.2x10^{-5}$/yr for long-term infiltrations corresponding to continuous glacial conditions and (2) a probability of $7.0x10^{-7}$/yr for infiltrations corresponding to continuous "present conditions" (see Table 6.1-1). These low frequencies of occurrence are important because the nuclear dynamics calculations in Section 4.4 indicated that the net fissions, and their corresponding increase in fission yield products (contribution to radiological source term), is also very small (the number of fissions per excursion is on the order of 10^{17} to 10^{20} fissions). To illustrate that the consequences due to criticality are small, Table 6.2-1 was constructed to determine the additional fissions and their impact on the radionuclide source term. In this table one can see that a wide range of probabilities for an initial criticality are displayed. The first two values (7.0×10^{-7}/yr and 2.2×10^{-5}/yr) correspond to short-term and long-term infiltration and the last two (1.0×10^{-3}/yr and 1.0×10^{-1}/yr) are presented for comparison purposes. (A.) The later comparison numbers were chosen as a test case to illustrate even large probability frequencies will yield insignificant results. A range of 10^{18} through 10^{20} fissions per criticality was used for nominal fissions expected from excursions. This number is based on a series of uncoupled nuclear dynamics (UDX) calculations performed with the NARK computer code and presented in Section 4.4. These values also are comparable to values that occurred in previous criticality accidents in the U. S. and in Russia (see Table B.2-1 and B.2-2). Also included in Table 6.2-1 are factors that identify the numbers of additional criticalities which might follow an initial criticality. The first factor is the amount of time assumed for repeated criticalities. The range is limited to 100 years, thus implying that is expected that geohydrology conditions are assumed to not remain the same for more than 100 years. The second factor is the assumed rate that is varied over a range of 5 to 100 criticalites per year (a conservative range, with a nominal value selected as 15 criticalities per year). If time scales longer than 100 years need to be investigated, values already existing in Table 6.2-1 could be directly scaled since these values correspond to a linear system. This range is based on values presented in Section 5.3. From that section, results of thermal geohydrology calculations (THX) performed with the BRAGFLO_T computer code are presented for various conditions. The results indicate that after a nominal criticality excursion, the immediate zone will experience a temperature rise and desaturation of the groundwater. The computational results indicate that the ground temperature recovers (returns to initial conditions) prior to the groundwater saturation recovery. The recovery times indicate that few criticalites would occur per year. This analysis is only for far-field geometries. Since thermal hydrology calculations have not yet been performed for in-situ geometries, the range for the rate of repeated criticalites is assumed to be comparable to that of the far-field (i.e., 1 to 10 criticalities per year, upper bounded at 15 criticalities per year).

In Table 6.2-1 nominal values for short-term infiltration are shown in bold. These values indicate an addition of 5.30×10^{15} fissions per year added to the source term (see Figure

7.2-1) would be a typical expected increase due to short-term infiltration scenarios (with frequency probability of 7.0×10^{-7} criticalites per year). The table also presents results corresponding to frequency probabilities of (1) 2.2×10^{-5} (long-term infiltration), (2) 10^{-3} and (3) 10^{-1} criticalites per year.

Table 6.2-1. Additional Fissions Due to Criticality of DOE-Owned Spent Nuclear Fuels

Probability of Initial Criticality (a) (crit/yr)	Number of Fissions per Criticality (b) (-)	Assumed Duration of Constant GeoHydrology (c) (yr)	Additional Fissions in DOE SNFs (fissions/yr) (bold values are nominal values used in Figure 1.1.5-1) — Assumed Rate of Repeated Criticalities (d) (criticalities/yr) 5.	10.	15.	25.	100.
			(fissions/year)				
7.0E-07 (short-term infiltration)	1.0E+17	10	3.50E+12	7.00E+12	1.05E+13	1.75E+13	7.00E+13
		50	1.75E+13	3.50E+13	5.25E+13	8.75E+13	3.50E+14
		100	3.50E+13	7.00E+13	1.05E+14	1.75E+14	7.00E+14
		500	1.75E+14	3.50E+14	5.25E+14	8.75E+14	3.50E+15
		1000	3.50E+14	7.00E+14	1.05E+15	1.75E+15	7.00E+15
	5.0E+18	10	1.75E+14	3.50E+14	5.25E+14	8.75E+14	3.50E+15
		50	8.75E+14	1.75E+15	2.62E+15	4.37E+15	1.75E+16
		100	1.75E+15	3.50E+15	**5.25E+15**	8.75E+15	3.50E+16
		500	8.75E+15	1.75E+16	2.63E+16	4.38E+16	1.75E+17
		1000	1.75E+16	3.50E+16	5.25E+16	8.75E+16	3.50E+17
	1.0E+20	10	3.50E+15	7.00E+15	1.05E+16	1.75E+16	7.00E+16
		50	1.75E+16	3.50E+16	5.25E+16	8.75E+16	3.50E+17
		100	3.50E+16	7.00E+16	1.05E+17	1.75E+17	7.00E+17
		500	1.75E+17	3.50E+17	5.25E+17	8.75E+17	3.50E+18
		1000	3.50E+17	7.00E+17	1.05E+18	1.75E+18	7.00E+18
2.2E-05 (long-term infiltration)	1.0E+17	10	1.10E+14	2.20E+14	3.30E+14	5.50E+14	2.20E+15
		50	5.50E+14	1.10E+15	1.65E+15	2.75E+15	1.10E+16
		100	1.10E+15	2.20E+15	3.30E+15	5.50E+15	2.20E+16
		500	5.50E+15	1.10E+16	1.65E+16	2.75E+16	1.10E+17
		1000	1.10E+16	2.20E+16	3.30E+16	5.50E+16	2.20E+17
	5.0E+18	10	5.50E+15	1.10E+16	1.65E+16	2.75E+16	1.10E+17
		50	2.75E+16	5.50E+16	8.25E+16	1.37E+17	5.50E+17
		100	5.50E+16	1.10E+17	1.65E+17	2.75E+17	1.10E+18
		500	2.75E+17	5.50E+17	8.25E+17	1.38E+18	5.50E+18
		1000	5.50E+17	1.10E+18	1.65E+18	2.75E+18	1.10E+19
	1.0E+20	10	1.10E+17	2.20E+17	3.30E+17	5.50E+17	2.20E+18
		50	5.50E+17	1.10E+18	1.65E+18	2.75E+18	1.10E+19
		100	1.10E+18	2.20E+18	3.30E+18	5.50E+18	2.20E+19
		500	5.50E+18	1.10E+19	1.65E+19	2.75E+19	1.10E+20
		1000	1.10E+19	2.20E+19	3.30E+19	5.50E+19	2.20E+20
1.0E-03 (e)	1.0E+17	10	5.00E+15	1.00E+16	1.50E+16	2.50E+16	1.00E+17
		50	2.50E+16	5.00E+16	7.50E+16	1.25E+17	5.00E+17
		100	5.00E+16	1.00E+17	1.50E+17	2.50E+17	1.00E+18
		500	2.50E+17	5.00E+17	7.50E+17	1.25E+18	5.00E+18
		1000	5.00E+17	1.00E+18	1.50E+18	2.50E+18	1.00E+19

Table 6.2-1. Additional Fissions Due to Criticality of DOE-Owned Spent Nuclear Fuels (Continued)

