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NUCLEAR CRITICALITY SAFETY ANALYSIS OF A SPENT FUEL WASTE PACKAGE IN A TUFF REPOSITORY

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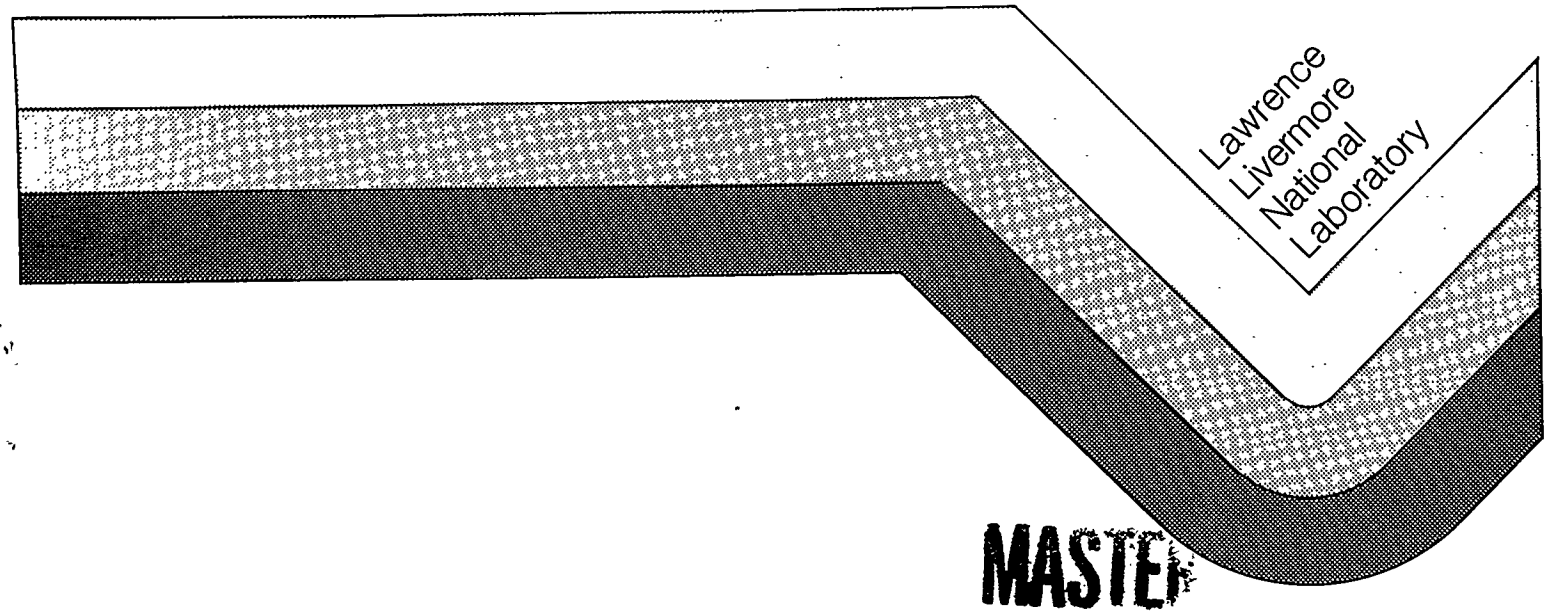

NOTICE

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Summary

An assessment has been performed of the criticality potential associated with the disposal of spent fuel in a tuff geology above the water table. Eleven potential configurations were defined which cover a vast range of geometries and conditions from the nominal configuration at emplacement to a hypothetical configuration thousands of years after emplacement in which the structure is gone, the fuel pellets disintegrated and the borehole flooded. Of these eleven configurations, four have been evaluated at this time.

The results of this evaluation indicate that even with very conservative assumptions (4.5 w/o fresh fuel), criticality is not a problem for the nominal configuration either dry or fully flooded. In the cases where the condition of the waste package is assumed to have severely deteriorated, over long times, calculations were performed with less conservative assumptions (depleted fuel). An assessment of these calculations indicates that criticality safety could be demonstrated if the depletion of the fissile inventory during fuel irradiation is taken into account.

A detailed discussion of the calculations performed is presented in this report. Also included are a description of the configurations which were considered, the analytical methods and models used, and a discussion of additional related work which should be performed.

1.0 Introduction

Lawrence Livermore National Laboratory (LLNL) is responsible for high-level nuclear waste package development as part of the Nevada Nuclear Waste Storage Investigations (NNWSI) Project. This project is part of the Department of Energy's Civilian Radioactive Waste Management (CRWM) Program. The waste package effort at LLNL is developing multibarriered packages for safe, permanent disposal in the proposed Yucca Mountain tuff repository.

As required by the Nuclear Waste Policy Act (NWPA) of 1982, the Nuclear Regulatory Commission (NRC) has established regulations for the licensing of a high level waste (HLW) repository (10 CFR Part 60). These regulations contain design criteria for repository systems which include the following criteria on 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." Section 60.131 (6)(7).

In 1983, conceptual designs for spent fuel waste packages for the vadose zone in tuff were developed at LLNL. THe canisters contain consolidated fuel elements from six PWR or 18 BWR spent fuel assemblies. An analytical effort by Westinghouse Electric Corporation's Waste Technology Services Division in Pittsburgh, PA, was subcontracted by LLNL to determine if these designs conformed to the 10 CFR 60 criticality safety requirements. The analytical study was limited to a few scenarios and configurations over long time periods in order to identify any initial or rearranged configurations and unlikely events which might prevent conformance to 10 CFR 60 requirements.

2.0 Background

The reference fuel for the purpose of this numerical analysis is unirradiated fuel rods from six Westinghouse PWR standard 17 x 17 fuel assemblies containing UO_2 fuel pellets enriched to 4.5 w/o U^{235}. The nominal configuration is closely-packed spent fuel rods, in a borehole in a tuff geology. The 1584 fuel rods from the six fuel assemblies are maintained in a closely-packed arrangement by a fabricated steel container, shown in Figure 1. This container is placed inside a 304 stainless steel canister which is inserted in a borehole. The canister and borehole are shown in Figure 2. The choices of fuel assembly type, enrichment and burnup will be discussed in Section 5.0 of this report.

In postulating potential configurations for evaluation, it was useful to think in terms of three time frames: 1) emplacement and short times (decades) thereafter; 2) intermediate times after emplacement (hundreds of years); and 3) long times (up to thousands of years after emplacement). It is reasonable to assume that in each successive time period, fewer controls would remain on the geometry of the waste form and on the waste form environment.

It is expected that, in the short term, the nominal geometry at emplacement will exist. It was assumed for this study, that as time passes, first the container and the canister corrode and are lost, then the fuel rod cladding fails, releasing the fuel pellets and finally the fuel pellets disintegrate to powder. At all times the potential for water intrusion must be considered. This scenario gave rise to eleven potential configurations, some dry and some flooded, which will be described in the following section of this report.

Current practice in safety analyses actually uses 0.95 as the upper limit for the effective neutron multiplication factor (K_{eff}). Many criticality studies have been performed for unmoderated (dry), fresh UO_2 fuel. In particular,