Probability of Initial Criticality (a) (crit/yr)	Number of Fissions per Criticality (b) (-)	Assumed Duration of Constant GeoHydrology (c) (yr)	Additional Fissions in DOE SNFs (fissions/yr) — Assumed Rate of Repeated Criticalities (d) (criticalities/yr) 5.	10.	15.	25.	100.
	5.0E+18	10	2.50E+17	5.00E+17	7.50E+17	1.25E+18	5.00E+18
		50	1.25E+18	2.50E+18	3.75E+18	6.25E+18	2.50E+19
		100	2.50E+18	5.00E+18	7.50E+18	1.25E+19	5.00E+19
		500	1.25E+19	2.50E+19	3.75E+19	6.25E+19	2.50E+20
		1000	2.50E+19	5.00E+19	7.50E+19	1.25E+20	5.00E+20
	1.0E+20	10	5.00E+18	1.00E+19	1.50E+19	2.50E+19	1.00E+20
		50	2.50E+19	5.00E+19	7.50E+19	1.25E+20	5.00E+20
		100	5.00E+19	1.00E+20	1.50E+20	2.50E+20	1.00E+21
		500	2.50E+20	5.00E+20	7.50E+20	1.25E+21	5.00E+21
		1000	5.00E+20	1.00E+21	1.50E+21	2.50E+21	1.00E+22
1.0E-01 (e)	1.0E+17	10	5.00E+17	1.00E+18	1.50E+18	2.50E+18	1.00E+19
		50	2.50E+18	5.00E+18	7.50E+18	1.25E+19	5.00E+19
		100	5.00E+18	1.00E+19	1.50E+19	2.50E+19	1.00E+20
		500	2.50E+19	5.00E+19	7.50E+19	1.25E+20	5.00E+20
		1000	5.00E+19	1.00E+20	1.50E+20	2.50E+20	1.00E+21
	5.0E+18	10	2.50E+19	5.00E+19	7.50E+19	1.25E+20	5.00E+20
		50	1.25E+20	2.50E+20	3.75E+20	6.25E+20	2.50E+21
		100	2.50E+20	5.00E+20	7.50E+20	1.25E+21	5.00E+21
		500	1.25E+21	2.50E+21	3.75E+21	6.25E+21	2.50E+22
		1000	2.50E+21	5.00E+21	7.50E+21	1.25E+22	5.00E+22
	1.0E+20	10	5.00E+20	1.00E+21	1.50E+21	2.50E+21	1.00E+22
		50	2.50E+21	5.00E+21	7.50E+21	1.25E+22	5.00E+22
		100	5.00E+21	1.00E+22	1.50E+22	2.50E+22	1.00E+23
		500	2.50E+22	5.00E+22	7.50E+22	1.25E+23	5.00E+23
		1000	5.00E+22	1.00E+23	1.50E+23	2.50E+23	1.00E+24

(a) Long-term and short-term infiltration values obtained from the PRA/SLAM model.

(b) Nuclear dynamic calculations performed with NARK (Section 6.4) and Tables B.2-1 & B.2-2 indicate that the expected number of fissions per excursion is 1.0E+17 → 1.0E+20.

(c) This range of time values indicates that it is expected that geohydrology scenarios are assumed not to remain the same for more than 1,000 years. (For this analysis, it was assumed that nominal conditions would be maintained for only 100 years.)

(d) Thermal-hydrology calculations performed with BRAGFLO_T (Section 5) indicate that substantial time is needed to recovery initial conditions and that only a few number of continuous criticalities per year could be achieved.

(e) These probability frequences are presented for comparison reasons only.

7.0 SUMMARY OF RESULTS

7.1 General Computational Results

The general findings from this study are as follows: Co-disposal of existing DOE SNF and HLW with commercial SNF are expected to result in intermixed leachate plumes, that have enrichments which are too low to form a critical assembly in far-field geometries. Near-field or internal criticality is possible only if significant separation of fissile material and neutron absorbers occur by chemical processes and/or mechanisms. The consequences of a critical excursion are minimal in terms of energy release (temperature rise) and impact on fission yield product inventories for plausible conditions. The probabilities for criticality initiators were estimated at the ROM (rough-order-of-magnitude) level and were determined to be very small. The net impact of resulting criticality fissions on the radiological source term is very small and may not contribute to overall repository performance assessment (contributions to the annual effective dose by criticality are less than the round-off for computed PA values). Several specific findings are itemized below in the following subsections:

7.1.1 Criticality Potential Parametric Study

Over 30,000 eigenvalue calculations for the fissile material/geometries were investigated using the CX model. These calculations were used to identify the relationship between fissile mass and fissile concentration necessary to yield a critical assembly. Figures 3.3-1 to 3.3-4 are examples of typical results identifying the relationship between fissile mass and concentrations (others can be found in Appendix E). In the NDCA study, S-curves were generated for over 30 scenarios corresponding to fissile material in near-fields consisting of rust and concrete "host rock" materials and also for far-fields consisting of Topopah Springs tuff host rock. The following key criticality features were identified from the S-curves:

A) Low enrichment fissile materials (less than 2% enrichment) do not achieve delayed criticality in far-field geometries, even for infinite geometries. Enrichments greater than 2% will require significant fissile mass quantities, which may not be possible to accumulate in a single concentrated far-field location. PA results should identify that required accumulation of fissile material is not possible.

B) Generating a critical assembly requires substantial fissile mass for far-field geometries (>60 kg) and for near-field geometries (>7 kg for highly-enriched uranium (HEU) fissile material without the presence of neutron poisons and fully-saturated/large porosity, >10 kg for HEU without neutron poisons under nominal conditions, and >14.4 kg for HEU with 1% of the original neutron poisons, see Appendix H).

C) There are combinations of fissile mass and concentration (for high enrichments) for which it is technically possible to achieve delayed criticality in near-field geometries that include a mixture of highly enriched fissile material and rust. However, the fissile concentrations (in the absence of neutron poisons) necessary to accomplish this are substantial (excess of 10 kg/m^3) and when considering the geochemistry in the repository environment and allowed fissile masses individual packages, it may not be plausible for these fissile concentrations to ever occur. PA results for container degradation will be needed to generate FEPs screening arguments for this scenario.

D) Results indicate that the presence of reflector material (the tuff host rock surrounding the critical zone) has a significant impact on the required critical mass but not on the fissile concentration. (Thus, the effect of the addition of a reflector is that the corresponding S-curve is moved down in fissile mass but not to the left or right in fissile concentration.) Models lacking in reflector geometries may overestimate minimum required fissile masses.

The nuclear criticality potential S-curves were generated for 36 case studies for near-filed, far-field, benchmarks, and special studies (see Tables 3.3-1 & 3.4-1 and Appendix E). The results of these case studies need to be analyzed from a PA perspective to identify which critical situations are physically possible. Some fissile concentrations are not attainable and/or the transport mechanisms to separate fissile material from neutron poisons are not sufficient. To further illustrate this point, uranium ore body concentrations have been identified from information in the open literature. Tables 7.1.1-1, 7.1.1-2, and 7.1.1-3 identify uranium concentrations for sandstone, volcanic, and epigenetic calcrete types of uranium ores. These tables identify that nominal uranium concentration values are expected in the range of 1 to 5 kg/m^3 for uranium concentration[1]. From the information identified in the S-curves for far-field geometries (especially Topopah Springs Tuff), it can be seen that the range of values seen in nature (natural analogs) correspond to non-optimal moderation cases. These cases are over-moderated scenarios and require substantially larger quantities of fissile mass in order to achieve a critical assembly. As can be seen from Figure E.3-34, for instance, a fissile concentration of 7.0 kg/m^3 would require a fissile mass (not including ^{238}U) greater than 600 kg assembled into a single location. This mass, and corresponding geometry radius, is substantial and the likelihood that this scenario could exist is very small. This information could be used, in conjunction with PA results for mass transport and fissile reconcentration, in the FEPs screening arguments.