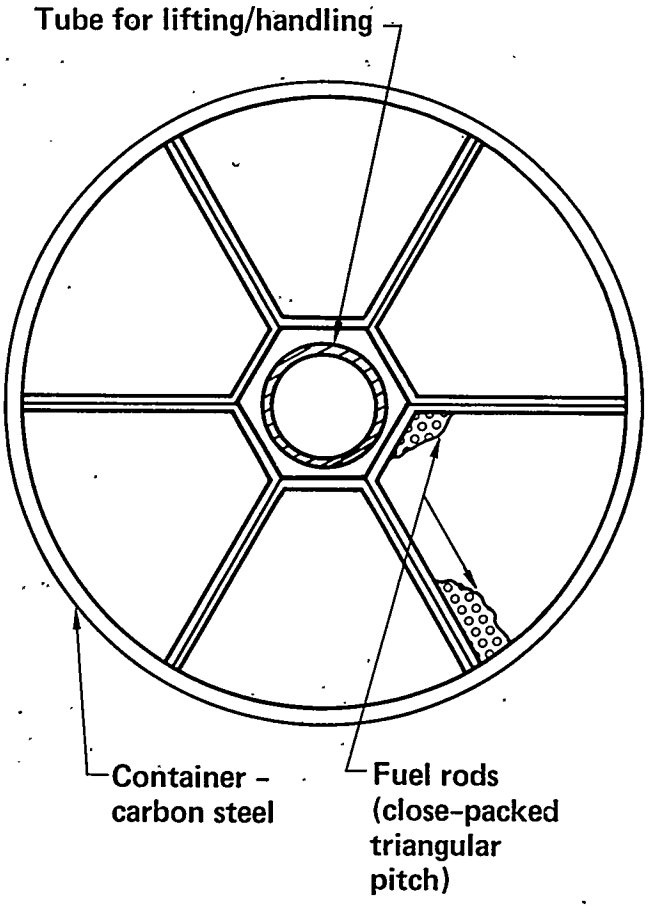


Fig. 1. Spent fuel container cross section

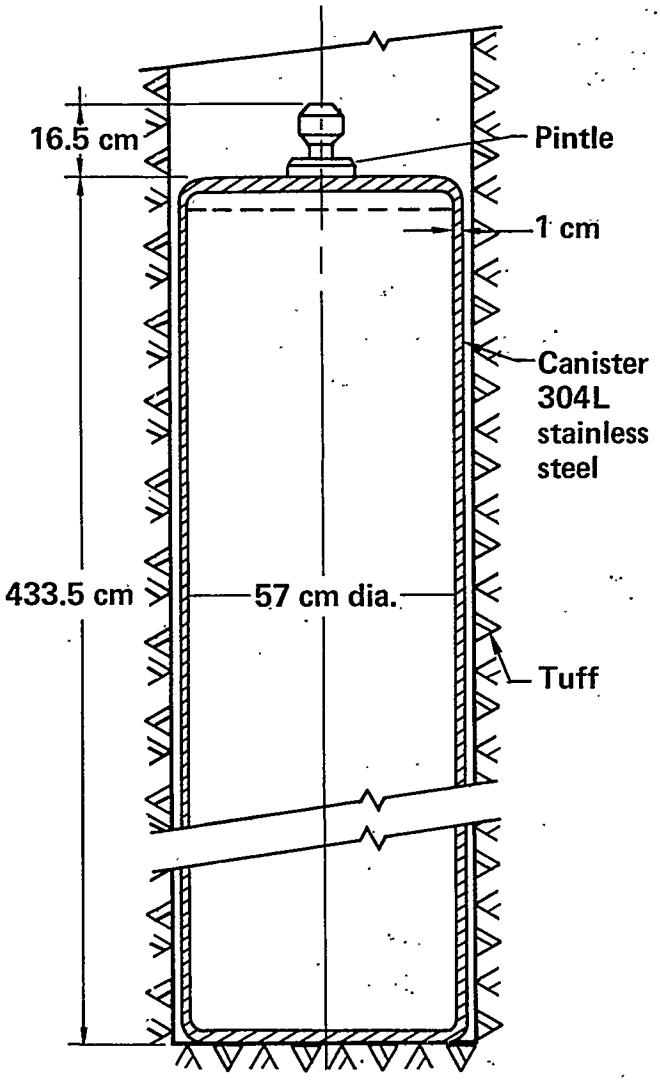


Fig. 2. Reference spent fuel waste package

particular, Reference 1 reports that no amount of fresh UO_2 enriched up to 7 w/o U^{235} can be made critical without moderation and that an infinite array of dry close-packed PWR fuel assemblies would have an effective neutron multiplication factor (K_{eff}) less than 0.8. Based on this and numerous other references not included here, it was concluded that all of the dry potential configurations would be subcritical.

Some of the flooded configurations were expected to be critical using the initial assumptions. Various studies, most notably References 2 and 3, conclude that demonstration of criticality safety in the geologic disposal of spent fuel will require taking credit for depletion (burnup) of the fissile inventory during irradiation. Those conclusions are confirmed by the results of this study.

3.0 Potential Configurations

Eleven potential configurations were identified and are summarized in Table 1. Each of these configurations will be described briefly. Configurations 1, 2, 6 and 10 were evaluated in this study.

Configurations 1, 2 and 3 - The basic geometry for configurations 1, 2 and 3 is that shown in Figures 1 and 2. Configuration 1 is assumed to be dry (unmoderated). Configuration 2 is assumed to be fully flooded; i.e. water has filled all void spaces around the fuel, inside the container and canister and between the borehole surface and the canister. Configuration 3 encompasses all partially flooded nominal configurations, such as flooding of the container but not the canister or borehole area around the canister or conversely flooding the borehole but not the inner container, etc. Studies reported in the literature (Reference 4) indicate that for casks containing multiple canisters, partial flooding (flooding of the canisters but not the cask) may be more reactive. However, for the single canister geometry under consideration, it is expected that Configuration 2 will be more reactive than Configuration 3. Configurations 1, 2 and 3 were expected to be subcritical with the initial assumptions. Configurations 1 and 2 were evaluated in this study and were found to be subcritical. A more detailed discussion of the results of this analysis is included in Section 7.0 of this report.

Configurations 4, 5 and 6 - Configurations 4, 5 and 6 represent potential configurations for the intermediate time frame of perhaps hundreds of years after emplacement. In this scenario, the container and canister structure is assumed to have been partially or totally lost, although the fuel rod structure remains. Configuration 4 assumes that the container and canister are gone and that the fuel rods are uniformly distributed throughout the borehole. This configuration dry (Number 4) is expected to be subcritical although flooded (Configuration 5) may be critical assuming fresh fuel. The reason for the

TABLE 1: POTENTIAL CONFIGURATIONS

CONFIGURATION NUMBER	DESCRIPTION
1	Nominal Configuration - Dry
2	Nominal Configuration - Flooded
3	Nominal Configuration - Partial Flooding
4	Structure* Gone - Rods Uniformly Spaced - Dry
5	Structure Gone - Rods Uniformly Spaced - Flooded
6	Container Partially Gone - Optimal Rearrangement of Rods - Flooded
7	Structure and Clad Gone - Pile of Pellets - Dry
8	Structure and Clad Gone - Pile of Pellets - Flooded
9	Structure and Clad Gone - Pellets Disintegrated to Powder - Dry
10	Clad and Disintegrated Pellets (Powder) Optimally Mixed - Flooded
11	Structure and Clad Gone - Pellets Disintegrated to Powder - Flooded

*Structure is defined as the container and canister.

uncertainty in Configuration 5 can be explained by considering Configuration 6, a partial loss of the container and rearrangement of the rods. With partial container failure, it is geometrically possible to construct an array of rods from two assemblies with a lattice pitch similar to that of intact assemblies such as shown in Figure 3. It is common fuel assembly design practice to select a rod pitch which results in a water/fuel ratio which is in the most reactive range. This, coupled with the fact that the assemblies are designed such that two assemblies of fresh fuel are critical in water, leads to the conclusion that failure to maintain the close-packed arrangement of the rods could result in hypothetical arrangements of the rods which would approach optimum moderation and would be critical if no compensatory factors (e.g. credit for fuel depletion, poisons, etc.) are included. This conclusion was confirmed by the results of this evaluation. It is not immediately obvious whether the uniform distribution of rods in Configuration 5 is sufficiently close-packed to remain subcritical.

For this analysis, Configuration 6 was evaluated, as shown in Figure 3, with the following assumptions: 1. the inner structure from two compartments in the container is lost; 2. two assemblies worth of rods are uniformly distributed throughout the central region and the two compartments at a pitch of 0.561 inches; 3. the remainder of the fuel rods remain closely-packed; and 4. the configuration is fully flooded. As expected, with the initial assumptions, this configuration was critical; therefore, an assessment of the reactivity decrease due to depletion was made.