[1] This information is speculative at the present time. Further investigation is necessary to confirm these values. Information was obtained from Dan McCarn, a specialist in uranium ore bodies.

Table 7.1.1-1. Sandstone Type Uranium Ore

No.	Redox (pH)	Location	Type	Setting	Trace Elements	Wt % (Kg/m^3)	References
1	Reduced (~7)	Grants Mineral Belt, NM	Syngenetic: Ambrosia Lake	Sandstone: Syngenetic Mo, V, Se -bearing uranium ores	V, Mo, Se	0.10% (2.5)	Saucier, 1979. pp.116-121
2	Reduced (~7)	Straz, Czech Republic	Syngenetic	Sandstone: Syngenetic U	-	0.05% (1.25)	McCarn, IAEA Report, 1997
3	Redox Front (~7)	Grants Mineral Best, NM	Crownpoint	Monometallic remobilized roll-front concentrated against regional redox (Fe^{+2}/Fe^{+3}) front	-	0.25% (6.25)	Saucier, 1979. pp.116-121; Adams & Saucier, 1981
4	Redox Front (~7)	Wyoming basins, WY, NB	Gas Hills Wyoming Roll-Type	Epigenetic sandstone	P, Se, Mo	0.20% (5.0)	Mickle & Mathews, 1978
5	Redox Front (~7)	South Texas	Texas Roll Front	Epigenetic sandstone	Se, Mo, V	0.20% (5.0)	Mickle & Mathews, 1978
6	Redox Front (~8)	Syr-Dahyr, Kazakhstan	Roll Front	Epigenetic sandstone	Rh, Se	0.20% (5.0)	Abakumov, 1983, p.163-176
7	Redox Front (~8)	Chu-Saryssu, Kazakhstan	Roll Front	Epigenetic sandstone	Rh, Se	0.20% (5.0)	Abakumov, 1983, p.163-176
8	Redox Front (~7)	Alamosa Basin (Basin & Range)	Roll Front	Epigenetic sandstone: Distal fan / interfingering with methanogenic lacustrine facies	-	0.20% (5.0)	Johnson et al, 1982
9	Oxid. / Red. (~7)	Colorado Plateau, CO, UT	Morison - Uravan	Sandstone: Oxidized V-bearing uranium ores	V	0.20% (5.0)	Mickle & Mathews, 1978
10	Oxid./Red. (~7)	Monument Valley / White Canyon	Peneconcordant Channel Controlled	Epigenetic sandstone occurring as both oxidized and reduced ore.	V, Cu	0.20% (5.0)	Mickle & Mathews, 1978
11	Oxidized (~7)	Grants Mineral Belt, NM	Poison Canyon	Sandstone: Oxidized V-bearing uranium ores	V	0.20% (5.0)	Mickle & Mathews, 1978

Table 7.1.1-2. Volcanic Type Uranium Ore

No.	Redox (pH)	Location	Type	Setting	Trace Elements	Wt % (Kg/m^3)	References
1		Hartford Hill Tuffs, NV	Volcanic – Hydroallogenic	U enriched fluids released from volcanic effusives & injected into adjacent rocks. Characterized by uranosilicates	Si, Th, V, Th	0.05% (1.25)	Mickle & Mathews, 1978; IAEA, 1988
2	Redox boundary	Pocos de Caldes, Brazil	Volcanic / laterization	E ore-body formed at redox boundary between oxidized, laterized sub-volcanic alkaline rocks & unweathered proto-ore. Protoore formed at brecciated vents / H_2S	Mo, Si	0.20% (5.0)	IAEA, 1998
3	H_2S	Pena Blanca, Mexico	Volcanic	Ore formed at breccia pipes (El Nopal I) or ignimbrites	Mo, F, Si, Th	0.20% (5.0)	Reyes-Cortéz, 1985
4		Spor Mountain, UT	Volcanic	A "topaz" –bearing volcanic	Be	0.05% (1.25)	Burt & Sheridan, 1985
5		Topaz Rhyolites, Western USA	Volcanic	Topaz-bearing rhyolites of the Basin & Range & Rio Grand Rift	F, Li, Rb, Cs, Be, Sn, W, Nb	0.01% (0.25)	Burt & Sheridan, 1985

Table 7.1.1-3. Pedogenic Uranium Ores – Calcretes & Silcretes

No.	Redox Character	Location	Type	Setting	Trace Elements	Wt % Kg/m^3	References
1	Oxidized	Colorado-Kansas	Ogallalla Silcrete	Sandstone with high tuffaceous content – Evaporative pumping	Si	0.01% (0.25)	Johnson et al, 1982
2	Oxidized	Boulder City, Nevada	Pedogenic Calcrete	Western Deserts: NM, AZ, NV: High rates of evaporation	V, Si	0.03% (0.75)	Carlisle, 1978
3	Oxidized	Yeelirrie	Pedogenic Calcrete	Valley-fill calcrete, western Australia, High rates of evaporation	V, Si	0.20% (5.0)	Carlisle, 1978

7.1.2 *Excursion Consequences*

A large parametric nuclear dynamics analysis was performed in this study using the DTHX and UDX models. The calculations were used to identify the relationship between net excursion fissions and criticality assembly parameters (i.e., mass, temperature feedback properties, etc.). These calculations were performed with these two models at different levels of detail. The more detailed model (DTHX) is termed "fully-coupled" nuclear dynamics. This model is sophisticated in that it couples the time behavior model for the neutron population (and hence power and fission production) with the transient multiphase model for the combined thermal hydrology and transport of unsaturated groundwater. The DTHX (nuclear dynamic/thermal hydrology) model is computationally intensive and is used for select studies for far-field criticality. The second consequence model is less detailed and is termed "Uncoupled" nuclear dynamics (UDX). This model analyzes only the time behavior of the neutron population and does not model spatial effects. Since it is computationally efficient, it was used for parametric sensitivity analysis. Comparison of this model to the "fully-coupled" nuclear dynamics indicated that its results are conservative and can be used for bounding calculations. Since the uncoupled nuclear dynamics is not related to the spatial geometry of the fissile mass, its results are applicable to in-situ, near-field, or far-field analysis. The UDX model results are used to identify the net impact upon the radiological source term due to a single nuclear excursion (in terms of additional fission yield products). The nuclear dynamics calculations (DTHX and UDX) identified the following:

A) The number of net fissions from a typical excursion are very low and are similar to values previously experienced in criticality accidents involving aqueous solutions with fissile material. Typical net-fissions are computed to be in the range of 10^{17} to 10^{20} fissions per excursion.

B) When comparing "fully-coupled" nuclear dynamics DTHX computational results to "Uncoupled" nuclear dynamics (UDX) results, it was identified that UDX results are conservative (see Figure 7.1.2-1). Since the UDX model does not include groundwater modeling, which is computationally intensive, the UDX model was used to investigate the sensitivity of excursion fissions upon various neutronic model parameters. The UDX calculations resulted in the further understanding of the nuclear excursions and yielded a simple scaling law (see Figure 7.1.2-2). An important feature of this scaling law is that the amount of net fissions is strongly dependent on the inventory of fissile material in a critical assembly. Since the fissile mass is limited by S-curve quantities, the fissions are expected to be very low for conceivable situations leading to an excursion.

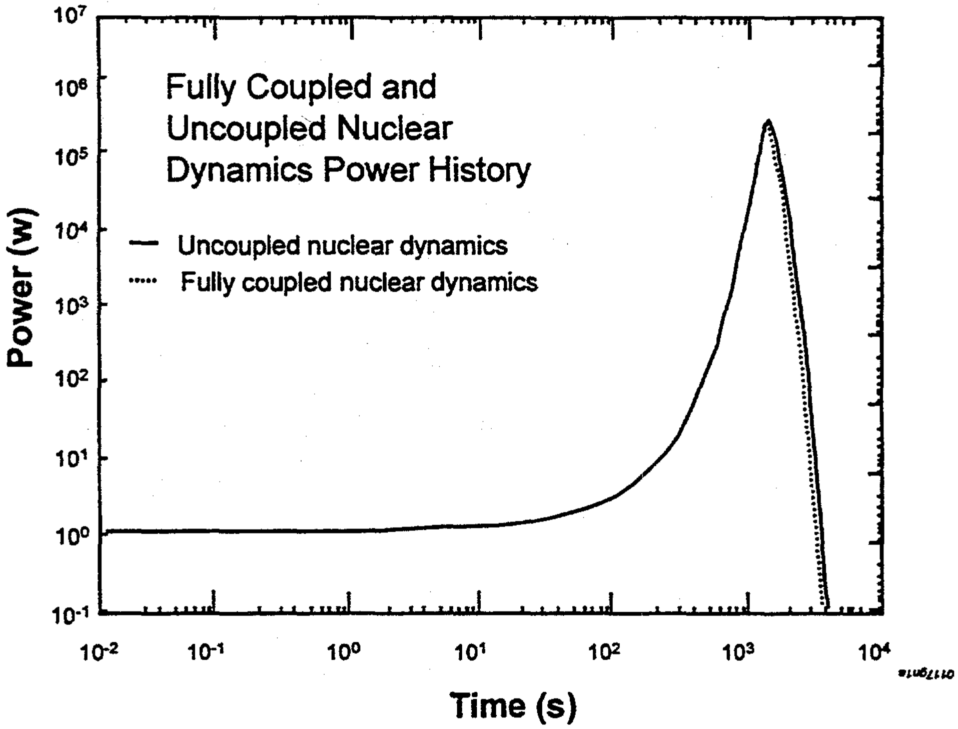


Figure 7.1.2-1. Comparison of fully-coupled nuclear dynamics results with uncoupled nuclear dynamics results (data for uranium in Topopah Springs tuff at nominal geologic conditions).

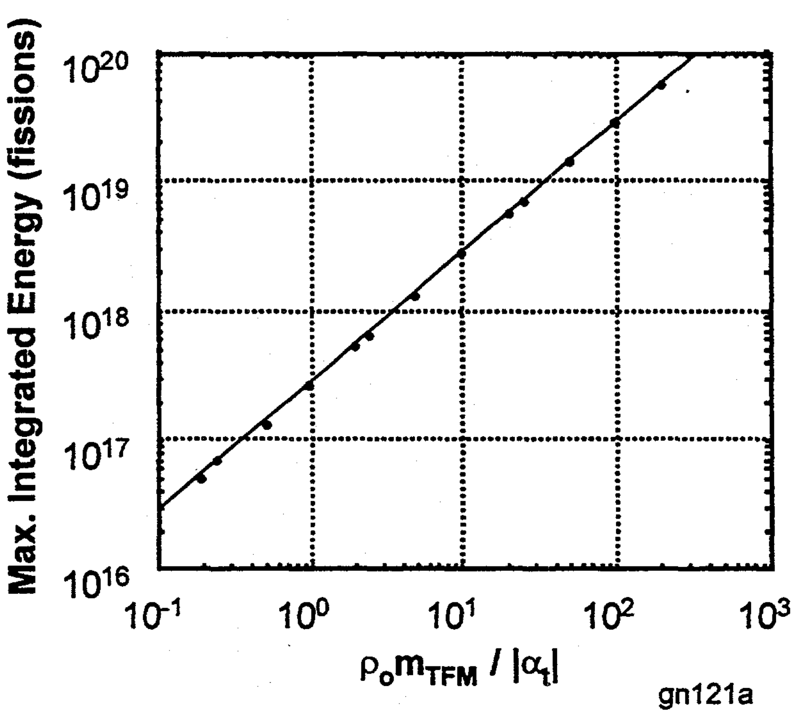


Figure 7.1.2-2. Scaling law for uncoupled nuclear dynamics calculations.

7.1.3 Thermal Hydrology Simulations

A small parametric study was performed with the THX model to investigate the transient response of the repository media during a nuclear excursion. Excursion power profiles correspond to typical energy released as predicted by the UDX and DTHX models. The thermal hydrology calculations were used for select far-field geometries to determine the temperature and saturation recycle times. These calculations allow estimation of the frequency of multiplier excursions that may occur after an initial critical assembly is generated. The thermal hydrology/groundwater transport calculations (THX) identified the following:

A) Even though the UDX and DTHX models indicated low net excursion fissions, there are significant groundwater temperature and saturation effects. Since it is necessary to restore the initial groundwater conditions to initiate another excursion, these effects are important in order to identify the bounding frequencies (recycle times) for occurrence of repeated nuclear excursions.

B) Computational results indicated that groundwater saturation recycle times are longer than groundwater temperature recycle times. Typical THX results can be seen in Figure 7.1.3-1. This figure presents a typical case that requires in excess of a hundred days to return to initial conditions. There considerable uncertainty in the THX computational results due to sensitivity to input parameters. A conservative (small) value for the overall recovery time of the thermal-hydrology is about 15 cycles per year. This conservative value is used in the identification of criticality risks.

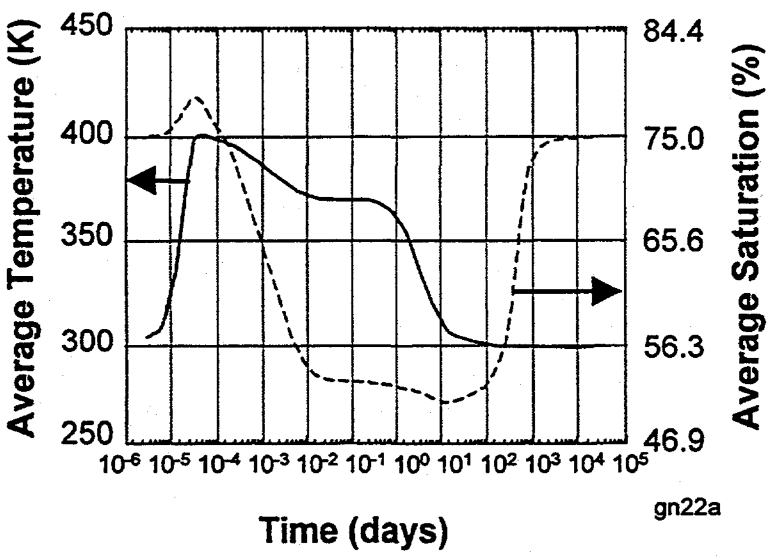


Figure 7.1.3-1. Typical thermal hydraulics/ groundwater transport computational results (data for uranium in Topopah Springs tuff at nominal geologic conditions).