Configurations 7 and 8 - Configurations 7 and 8 represent the next step in the degeneration from the nominal geometry. In these configurations, the fuel clad is assumed to be gone in addition to the steel container/canister structure. The result is assumed to be a pile of fuel pellets in the bottom of the borehole. The dry configuration (Number 7) was expected to be subcritical. Reference 5 evaluated a potential scenario in which one assembly's worth of fuel pellets fell to the bottom of a cylindrical canister and assumed a random orientation. This was found to be a more compact configuration and (assuming flooding) quite undermoderated compared to a normal reactor lattice. Although

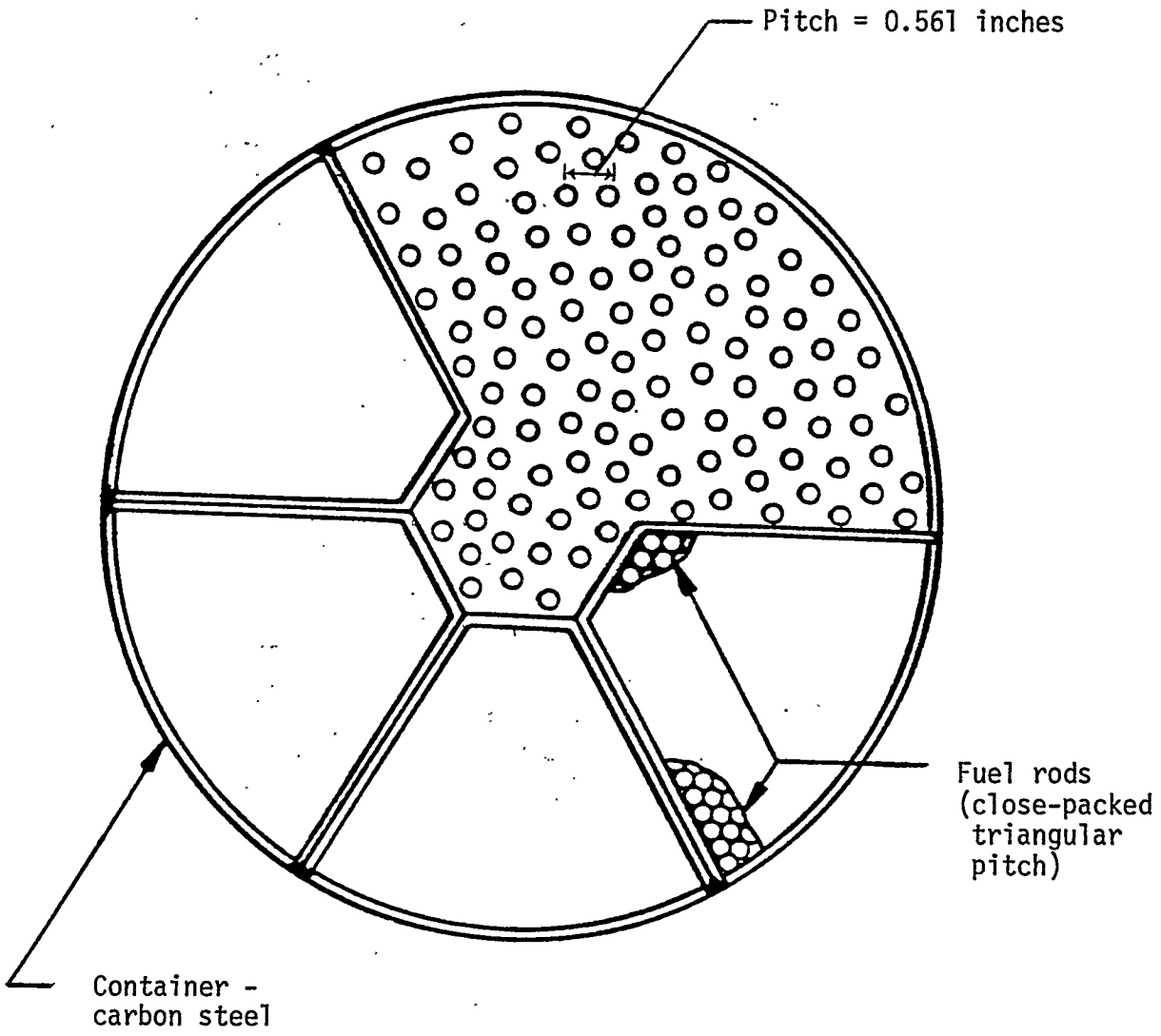


Fig. 3. Configuration 6 - Partial Container Failure

this evaluation would have to be extended to cover an increased number of pellets (up to six assemblies worth) and a different canister geometry, it is expected that potential configuration 8 would be shown to be subcritical.

Configuration 9, 10 and 11 - Configurations 9, 10, and 11 represent the long term potential configurations. In this time frame, the steel container and canister are assumed to be gone, the fuel rod cladding has failed allowing the fuel pellets to disintegrate and undergo additional oxidization. Consideration has been given to the composition of the fuel powder (UO_2, UO_3, U_3O_8 or combinations). The choice of U_3O_8 is discussed in Section 5.0 of this report. The extreme assumptions of Configurations 9 and 11, that all of the cladding is gone and that only fuel powder (Configuration 9) or an optimal mixture of fuel powder and water (Configuration 11) remains are apparently unrealistic since it is believed that the cladding will not be leached away faster than the fuel. A more realistic configuration (Number 10) is thought to be some mixture of cladding, fuel powder and water in the bottom of a borehole with the remaining cladding and more water above as shown in Figure 4. To determine the proportions in the fuel/clad/water mixture, it was assumed that all of the fuel was in powdered form in a cylinder the diameter of the borehole, the height of the cylinder determined so as to accommodate all of the fuel plus the volume of cladding which would normally be included in that height. The water volume fraction was assumed to be that of the void fraction in dry powder (i.e. water would fill the void spaces in the powder as opposed to assuming optimum moderation). The remaining clad and water were assumed to be present in a layer above the fuel/clad/water mixture. Configuration 9 (dry) will be subcritical. According to Reference 4, with no cladding, a cylinder diameter of ten inches or less of optimally moderated 3.5 w/o enriched UO_2 would be required to achieve an acceptable reactivity. Thus Configuration 11 was expected to be critical assuming fresh fuel. Configuration 10 was found to be critical as anticipated and assessment of the burnup effects was made.

The potential configurations and the anticipated results are summarized in Table 2. Configurations 1, 2, 6 and 10 were explicitly evaluated in this waste package criticality study. It was intended that the four configurations