7.1.4 Probability for Criticality Initiators

A Monte Carlo simulation was performed in the PRA model for events (such as groundwater infiltration, container corrosion, etc.) that may cumulatively result in the generation of an initial criticality. These probability values, when multiplied with the consequences of multiple excursions (for only those SNFs that have the potential to yield a critical assembly), will yield "risk". The metric used in this study for risk is "additional fissions" which can be directly compared to the initial radiological source term. The PRA model added valuable information on the probability for an initial criticality. This PRA model, using the SLAM code, computed criticality probability frequencies under glacial and non-glacial conditions. The results indicated a "worst case" (under persistent glacial conditions) probability of 2.2 containers undergoing criticality over 100,000 year duration (2.2×10^{-5}/yr). "Present day" conditions yielded a probability frequency of only 0.07 containers undergoing criticality over 100,000 year duration (7×10^{-7}/yr). Thus, the PRA model (using PA corrosion submodels and results) identified that these fissile masses and their corresponding concentrations have very small probabilities of occurrence.

To further understand the meaning of the values presented in Table 6.2-1, a comparison was made to the initial source term values. This comparison was made in Table 7.1.4-1. The important factor in constructing this table is that the initial source term is estimated to be 6.43×10^{31} fissions (see Appendix C). Thus, Table 7.1.4-1 presents the elapsed time of recurring fissioning events (as presented in Table 6.2-1) to increase the initial source term by one percent (i.e., 6.43×10^{29} fissions). This one percent limit was chosen because it is the assumed round-off in the source term inventory. Any contributions less than this diminutive value would essentially be considered to be less than the round-off for the initial source term and would have a negligible contribution. As can be seen from Table 7.1.4-1, the amount of time necessary to result in a one-percent increase is very long. Even at a probability of 10^{-1} criticalities per year, the corresponding cumulative time is on the order of a billion years. This means that existing burnup of the SNFs in the inventory is massive since these fuels underwent extensive numbers of fissions when they were burned up in nuclear reactors. Any additional fissions in a repository would be lost in comparison. Basically the lack of (1) moderation, (2) containment, and (3) heat transfer mechanisms preclude any significant amount of additional fissions. In order to present the data from Table 6.2-1 in a simple form, dose releases to the biosphere were extracted from Rechard 1997 and were used to generate Table 7.1.4-2. Then using this table, first order estimates of releases to the biosphere due to criticality only were calculated and are presented in Table 7.1.4-3. This table presents risks in the common metric of "mrem/yr". These units are easier for scientists to understand than the additional fission rates. As can be seen, these risks are very small in comparison to the AEDE doses (Table 7.1.4-2) due to the repository performance assessment results from the initial source term.

As mentioned previously, the PRA analysis results presented in this section represent the best model to date. We have good confidence in the calculations, but we add caution in that there is significant uncertainty in the input values and submodels. It is anticipated that the fault tree/event tree models will be updated at INEEL in the near future using the latest available submodels and input data. The PRA model itself may be upgraded from SLAM to SAPHIRE (NUREG, 1994), which is considered to be more responsive, easy to change, have minimal problems in quantifications and is accepted in the PRA community. When new computational values become available, they should be considered to supercede all probabilities presented in this section.

Table 7.1.4-1. Number of Years of Continuous Criticalities Needed in Order to Increase Initial Source Term by One Percent

Probability of Initial Criticality (b)	Time to Increase Initial Source Term by 1% Due to Continuous Criticalities (a) (years)						
	Number of Fissions per Criticality (c)	Assumed Duration of Constant GeoHydrology (d)	Assumed Rate of Repeated Criticalities (e) (criticalities/yr)				
(crit/yr)	(-)	(yr)	5.	10.	15.	25.	100.
			(years)				
7.0E-07 (short-term infiltration)	1.0E+17	10	1.84E+17	9.19E+16	6.12E+16	3.67E+16	9.19E+15
		50	3.67E+16	1.84E+16	1.22E+16	7.35E+15	1.84E+15
		100	1.84E+16	9.19E+15	6.12E+15	3.67E+15	9.19E+14
		500	3.67E+15	1.84E+15	1.22E+15	7.35E+14	1.84E+14
		1000	1.84E+15	9.19E+14	6.12E+14	3.67E+14	9.19E+13
	5.0E+18	10	3.67E+15	1.84E+15	1.22E+15	7.35E+14	1.84E+14
		50	7.35E+14	3.67E+14	2.45E+14	1.47E+14	3.67E+13
		100	3.67E+14	1.84E+14	1.22E+14	7.35E+13	1.84E+13
		500	7.35E+13	3.67E+13	2.45E+13	1.47E+13	3.67E+12
		1000	3.67E+13	1.84E+13	1.22E+13	7.35E+12	1.84E+12
	1.0E+20	10	1.84E+14	9.19E+13	6.12E+13	3.67E+13	9.19E+12
		50	3.67E+13	1.84E+13	1.22E+13	7.35E+12	1.84E+12
		100	1.84E+13	9.19E+12	6.12E+12	3.67E+12	9.19E+11
		500	3.67E+12	1.84E+12	1.22E+12	7.35E+11	1.84E+11
		1000	1.84E+12	9.19E+11	6.12E+11	3.67E+11	9.19E+10
2.2E-05 (long-term infiltration)	1.0E+17	10	5.85E+15	2.92E+15	1.95E+15	1.17E+15	2.92E+14
		50	1.17E+15	5.85E+14	3.90E+14	2.34E+14	5.85E+13
		100	5.85E+14	2.92E+14	1.95E+14	1.17E+14	2.92E+13
		500	1.17E+14	5.85E+13	3.90E+13	2.34E+13	5.85E+12
		1000	5.85E+13	2.92E+13	1.95E+13	1.17E+13	2.92E+12
	5.0E+18	10	1.17E+14	5.85E+13	3.90E+13	2.34E+13	5.85E+12
		50	2.34E+13	1.17E+13	7.79E+12	4.68E+12	1.17E+12
		100	1.17E+13	5.85E+12	3.90E+12	2.34E+12	5.85E+11
		500	2.34E+12	1.17E+12	7.79E+11	4.68E+11	1.17E+11
		1000	1.17E+12	5.85E+11	3.90E+11	2.34E+11	5.85E+10
	1.0E+20	10	5.85E+12	2.92E+12	1.95E+12	1.17E+12	2.92E+11
		50	1.17E+12	5.85E+11	3.90E+11	2.34E+11	5.85E+10
		100	5.85E+11	2.92E+11	1.95E+11	1.17E+11	2.92E+10
		500	1.17E+11	5.85E+10	3.90E+10	2.34E+10	5.85E+09
		1000	5.85E+10	2.92E+10	1.95E+10	1.17E+10	2.92E+09
1.0E-03 (f)	1.0E+17	10	1.29E+14	6.43E+13	4.29E+13	2.57E+13	6.43E+12
		50	2.57E+13	1.29E+13	8.57E+12	5.14E+12	1.29E+12
		100	1.29E+13	6.43E+12	4.29E+12	2.57E+12	6.43E+11
		500	2.57E+12	1.29E+12	8.57E+11	5.14E+11	1.29E+11
		1000	1.29E+12	6.43E+11	4.29E+11	2.57E+11	6.43E+10

Table 7.1.4-1. Number of Years of Continuous Criticalities Needed in Order to Increase Initial Source Term by One Percent (Continued)

Probability of Initial Criticality (b) (crit/yr)	Number of Fissions per Criticality (c) (-)	Assumed Duration of Constant GeoHydrology (d) (yr)	Time to Increase Initial Source Term by 1% Due to Continuous Criticalities (a) (years) — Assumed Rate of Repeated Criticalities (e) (criticalities/yr) 5.	10.	15.	25.	100.
	5.0E+18	10	2.57E+12	1.29E+12	8.57E+11	5.14E+11	1.29E+11
		50	5.14E+11	2.57E+11	1.71E+11	1.03E+11	2.57E+10
		100	2.57E+11	1.29E+11	8.57E+10	5.14E+10	1.29E+10
		500	5.14E+10	2.57E+10	1.71E+10	1.03E+10	2.57E+09
		1000	2.57E+10	1.29E+10	8.57E+09	5.14E+09	1.29E+09
	1.0E+20	10	1.29E+11	6.43E+10	4.29E+10	2.57E+10	6.43E+09
		50	2.57E+10	1.29E+10	8.57E+09	5.14E+09	1.29E+09
		100	1.29E+10	6.43E+09	4.29E+09	2.57E+09	6.43E+08
		500	2.57E+09	1.29E+09	8.57E+08	5.14E+08	1.29E+08
		1000	1.29E+09	6.43E+08	4.29E+08	2.57E+08	6.43E+07
1.0E-01 (f)	1.0E+17	10	1.29E+12	6.43E+11	4.29E+11	2.57E+11	6.43E+10
		50	2.57E+11	1.29E+11	8.57E+10	5.14E+10	1.29E+10
		100	1.29E+11	6.43E+10	4.29E+10	2.57E+10	6.43E+09
		500	2.57E+10	1.29E+10	8.57E+09	5.14E+09	1.29E+09
		1000	1.29E+10	6.43E+09	4.29E+09	2.57E+09	6.43E+08
	5.0E+18	10	2.57E+10	1.29E+10	8.57E+09	5.14E+09	1.29E+09
		50	5.14E+09	2.57E+09	1.71E+09	1.03E+09	2.57E+08
		100	2.57E+09	1.29E+09	8.57E+08	5.14E+08	1.29E+08
		500	5.14E+08	2.57E+08	1.71E+08	1.03E+08	2.57E+07
		1000	2.57E+08	1.29E+08	8.57E+07	5.14E+07	1.29E+07
	1.0E+20	10	1.29E+09	6.43E+08	4.29E+08	2.57E+08	6.43E+07
		50	2.57E+08	1.29E+08	8.57E+07	5.14E+07	1.29E+07
		100	1.29E+08	6.43E+07	4.29E+07	2.57E+07	6.43E+06
		500	2.57E+07	1.29E+07	8.57E+06	5.14E+06	1.29E+06
		1000	1.29E+07	6.43E+06	4.29E+06	2.57E+06	6.43E+05

(a) Time values determined by using additional fission rates from Table 6.2-1 and the initial source term value estimated to be ~ 6.43E+31 fissions (see Appendix C).

(b) Long-term and short-term infiltration values obtained from PRA model (see Appendix H).

(c) Nuclear dynamic calculations performed with NARK (Section 4.) indicate that the expected number of fissions per excursion is 1.0E+17 → 1.0E+20. (For comparison to small excursion accidents, see Tables B.2-1 and B.2-2.)

(d) This range of time values indicates that it is expected that geohydrology scenarios are not expected to remain the same after 1,000 years. (For this analysis, it was assumed that nominal conditions conditions would be maintained for only 100 years.)

(e) Thermal hydrology calculations performed with BRAGFLO_T (Section 5.) indicate that substantial time is needed to recovery initial conditions and that only a few number of continuous criticalities per year could be achieved.

(f) These probability frequences are presented for comparison reasons only.

Table 7.1.4-2. Releases Determined in 1997 INEEL Performance Performance Assessment of Spent Nuclear Fuels (a)

Instantaneous Release (Ci/yr)			
Nuclide	[@ 10,000 yr]	[@ 50,000 yr]	[@ 100,000 yr]
I-129	9.77E-09	2.22E-05	4.10E-06
Tc-99	3.87E-06	7.45E-03	1.17E-03
Np-237	3.46E-10	2.06E-06	1.42E-05
Cumulative Release (Ci)			
Nuclide	[@ 10,000 yr]	[@ 50,000 yr]	[@ 100,000 yr]
I-129	6.48E-05	4.40E-01	1.16E+00
Tc-99	2.57E-02	1.54E+02	3.92E+02
Np-237	2.34E-06	3.86E-03	5.33E-01
Mean Annual Dose Rate (AEDE) at 5 km Boundary (mrem/yr)			
Nuclide	[@ 10,000 yr]	[@ 50,000 yr]	[@ 100,000 yr]
I-129	1.80E-02	5.20E+01	1.70E+00
Tc-99	6.36E-02	1.60E+02	4.41E+00
Np-237	3.75E-03	6.30E+00	3.76E+02
Total	8.53E-02	2.18E+02	**3.82E+02 (b)**

(a) Release rates obtained from electronic database for Ref. Rechard 1997.

(b) Near-field criticality risks (cumulative AEDE @ 100,000 yr) calculated with: *Risk (mrem/yr)* = [*AEDE dose rate (mrem/yr)* × *Time (yr)* × *Fission Rate (fis/yr)*] / [*Initial Fissions (fis)*] = [3.82*E*+02(*mrem/yr*) × 100,000(*yr*) × *Fission Rate (fis/yr)*] / [6.43*E*+31(*fis*)] = [5.94*E*−25 × *Fission Rate*](*mrem/yr*).

Table 7.1.4-3. Risks Due to Criticality of Spent Nuclear Fuels

Probability of Initial Criticality (b)	Risks of Additional Fissions in SNFs (a) (mrem/yr)						
	Number of Fissions per Criticality (c)	Assumed Duration of Constant GeoHydrology (d)	Assumed Rate of Repeated Criticalities (e) (criticalities/yr)				
(crit/yr)	(-)	(yr)	5.	10.	15.	25.	100.
			(mrem/year)				
7.0E-07	1.0E+17	10	2.08E-12	4.16E-12	6.24E-12	1.04E-11	4.16E-11
(short-		50	1.04E-11	2.08E-11	3.12E-11	5.20E-11	2.08E-10
term		100	2.08E-11	4.16E-11	6.24E-11	1.04E-10	4.16E-10
infiltration)		500	1.04E-10	2.08E-10	3.12E-10	5.20E-10	2.08E-09
		1000	2.08E-10	4.16E-10	6.24E-10	1.04E-09	4.16E-09
	5.0E+18	10	1.04E-10	2.08E-10	3.12E-10	5.20E-10	2.08E-09
		50	5.20E-10	1.04E-09	1.56E-09	2.60E-09	1.04E-08
		100	1.04E-09	2.08E-09	3.12E-09	5.20E-09	2.08E-08
		500	5.20E-09	1.04E-08	1.56E-08	2.60E-08	1.04E-07
		1000	1.04E-08	2.08E-08	3.12E-08	5.20E-08	2.08E-07
	1.0E+20	10	2.08E-09	4.16E-09	6.24E-09	1.04E-08	4.16E-08
		50	1.04E-08	2.08E-08	3.12E-08	5.20E-08	2.08E-07
		100	2.08E-08	4.16E-08	6.24E-08	1.04E-07	4.16E-07
		500	1.04E-07	2.08E-07	3.12E-07	5.20E-07	2.08E-06
		1000	2.08E-07	4.16E-07	6.24E-07	1.04E-06	4.16E-06
2.2E-05	1.0E+17	10	6.53E-11	1.31E-10	1.96E-10	3.27E-10	1.31E-09
(long-		50	3.27E-10	6.53E-10	9.80E-10	1.63E-09	6.53E-09
term		100	6.53E-10	1.31E-09	1.96E-09	3.27E-09	1.31E-08
infiltration)		500	3.27E-09	6.53E-09	9.80E-09	1.63E-08	6.53E-08
		1000	6.53E-09	1.31E-08	1.96E-08	3.27E-08	1.31E-07
	5.0E+18	10	3.27E-09	6.53E-09	9.80E-09	1.63E-08	6.53E-08
		50	1.63E-08	3.27E-08	4.90E-08	8.17E-08	3.27E-07
		100	3.27E-08	6.53E-08	9.80E-08	1.63E-07	6.53E-07
		500	1.63E-07	3.27E-07	4.90E-07	8.17E-07	3.27E-06
		1000	3.27E-07	6.53E-07	9.80E-07	1.63E-06	6.53E-06
	1.0E+20	10	6.53E-08	1.31E-07	1.96E-07	3.27E-07	1.31E-06
		50	3.27E-07	6.53E-07	9.80E-07	1.63E-06	6.53E-06
		100	6.53E-07	1.31E-06	1.96E-06	3.27E-06	1.31E-05
		500	3.27E-06	6.53E-06	9.80E-06	1.63E-05	6.53E-05
		1000	6.53E-06	1.31E-05	1.96E-05	3.27E-05	1.31E-04
1.0E-03	1.0E+17	10	2.97E-09	5.94E-09	8.91E-09	1.49E-08	5.94E-08
(f)		50	1.49E-08	2.97E-08	4.46E-08	7.43E-08	2.97E-07
		100	2.97E-08	5.94E-08	8.91E-08	1.49E-07	5.94E-07
		500	1.49E-07	2.97E-07	4.46E-07	7.43E-07	2.97E-06
		1000	2.97E-07	5.94E-07	8.91E-07	1.49E-06	5.94E-06