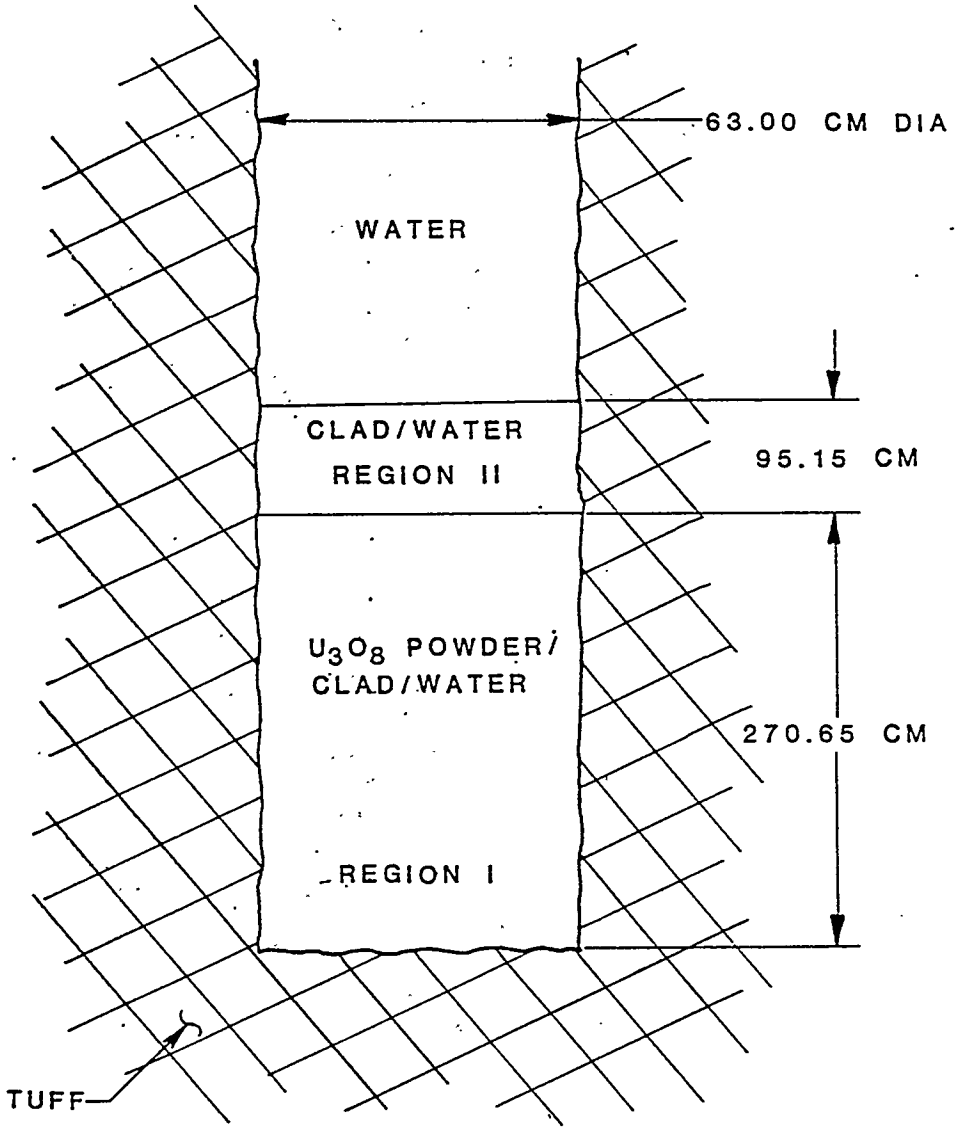


Figure 4. Configuration 10 Geometry

TABLE 2: POTENTIAL CONFIGURATIONS - EXPECTED RESULTS

CONFIGURATION NUMBER	DESCRIPTION	EXPECTED RESULTS ASSUMING FRESH FUEL	CREDIT FOR DEPLETION
1**	Nominal Configuration - Dry	Subcritical	Subcritical
2**	Nominal Configuration - Flooded	Subcritical	Subcritical
3	Nominal Configuration - Partial Flooding	Subcritical	Subcritical
4	Structure* Gone - Rods Uniformly Spaced - Dry	Subcritical	Subcritical
5	Structure Gone - Rods Uniformly Spaced - Flooded	Uncertain	Subcritical
6**	Container Partially Gone - Optimal Rearrangement of Rods - Flooded	Critical	Subcritical
7	Structure and Clad Gone - Pile of Pellets - Dry	Subcritical	Subcritical
8	Structure and Clad Gone - Pile of Pellets - Flooded	Subcritical	Subcritical
9	Structure and Clad Gone - Pellets Disintegrated to Powder - Dry	Subcritical	Subcritical
10**	Clad and Disintegrated Pellets (Powder) Optimally Mixed - Flooded	Uncertain	Subcritical
11	Structure and Clad Gone - Pellets Disintegrated to Powder - Flooded	Critical	Subcritical

*Structure is defined as container and canister.
**Denotes configurations evaluated.

selected for evaluation would provide an initial assessment covering the wide range of potential configurations and conditions from the nominal case to a worst case. Configurations 1, 2, 6 and 10 provide a logical sequence in increasingly deteriorated conditions. Configuration 1 is the nominal configuration at emplacement and is of obvious interest as the base case. Configuration 2 represents what is probably the most severe, in terms of reactivity increase, single abnormal occurrence - flooding. Configuration 6 represents a class of potential configurations which result from two abnormal occurrences, that is, failure to maintain the tightly-packed rod geometry and flooding. For completeness, Configuration 10 represents a worst case scenario, assuming multiple failures; in this case, structure failure, clad failure, pellet disintegration and flooding.

4.0 Method of Analysis

The nuclear criticality analyses employed the current version of the AMPX modular code system, which includes a 218 group cross section library, and the KENO-IV Monte Carlo criticality program, all developed by the Oak Ridge National Laboratory. The cross section set and codes were thoroughly qualified by the Westinghouse Nuclear Fuel Division by comparing predicted results with critical experiments (References 6 and 7). AMPX and KENO-IV are used extensively in the licensing process in the nuclear industry, especially for criticality safety calculations.

The accuracy of AMPX-KENO is excellent as judged by comparing its predictions of k-effective to critical experiments. Fifteen criticals of thermal systems were analyzed with the result that the average k-effective predicted by AMPX-KENO was 0.9986 with a sample population standard deviation of the k-effective values being 0.005.

The several codes used in these analyses are shown in Figure 5 and a summary of each code used in the analyses follows.

4.1 Cross Section Library

A 218 group cross section library developed by Oak Ridge, (Reference 8), from ENDF/B-IV data, (Reference 9), was used in the criticality analyses. Unresolved resonances are implicitly included. The 218 energy group structure consists of 140 fast groups and 78 thermal groups below 3.05 eV which contain upscatter cross sections.

4.2 NITAWL

The 218 group library does not contain resolved resonance cross sections; these are dependent on the geometry of the configuration being studied. NITAWL (Nordheim's Integral Treatment and Working Library Production), (Reference 10),

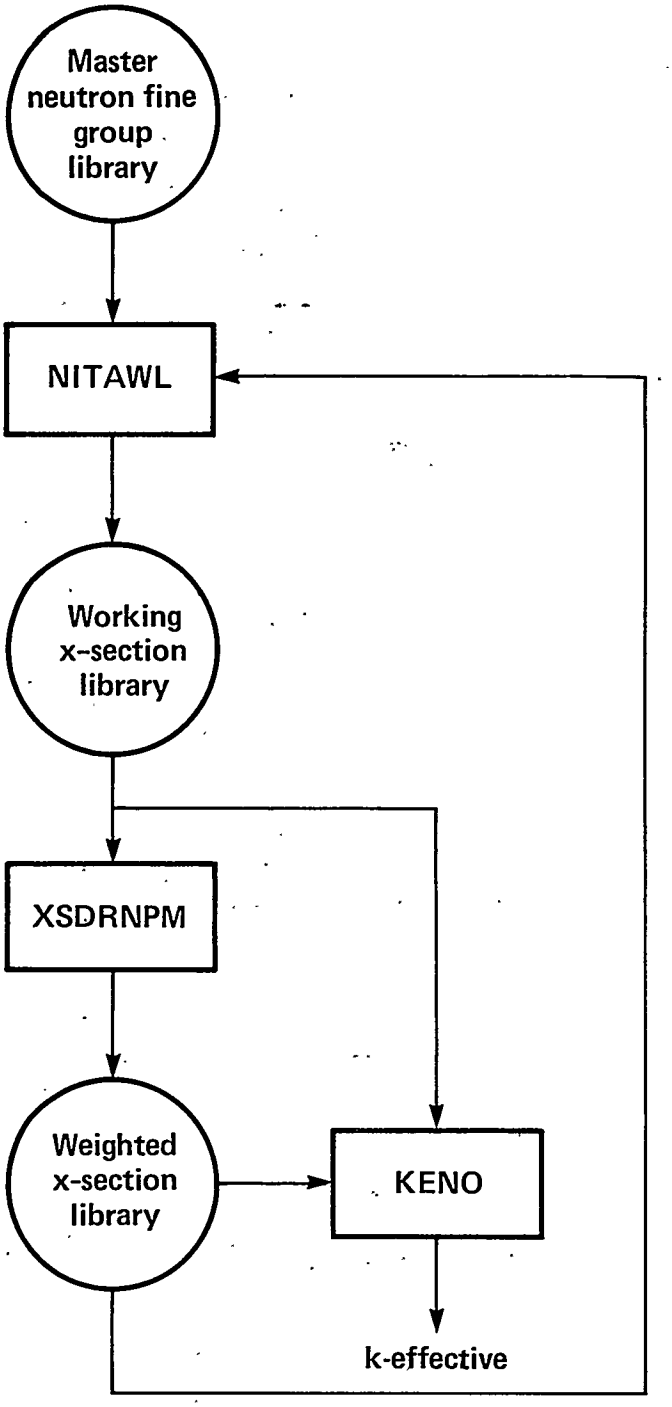


Fig. 5. Modules of the AMPX-KENO system

performs resonance self-shielding calculations and collects data into working libraries for use in either the XSDRNPM module of the AMPX system or the KENO-IV Monte Carlo code.

4.3 XSDRNPM

XSDRNPM (XSDRN with Petrie Modifications), (Reference 10), is a one-dimensional S_n transport theory code which is used to generate 19 group cross sections for use by KENO from the 218 group library generated by NITAWL. The 19 group energy structure, suggested by Oak Ridge, contains 12 fast groups and 7 thermal (below 3.05 eV) groups. It is similar to the Hansen-Roach 16 group structure except that there are more thermal groups in the Oak Ridge 19 group set, thereby making it more appropriate for use in thermal systems. Hence, XSDRNPM is principally used to energy and spatially collapse the 218 group cross sections to a 19 group set. The collapsed cross sections from XSDRNPM are output in a format for use in either the NITAWL or KENO-IV codes.

4.4 KENO-IV

KENO-IV, (Reference 11), is a multigroup Monte Carlo criticality program used to calculate the multiplication factor (k-effective) of systems having even complex three-dimensional geometries. The code is limited to P_1 order of scattering. KENO-IV utilizes a weighted tracking method and the weights are specified by region and group. The purpose of weighting is to improve the statistical accuracy of k-effective per unit tracking time.

4.5 Uncertainty Analysis

The uncertainty in the KENO-IV nominal calculated K_{eff}, at a 95% probability, 95% confidence level, was computed using the following equations:

$$U = ((U_b)^2 + (U_K)^2)^{1/2} \quad (1)$$

$$U = ((U_b)^2 + (U_K)^2 + (U_p)^2 + (U_I)^2)^{1/2} \quad (2)$$

where:

U = 95/95 total uncertainty,
U_b = 95/95 uncertainty in the method relative to "benchmarking" the code,
U_K = 95/95 uncertainty in the individual KENO-IV calculation,
U_p = 95/95 uncertainty in plutonium reactivity,
U_I = 95/95 uncertainty in reactivity as a function of fuel irradiation.