Table 7.1.4-3. Risks Due to Criticality of Spent Nuclear Fuels (Continued)

Probability of Initial Criticality (b) (crit/yr)	Number of Fissions per Criticality (c) (-)	Assumed Duration of Constant GeoHydrology (d) (yr)	Risks of Additional Fissions in SNFs (a) (mrem/yr) — Assumed Rate of Repeated Criticalities (e) (criticalities/yr) 5.	10.	15.	25.	100.
	5.0E+18	10	1.49E-07	2.97E-07	4.46E-07	7.43E-07	2.97E-06
		50	7.43E-07	1.49E-06	2.23E-06	3.71E-06	1.49E-05
		100	1.49E-06	2.97E-06	4.46E-06	7.43E-06	2.97E-05
		500	7.43E-06	1.49E-05	2.23E-05	3.71E-05	1.49E-04
		1000	1.49E-05	2.97E-05	4.46E-05	7.43E-05	2.97E-04
	1.0E+20	10	2.97E-06	5.94E-06	8.91E-06	1.49E-05	5.94E-05
		50	1.49E-05	2.97E-05	4.46E-05	7.43E-05	2.97E-04
		100	2.97E-05	5.94E-05	8.91E-05	1.49E-04	5.94E-04
		500	1.49E-04	2.97E-04	4.46E-04	7.43E-04	2.97E-03
		1000	2.97E-04	5.94E-04	8.91E-04	1.49E-03	5.94E-03
1.0E-01 (f)	1.0E+17	10	2.97E-07	5.94E-07	8.91E-07	1.49E-06	5.94E-06
		50	1.49E-06	2.97E-06	4.46E-06	7.43E-06	2.97E-05
		100	2.97E-06	5.94E-06	8.91E-06	1.49E-05	5.94E-05
		500	1.49E-05	2.97E-05	4.46E-05	7.43E-05	2.97E-04
		1000	2.97E-05	5.94E-05	8.91E-05	1.49E-04	5.94E-04
	5.0E+18	10	1.49E-05	2.97E-05	4.46E-05	7.43E-05	2.97E-04
		50	7.43E-05	1.49E-04	2.23E-04	3.71E-04	1.49E-03
		100	1.49E-04	2.97E-04	4.46E-04	7.43E-04	2.97E-03
		500	7.43E-04	1.49E-03	2.23E-03	3.71E-03	1.49E-02
		1000	1.49E-03	2.97E-03	4.46E-03	7.43E-03	2.97E-02
	1.0E+20	10	2.97E-04	5.94E-04	8.91E-04	1.49E-03	5.94E-03
		50	1.49E-03	2.97E-03	4.46E-03	7.43E-03	2.97E-02
		100	2.97E-03	5.94E-03	8.91E-03	1.49E-02	5.94E-02
		500	1.49E-02	2.97E-02	4.46E-02	7.43E-02	2.97E-01
		1000	2.97E-02	5.94E-02	8.91E-02	1.49E-01	5.94E-01

(a) Near-field risks (cumulative AEDE @ 100,000 yr) calculated with: $Risk\,(mrem/yr) = [AEDE\ dose\ rate\,(mrem/yr) \times Time\,(yr) \times Fission\ Rate\,(fis/yr)]\ /\ [Initial\ Fissions\,(fis)] = [3.82E{+}02(mrem/yr) \times 100{,}000(yr) \times Fission\ Rate\,(fis/yr)]\ /\ [6.43E{+}31\,(fis)] = [5.94E{-}25 \times Fission\ Rate]\,(mrem/yr)$.

(b) Long-term and short-term infiltration values obtained from PRA model (see Appendix H).

(c) Nuclear dynamic calculations performed with NARK (Section 4.) indicate that the expected number of fissions per excursion is 1.0E+17 → 1.0E+20. (For comparison to small excursion accidents, see Tables B.2-1 and B.2-2.)

(d) This range of time values indicates that it is expected that geohydrology scenarios are assumed not to remain the same for more than 1,000 years. (For this analysis, it was assumed that nominal conditions would be maintained for only 100 years.)

(e) Thermal-hydrology calculations performed with BRAGFLO_T (Section 5.) indicate that substantial time is needed to recovery initial conditions (only a few number of continuous criticalities per year can be achieved).

(f) These probability frequences are presented for comparison reasons only.

7.1.5 General Results

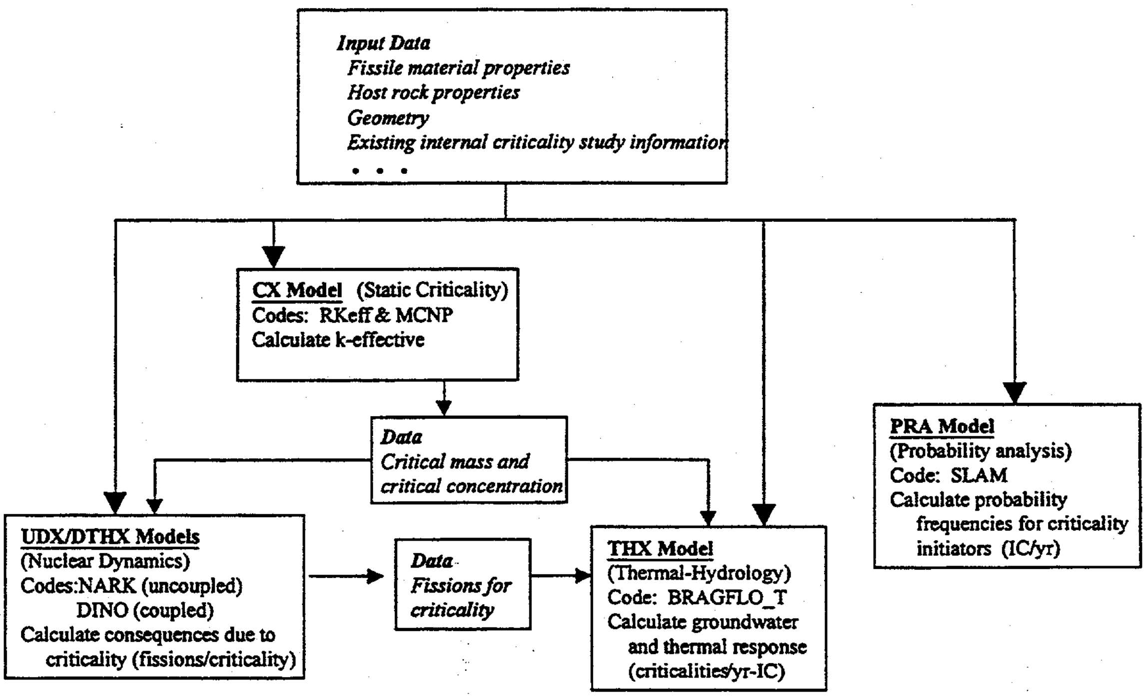
The major NDCA findings indicate that the disposal of DOE SNF in volcanic tuff *typical* of the Yucca Mountain Site (YMS) result in: (1) probability frequency of initial criticality of $7x10^{-7}$ criticality initiators/yr (under present day conditions), (2) range of 3 to 30 criticalities/yr (limited by geohydrology), and (3) range of 10^{17} to 10^{20} fissions/criticality. Thus the nominal risk associated with criticality is given by: Risk = Consequences x Frequency = $5x10^{18}$ (fissions/criticality) x $7x10^{-7}$ (initial criticalities/yr) x 15 (criticalities/yr-initial criticality) x 100 yr (assumed duration of repeated criticalities) = $5.3x10^{15}$ additional fissions per year. This risk is extremely small when compared to the initial YMS source term of ~$6x10^{31}$ fissions.