Equation 1 applies to those problems with fuel enriched at 4.5 w/o U^{235}. Equation 2 applies to those problems with fuel enrichments less than 4.5 w/o U^{235} for which fuel burnup credit was assumed.

The uncertainties, U_p and U_I, in Equation 2 are involved with the equivalencing of low U^{235} enrichments in fuel for which burnup credit has been applied.

In this analysis the values used for the above uncertainties were determined to be:

U_b = 0.0133
U_K = 2 standard deviations from KENO (see Table 8)
U_p = .009
U_I = .009

Table 3 shows the calculational statistics obtained from analyses of the Battelle criticals, (References 6 and 7) (wet) using the AMPX-KENO methodology. U_b was calculated using these statistics. U_p and U_I were obtained from previous Westinghouse Nuclear Fuel Division work (Reference 12).

4.6 Accounting for Fissile Inventory Depletion

The assumption of fresh fuel for spent fuel storage criticality studies has been shown to be a very conservative assumption. Although this approach is the simplest and is used typically where acceptable results are obtained, recently-licensed designs of spent fuel storage racks have been based on taking credit for the fissile inventory depletion which results from irradiation of the

TABLE 3: BENCHMARK CALCULATION STATISTICS

	Battelle Criticals (wet)
Number of Experiments	15
Average k_{eff} ($\overline{k}_{eff}$) calculated using the AMPX-KENO methodology	0.9986*
Standard Deviation (S_1)	0.0052
One-Sided Tolerance Limit Factor for 95-95 (K_1)	2.57
Bias ($1.0-\overline{k}_{eff}$)	0.0014
$U_b = K_1 S_1$	0.0133

*Note that the accuracy of AMPX-KENO is excellent when comparing its predictions of k-effective to the Battelle critical experiments.

fuel. Demonstration of criticality safety in the geologic disposal of spent fuel will also require taking credit for fuel burnup.

A concept referred to as reactivity equivalencing was used by Westinghouse Nuclear Fuel Division (NFD) personnel in the design and licensing of spent fuel storage racks for Arkansas Power and Light, Reference 12. As the fuel is irradiated, the amount of fissile material becomes depleted. For a given geometry, for example - an intact fuel assembly in water, the reactivity of that configuration is determined largely by the amount of fissile material present. It follows then that a fuel assembly which was initially 4.5 w/o U^{235}, but has been irradiated to 36,000 MWD/MTU would have a lower reactivity than a similar assembly with fresh fuel (zero burnup). Likewise, an assembly with some lower initial enrichment, say 3.5 w/o, and a lower burnup, perhaps 28,000 MWD/MTU would have the same reactivity as the depleted 4.5 w/o initial enrichment assembly. Similarly an assembly of initial enrichment of 2.0 w/o depleted to 8,000 MWD/MTU could also have the same reactivity. As a limit, there is an initial enrichment (in this example, 1.4 w/o) at which the assembly has the same reactivity at zero burnup. For a given configuration, if the assembly burnup is plotted versus the initial enrichment which yields the desired reactivity value, a constant reactivity contour can be constructed, as shown in Figure 6. In this example, the reactivity contour ranges from 4.1 w/o initial enrichment and 36,000 MTU/MWD burnup to 1.4 w/o initial enrichment and zero burnup. (This contour is for a spent fuel storage rack design, not a single assembly.) Any initial enrichment/burnup combination to the left or above the contour would have a lower reactivity, and therefore be acceptable; but any combination to the right or below the contour would have an unacceptable higher reactivity. The term reactivity equivalencing refers to the method used to construct the constant reactivity contour.

The motivation for undertaking this effort is derived from the limitation of existing Monte Carlo computer codes, such as KENO-IV. These codes do not calculate fuel depletion or include fission products in the cross section libraries. Thus, while KENO-IV is the preferred code for reactivity determination, it is limited to evaluation of fresh fuel configurations. By using the

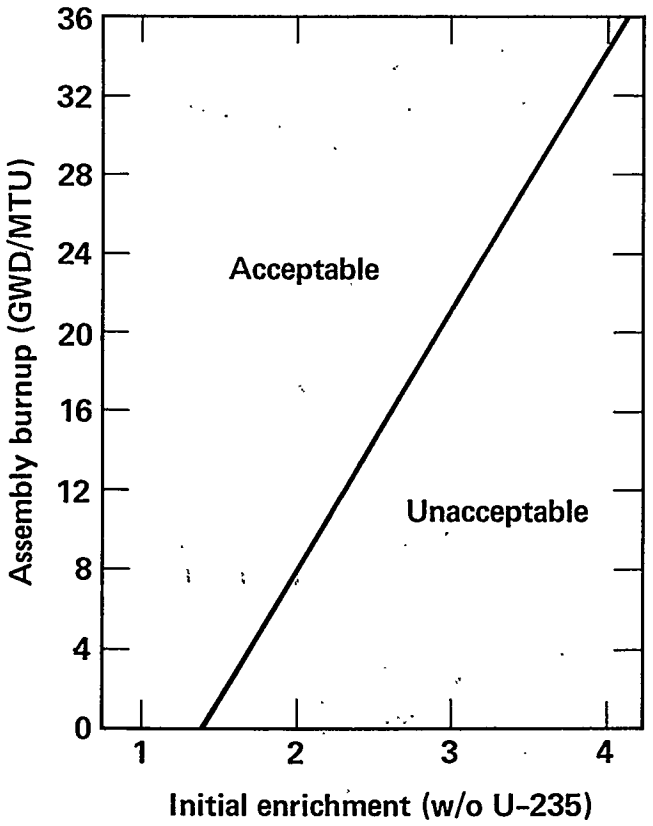


Fig. 6. Minimum burnup vs. initial enrichment

equivalent zero burnup initial enrichment, obtained by reactivity equivalencing, in the KENO-IV code, the reactivity of a configuration actually containing depleted fuel can be calculated.

In reactivity equivalencing, depletion codes are used to calculate the isotopic compositions and cross sections of the fuel as a function of irradiation history and subsequent decay time. These cross sections are input to a diffusion code which is used to determine the reactivity of the configuration of interest assuming various combinations of initial enrichment and burnup. A constant reactivity contour is constructed of burnup versus initial enrichment. The enrichment which corresponds to the zero burnup intercept is then used in a Monte Carlo code to perform a detailed reactivity calculation of the configuration being evaluated.

Westinghouse NFD personnel use the CINDER and LEOPARD depletion codes (References 13 and 14, respectively) and the TURTLE diffusion code (Reference 15) for reactivity equivalencing and AMPX-KENO for the actual reactivity calculations. One advantage of this approach is that CINDER/LEOPARD/TURTLE are used only to calculate relative reactivities as a function of irradiation (a calculational ability qualified by many years of reactor design experience) while the actual reactivity determination is performed by the more powerful AMPX-KENO method.

The actual reactivity change which results from accounting for fuel burnup is, of course, dependent upon many parameters including the fuel type, geometry, initial enrichment and burnup. The significance of taking credit for fuel burnup is demonstrated by Reference 1 and 12 results. These studies showed, respectively, a reduction of approximately 0.01 ΔK per 1000 MWD/MTU for PWR assemblies and a 0.188 ΔK reduction for a fresh to 21,000 MWD/MTU burnup B&W 15 x 15, 3.1 w/o U^{235} initial enrichment assembly.

For this study, where the assumption of fresh fuel resulted in a reactivity which is unacceptable from a criticality safety point of view, additional KENO calculations were performed for those configurations to define the maximum acceptable equivalent zero burnup enrichment. Additional CINDER/LEOPARD/TURTLE

calculations are beyond the scope of this evaluation; therefore, the maximum acceptable zero burnup enrichments were compared with existing reactivity equivalence results. It is concluded that, based on this comparison, sufficient information exists to provide an assessment of the criticality safety including credit for fissile inventory depletion. It is also possible to determine the usefulness of performing the reactivity equivalencing calculations for these configurations.

5.0 Selection of Parameters

The present design of waste packages for disposal of spent fuel in a tuff geology is dictated by, among other things, a desire to accommodate the many types of fuel assemblies which will require disposal. Because detailed evaluation of all the fuel configurations was beyond the scope of this study, a reference fuel/package concept was chosen.

Definition of this typical or reference fuel assembly required selection of numerous parameters including: 1. fuel type (PWR vs BWR); 2. assembly manufacturer (Westinghouse, General Electric, etc.); 3. assembly size (15 x 15, 17 x 17, etc.); 4. fuel enrichment; and 5. burnup of fuel (fresh or depleted). Once the reference fuel assembly was chosen, this determined the number of assemblies per containers (i.e. number of fuel rods) and the dimensions of the container structure. The choice of the reference fuel assembly was predicated on a desire to obtain results which are conservative but within the realm of realism and, as much as possible, typical. The reference fuel assembly was chosen to be a Westinghouse PWR standard 17 x 17 assembly with fresh UO_2 enriched to 4.5 w/o U^{235}. The reference waste package contains 1584 spent fuel rods (six assemblies worth of rods).

The choice of PWR over BWR fuel was relatively straight forward. In general, PWR fuel assemblies are more reactive than BWR assemblies. The PWR assemblies have higher initial uranium loadings (475 kg typical PWR, 197 kg typical BWR) and higher average U^{235} enrichments (3.5 w/o PWR, 2.6 w/o BWR). Studies reported in the literature have shown a standard PWR assembly to be more reactive than two and three BWR assemblies (References 1 and 4, respectively). On the other hand, the reference package would contain eighteen BWR assemblies versus only six PWR assemblies and the reference configuration is for consolidated rather than boxed fuel rods. As a result the total U^{235} content for the two packages would be similar, and the BWR configuration should be evaluated at a later date.

The Westinghouse 17 x 17 fuel assembly was selected as being a "typical" PWR assembly. It is, at present, the most populus type of assembly for disposal and has been used most frequently in relevant criticality studies reported in the literature.

The choice of 4.5 w/o U^{235} fresh fuel was made to ensure applicability of the results of this evaluation to the newer fuels now being designed and put into use. Historically, 3.5 w/o U^{235} has been used as a conservative average PWR fuel enrichment. However, fuel is now being designed for higher burnups and therefore includes higher initial enrichment. Present designs assume 4.0 w/o with plans to increase the enrichment to 4.2 to 4.4 w/o in coming years. Use of a 4.5 w/o reference enrichment should provide realistic results but with adequate conservatism to cover all of the old and newer fuel assembly designs.

The assumption of fresh UO_2 fuel is certainly more conservative than depleted fuel for criticality studies. Where results allow, this method is more straightforward; but as previously stated, some of the configurations were found to be critical assuming fresh fuel. Also as previously discussed, the reactivity worth of accounting for depletion was assessed as needed using methods currently accepted for spent fuel storage licensing.

Consideration was also given to the composition of the fuel following disintegration of the fuel pellets. The actual composition would be dependent upon the specific geochemical conditions under which the disintegration occurred. Scenarios could be developed in which various combinations of UO_2, UO_3, U_4O_9, U_3O_8 and other intermediate states would occur. But, based on discussions with Westinghouse Nuclear Fuel Division personnel, it is judged that the reactivity of this configuration will not be very sensitive to the actual composition. For example, a variation of less than one percent in reactivity would be expected in assuming UO_2 versus U_3O_8. Assuming a fixed amount of uranium present, the geometry is determined by the assumed porosity of the fuel powder. This porosity would not change significantly with choice of fuel composition. The porosity in turn determines the amount of water present which is a much more significant parameter in the criticality analysis. The choice of fuel

composition only effects the density of uranium in the mixture (slightly) and the concentration of the oxygen (UO_2 or $UO_{2.25}$ ($=U_4O_9$) or $UO_{2.67}$ ($=U_3O_8$)). To maximize the amount of water and the diameter of the configuration (i.e., increase the reactivity), all of the container and canister were assumed to be gone. A powder porosity of 50 percent and a uranium to oxygen ratio of 2.67 (consistent with U_3O_8) were assumed. The expected small variations due to powder composition could be determined after the more significant uncertainties in powder porosity and credible disintegration scenarios have been addressed.

6.0 Analytical Models

Each of the four configurations analyzed required a somewhat different application of the computer codes discussed in the methods of analysis section. This section describes the specifics relative to each analytical model. The basic fuel parameters upon which the analyses are based are given in Table 4. The basic material parameters for the canister, container, and tuff are given in Table 5.

6.1 Configuration 1

6.1.1 KENO-IV Geometry

Figure 7 is a section through the borehole in tuff showing one half of the canister and three of the six sections of the fuel rod container. The canister is a stainless steel right circular cylinder, 1 cm thick, with an inside radius of 27.5 cm. It is located at the center of a borehole in a tuff environment. The radius of the borehole is 31.5 cm. The container which holds the fuel rods, 264 rods per section, is made of carbon steel with a wall thickness of 0.198 cm, resulting in 0.396 cm of steel between adjacent fuel zones. The inside distance across the flats of the hexagon formed by the six sections is 26.24 cm and the outside radius of the cylinder formed by the six sections is 25.569 cm. The computer model used the surface equations shown on Figure 7 which is to scale. The KENO-IV geometry for Configuration 1 is exactly as shown on Figure 7 since the equations input to KENO-IV are identical to those shown on the sketch with the exception of the outside boundaries of the tuff region. The tuff extends from x = -61.5 cm to x = +61.5 cm and from y = 0.0 to y = 61.5 cm. It forms a square in the x-y plane when reflected by the reflective surface in KENO-IV. Top and bottom planes in the Z dimension enclose the configuration; both are specified as "reflective", which in effect extend the geometry to infinity in the "Z" (axial) dimension. The outside lat- eral sides of the tuff zone are specified as vacuum boundaries. However, the

TABLE 4: BASIC FUEL ROD PARAMETERS

BASIC FUEL ROD PARAMETERS

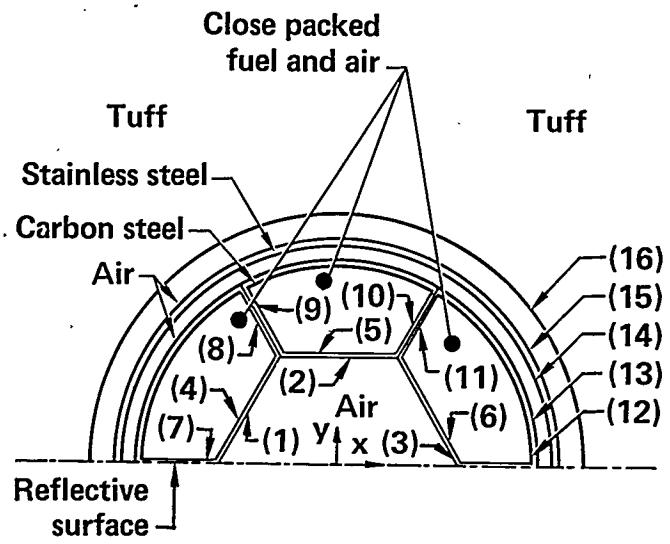
TYPE OF FUEL	= WESTINGHOUSE 17x17 STD.
ENRICHMENT	= 4.5 W/O U-235
FUEL PELLET OD	= .3225 IN. (.81915 CM)
CLAD OD	= .374 IN. (.94996 CM)
CLAD THICKNESS	= .0225 IN. (.05715 CM)
FUEL PELLET DENSITY	= 95% THEORETICAL (10.412 GM/CC)
PELLET DISHING	= 1.2012%
PELLET STACK DENSITY	= 10.287 GM/CC

TABLE 5: BASIC MATERIAL COMPOSITIONS USED IN ANALYSES

BASIC MATERIAL COMPOSITIONS USED IN ANALYSIS

ITEM	MATERIAL	COMPOSITIONS (W/O)	
Canister	Stainless Steel (density = 7.9 g/cm^3)	Cr	18.0
		Mn	1.0
		Ni	8.0
		Fe	72.0
		Traces	1.0
Container	Carbon Steel (density = 7.88 gm/cc)	Fe	98.92
		C	0.18
		Mn	0.90
Rock	Tuff (dry)* (density = 2.2 gm/cc)	SiO_2	69.7
		Al_2O_3	15.6
		Fe_2O_3	1.1
		FeO	0.58
		MgO	0.64
		CaO	1.1
		Na_2O	4.1
		K_2O	6.6
		Others	.58

*Wet Tuff contains 2.2 grams of rock plus 0.26 grams of water per cubic centimeter.