7.2 Identification of Risk

The calculation for risk (expressed in units of additional fissions) due to post-closure criticality is identified in Figure 7.2-1. This figure uses nominal values for criticality consequences and its associated probability frequency. The overall results of the NDCA study is that the risks associated with criticality of DSNFs in the YMP repository are only 5×10^{15} additional fissions per year. Even though the criticality probability frequencies calculated with the PRA model are ROM (rough-order-of-magnitude) values, the overall computed risk is very small. Thus, even if the ROM values are good to only several orders of magnitude, the risks will still be negligible in comparison to the risk associated to the radionuclide inventory of the initial source term.

7.3 Comparison of Criticality Risk to Initial Source Term

As mentioned in Section 6. the risks associated with post-closure criticality of DSNFs in the YMP repository are very small. The test used to determine if the risks due to post-closure criticality are significant is identified in Figure 1.1.3-2. This test corresponds to identifying if the addition fissions due to criticality are greater than one percent of the initial repository inventory. This level was chosen since that level corresponds to the estimated roundoff of the data available on the source term. Any values less than this value would impact repository releases after they have been computed and rounded off to their number of significant digits. Thus the important factor for the risk level test is the estimated source term, estimated in units of fissions. This was analyzed in Appendix C and yielded an estimated initial inventory of 6.43×10^{31}. Thus, the risk is: 100% x (5.3×10^{15} fissions/yr) x (10,000 yr) / (6.43×10^{31} fissions) = 8.24×10^{-11}% of the original source term for a regulatory timeframe of 10,000 yr. This result indicates that it nearly impossible to have post-closure fissions that could come close in comparison to the massive reactor burnup that fissile materials have experienced in an engineered reactor environment, which is under severe conditions of pressure, containment, etc.



RISKS = CONSEQUENCES X FREQUENCY

$$= 5 \times 10^{18} \left(\frac{\text{fissions}}{\text{criticality}}\right) \times 15 \left(\frac{\text{criticalities}}{\text{yr - initial criticality}}\right) \times 100 \text{ (yrs)} \times 7\times10^{-7} \left(\frac{\text{Initial criticalities}}{\text{yr}}\right)$$

$$= 5 \times 10^{15} \left(\frac{\text{fissions}}{\text{yr}}\right)$$

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Figure 7.2-1 Identification of risks due to criticality.

8.0 CONCLUSIONS AND RECOMMENDATIONS

8.1 Conclusions

The overall finding of this report is that nuclear criticality is not a significant contributor to post-closure repository releases to the accessible environment. The results presented in this study indicate that it is nearly impossible to generate a critical assembly in near- and far-field geometries and that the currently estimated risks of criticality are below the round-off for the radionuclide inventory source term. Basically it highly unlikely, in a geologic repository, that additional burnup of spent nuclear fuel will occur that is within an the order of magnitude of that resulting from engineered nuclear reactors, which have significant containment and heat transfer mechanisms. .

Since the risks are below the "noise", there is not a risk-based justification for application of criticality safety (k_{eff} <0.95) guidelines for repository post-closure conditions. This conclusion would recommend that resources are better applied to engineered features that may reduce annual effective doses due to groundwater transport of radionuclide inventory.

Significant results are summarized below:

- **Nominal additional fissions due to criticality are approximately 5.3×10^{15} fissions per year.**
- **The dose equivalent for the additional fissions corresponds to approximately 10^{-06} mrem per year.**

8.2 Recommendations

Much of the technical work in this study is preliminary. Future work is not going to significantly affect the technical findings, but it may aid in the defensibility of the models. There are three areas where NDCA model enhancements would be beneficial:

1) <u>PRA Model</u>
   Upgrading the PRA model would result in better confidence for criticality probability frequencies. At present, the model uses preliminary corrosion data and incomplete corrosion submodels. These submodels are currently being upgraded within the Yucca Mountain PA project and may be available in the near future. These updated models along with refinement in the input data will aid the defensibility of the PRA model. Results, if accepted, should continue to indicate that criticality does not have a significant impact to the releases to the accessible environment.

The upgraded PRA model could also be used to investigate over-moderated wet criticality scenarios. Of particular interest is the identification of the risks due to these auto-catalytic scenarios. A current conjucture is that while the consequences may increase over that of nominal cases, the probability is much lower than that of nominal cases. Thus, the risks of these auto-catalytic scenarios may be shown to be less than that of nominal cases.

Significant attention should given to the internal (*in situ*) geometries when upgrading the PRA model since these geometries would have the largest probability of resulting in a criticality for post-closure conditions.

2) <u>Nuclear Cross Sections</u>
For highly enriched materials, enrichments close to pure ^{235}U, nuclear cross sections may be processed for use in evaluation the Doppler temperature coefficient (DTC). This evaluation, plus static criticality calculations for non-leakage probabilities, could be used to show that the range of the overall prompt feedback coefficient used in this study (sensitivity analyses performed with the UDX model) include the fuel type in question.

3) <u>PA Models</u>
Repository performance assessment results for the transport of fissile and neutron poison materials could be used to determine the mass and concentration of fissile material in an assembly. These data can be directly compared with the criticality S-curves. Based on probability, the near-field and far-field scenarios may be "screened out" with corresponding FEPs screening arguments.

PA models could be used to generate estimated reactivity insertion rates due to groundwater infiltration into internal, near-field and far-field geometries.

Detailed analysis with the PA models could be used to identify the expected duration of time that a near-field or far-field critical assembly could continuously experience critical excursions. (Risk tables in Sections 6. and 7. assumed a duration of 100 years before host rock pore spaces would become clogged or other geologic mechanisms would result in a terminal shutdown of the fissile assembly.)

9.0 REFERENCES

Included in this list of references are significant references not discussed in detail in the main body of the report. These additional references provide valuable information in the following areas: (1) natural analogues and geological systems, (2) nuclear accident analysis, (3) numerical solution of nuclear dynamic systems, (4) the Oklo phenomena, (5) autocatalytic nuclear criticality in a geologic repository and (6) rebuttals to the autocatalytic conjecture.

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