N	Equation for surface (N)
1	$1.73205X - Y + 26.2445 = 0$
2	$Y - 13.12 = 0$
3	$1.73205X + Y - 26.2445 = 0$
4	$1.73205X - Y + 26.6405 = 0$
5	$Y - 13.318 = 0$
6	$1.73205X + Y - 26.6405 = 0$
7	$Y - 0.198 = 0$
8	$1.73205X + Y + 0.396 = 0$
9	$1.73205X + Y - 0.396 = 0$
10	$1.73205X - Y + 0.396 = 0$
11	$1.73205X - Y - 0.396 = 0$
12	$X^2 + Y^2 - 643.6876 = 0$
13	$X^2 + Y^2 - 653.7738 = 0$
14	$X^2 + Y^2 - 756.25 = 0$
15	$X^2 + Y^2 - 812.25 = 0$
16	$X^2 + Y^2 - 992.25 = 0$

Fig. 7. KENO geometry for configuration 1

thickness of the tuff in the lateral dimension (minimum of 30 cm) virtually eliminates any significant neutron leakage from the KENO-IV geometry model.

The atom densities for the KENO zones shown on Figure 7 are tabulated in Tables 6 and 7 for fuel and nonfuel zones, respectively. These tables are self-explanatory and also include atom densities of KENO-IV zones for the other three configurations.

6.1.2 Cross Sections

To prepare cross sections for Configuration 1, two NITAWL calculations and two XSDRNPM calculations were required. The first NITAWL using the 218 group library previously discussed, does resonance self-shielding calculations for isotopes of concern and produces a 218 neutron group working library. The NITAWL calculations are sensitive both to fuel rod parameters (Table 4) and to the rod packing configuration of an array of rods. For Configuration 1, the rods are packed in a triangular pitch in each container section. Calculations, based on 284 rods per container section, show that the volume fraction of rods in the container inside space is 0.8113 which yields an equivalent triangular pitch of 1.0044 cm. (This value may be compared to a triangular pitch of 0.94996 cm which assumes that the rods are all in contact with each other.) The input data for NITAWL was based on the larger value of pitch.

Two XSDRNPM calculations were performed to reduce the 218 neutron group cross sections to 19 groups for the KENO-IV code. The first XSDRNPM problem was a cylindrical unit cell model explicitly defining the fuel pellet, gap and clad, and air space outside the clad preserving the rod volume fraction of 0.8113. The cross sections for the fuel zone materials were weighted over the entire cell since the KENO-IV code models the fuel zone as an homogenized mixture of isotopes bounded by the carbon steel container. The second XSDRNPM problem is a large cylindrical model based on the Figure 7 geometry which contains the following 8 zones beginning at the center: air, carbon steel, homogenized fuel zone, carbon steel, air, stainless steel, air, and tuff. Referring to Figure 7, the hexagonal air space and the inner container steel plates were modeled in the XSDRNPM as a right circular cylinder and annulus by preserving the cross

TABLE 6: FUEL ZONE ATOM DENSITIES (ATOMS/BARN-CM) USED IN KENO ANALYSES

TIGHT PACKED RODS (CONFIGURATIONS 1, 2 & 6)

	4.5 W/O*		1.0 W/O	2.0 W/O
	DRY	FLOODED	FLOODED	FLOODED
U-235	6.3085(-4)	6.3085(-4)	1.4020(-4)	2.8040(-4)
U-238	1.3220(-2)	1.3220(-2)	1.3705(-2)	1.3567(-2)
O-16	2.7703(-2)	3.4010(-2)	3.400(-2)	2.4003(-2)
Zr	7.9380(-3)	7.9380(-3)	7.9380(-3)	7.9380(-3)
H	--	1.2619(-2)	1.2619(-2)	1.2691(-2)
N	8.0800(-6)	--	--	--

LOOSE DISPERSED RODS (CONFIGURATION 6)(FLOODED)

	4.5 W/O	1.0 W/O	2.0 W/O
U-235	2.7154(-4)	6.0349(-5)	1.2070(-4)
U-238	5.6903(-3)	5.8992(-3)	5.8396(-3)
O-16	3.3686(-2)	3.3681(-2)	3.3682(-2)
Zr	3.4168(-3)	3.4168(-3)	3.4168(-3)
H	4.3524(-2)	4.3524(-2)	4.3524(-2)

FUEL POWDER/CLAD/WATER MIX (CONFIGURATION 10)

	4.5 W/O	1.6 W/O
U-235	3.7730(-4)	1.3416(-4)
U-238	7.9057(-3)	8.1467(-3)
O-16	3.7447(-2)	3.7441(-2)
Zr	3.5210(-3)	3.521(-3)
H	3.0718(-2)	3.0718(-2)

*W/O Refers to U-235 Enrichment of Uranium

Note: Numbers in Parentheses refer to Powers of 10.

TABLE 7: NONFUEL ZONE ATOM DENSITIES (ATOMS/BARN-CM) USED IN KENO ANALYSES

ELEMENT	DRY TUFF	FLOODED TUFF	CARBON STEEL	STAINLESS STEEL	WATER	WATER + CLAD*	AIR
O-16	3.540(-2)	4.409(-2)			3.344(-2)	3.072(-2)	9.600(-6)
H		1.739(-2)			6.688(-2)	6.144(-2)	
Zr						3.521(-3)	
N							4.280(-5)
Si	1.537(-2)	1.537(-2)					
Fe	1.983(-4)	1.983(-4)	8.408(-2)	6.134(-2)			
Cr				1.647(-2)			
Ni				6.485(-3)			
Mn			7.761(-4)	8.660(-4)			
Ca	2.599(-4)	2.599(-4)					
K	9.284(-4)	9.284(-4)					
Mg	2.104(-4)	2.104(-4)					
Na	8.765(-4)	8.765(-4)					
Al	2.027(-3)	2.027(-3)					
C			7.100(-4)				

* This represents the zone above the fuel zone in Configuration 10.

Note: Numbers in parentheses refer to Powers of 10.

sectional area of the air and steel zones. All other radial dimensions of the XSDRNPM zones are exact relative to the geometry shown in Figure 7. The tuff was modeled as a 30 cm thick annulus. In this XSDRNPM problem, the cross sections were zone weighted over the fluxes in the zones of interest (i.e., all zones excluding the fuel zone) to produce 19 group region dependent cross sections for all elements in zones outside the fuel.

The purpose of the second NITAWL problem was to combine the results from the two XSDRNPM problems to produce a library of cross sections for use in the KENO-IV code.

6.2 Configuration 2

6.2.1 KENO-IV Geometry

Figure 8 shows the geometry for Configuration 2 which is identical to Configuration 1 except the air has been replaced by water. The KENO-IV input data from a geometry viewpoint is identical to that used in Configuration 1. From a material composition standpoint, the atom densities used for Configuration 2 regions are tabulated in Tables 6 and 7.

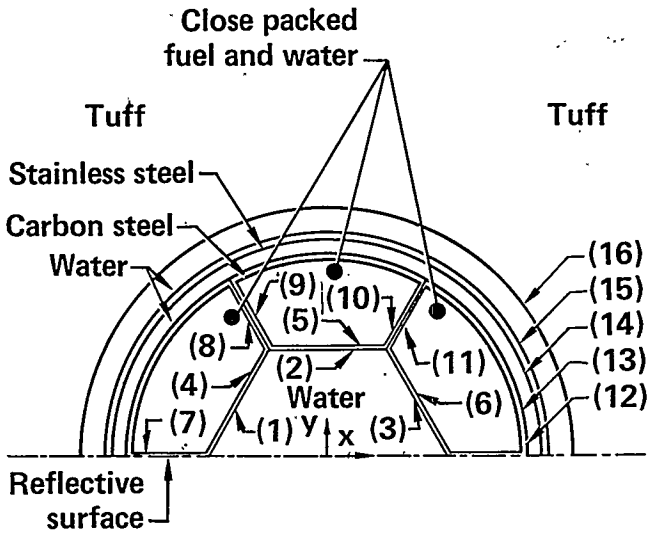
6.2.2 Cross Sections

The addition of water to this configuration required that a different set of neutron cross sections be developed relative to those used in Configuration 1. The same techniques were applied as previously discussed; i.e., a NITAWL problem to calculate resonances, two XSDRNPMs, one to reduce the 218 group library to 19 groups for cell-weighted fuel zone elements and the other to prepare zone-weighted cross sections for nonfuel zones.

6.3 Configuration 6

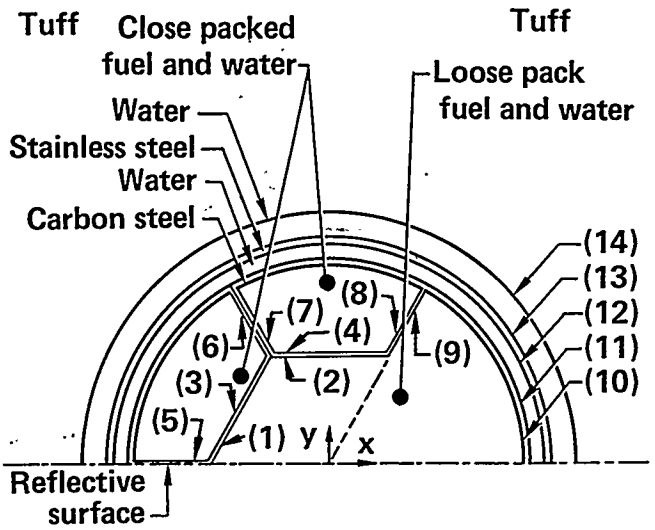
6.3.1 KENO-IV Geometry

Figure 9 shows the Configuration 6 geometry which is similar to Configurations 1 and 2 except that two adjacent sections of the container have failed, thus allowing the inventory of rods in those two sections to disperse into the central zone of the configuration, indicated as loose packed fuel and water in



N	Equation for surface (N)
1	$1.73205X - Y + 26.2445 = 0$
2	$Y - 13.12 = 0$
3	$1.73205X + Y - 26.2445 = 0$
4	$1.73205X - Y + 26.6405 = 0$
5	$Y - 13.318 = 0$
6	$1.73205X + Y - 26.6405 = 0$
7	$Y - 0.198 = 0$
8	$1.73205X + Y + 0.396 = 0$
9	$1.73205X + Y - 0.396 = 0$
10	$1.73205X - Y + 0.396 = 0$
11	$1.73205X - Y - 0.396 = 0$
12	$X^2 + Y^2 - 643.6876 = 0$
13	$X^2 + Y^2 - 653.7738 = 0$
14	$X^2 + Y^2 - 756.25 = 0$
15	$X^2 + Y^2 - 812.25 = 0$
16	$X^2 + Y^2 - 992.25 = 0$

Fig. 8. KENO geometry for configuration 2



N	Equation for surface (N)
1	$1.73205X - Y + 26.2445 = 0$
2	$Y - 13.12 = 0$
3	$1.73205X - Y + 26.6405 = 0$
4	$Y - 13.318 = 0$
5	$Y - 0.198 = 0$
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12	$X^2 + Y^2 - 756.25 = 0$
13	$X^2 + Y^2 - 812.25 = 0$
14	$X^2 + Y^2 - 992.25 = 0$

Fig. 9. KENO geometry for configuration 6

Figure 9. Note on Figure 9 that only one section is shown as failed. However, the reflective surface in the model implies the other failed container section as well as the other two intact sections. The reactivity of the array of dispersed rods depends strongly on the degree of dispersal. Calculations show that if the 528 rods uniformly fill all of the available space as shown on Figure 9, an equivalent square rod pitch would be 1.4246 cm. For comparison, the rod pitch of the Westinghouse 17 x 17 standard fuel assembly is 1.2598 cm. It might be postulated that the dispersed rods would be more reactive if the available space were not quite filled with dispersed rods. However, calculations have indicated that the reactivity for an array of rods increases if the standard rod pitch is increased and peaks at a pitch greater than the 1.4246 cm computed for uniform dispersal. Therefore, for the sake of conservatism, the KENO-IV model was based on the rods uniformly filling the available space with an equivalent rod pitch of 1.4246 cm. The atom densities for Configuration 6 are given on Tables 6 and 7.

6.3.2 Cross Sections

For Configuration 6 with fuel at 4.5 w/o U^{235} enrichment, it was possible to use cross sections already developed for Configuration 2, i.e., fuel zone isotopes for the tight parked fuel zones and those in zones outside the fuel zones. It was, however, necessary to compute, using the NITAWL/XSDRNPM technique, cross sections for isotopes in the dispersed rod fuel zone. The XSDRNPM problem for this case used the cell-weighting technique for the fuel zone isotopes in a unit cell based on an equivalent rod pitch of 1.4246 cm.

As shown on Table 6, Configuration 6 was also analyzed for fuel enrichments of 1.0 and 2.0 w/o U^{235} enrichments. Consequently, it was necessary to develop cross sections for fuel zones at those enrichments using the NITAWL/XSDRNPM codes for the fuel zones, both close packed and dispersed rod zones. The cross sections for zones outside the fuel zones did not need to be recalculated; hence, the same set was used that had been employed for Configuration 2.

6.4 Configuration 10

6.4.1 KENO-IV Geometry

Figure 10 shows a vertical section of Configuration 10 as modeled in KENO-IV. The drawing is to scale and is self-explanatory. The atom densities used in KENO-IV are given on Tables 6 and 7. It can be inferred from the drawing that a minimum thickness of tuff of 30 cm is modeled on the side and bottom. All external surfaces were specified as "vacuum" boundaries, but the relatively large path from the fuel to the boundaries eliminates any significant neutron leakage from the system.

6.4.2 Cross Sections

The cross sections used for the wet tuff for Configuration 10 were the same as those developed for the wet tuff in Configuration 2. This model has a truly homogenized fuel zone and, consequently, the NITAWL run which computes the resonances was run using the homogenous Nordheim treatment instead of the cylindrical model used for the Configurations 1, 2 and 6 fuel rods.

The XSDRNPM problem for Configuration 10 also was run differently than for Configurations 1, 2 and 6. For Configuration 10, a slab geometry was modeled with a slab of fuel and a slab of water/clad mixture. The cross sections for elements in the fuel zone and water/clad zone were zone weighted over the fluxes in the respective zones to produce the 19 group cross sections required in KENO-IV.

Configuration 10 was analyzed for two fuel enrichments, 4.5 and 1.6 w/o U^{235}, and a different set of cross sections was developed for each case.

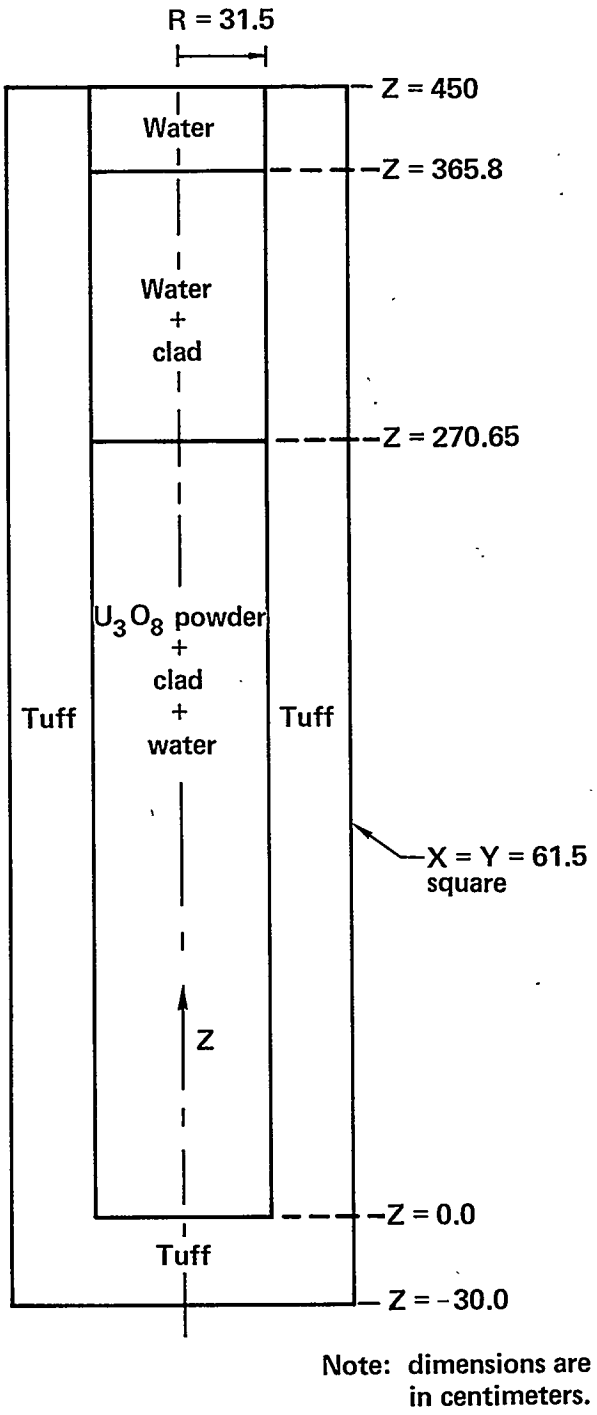

Fig. 10. KENO geometry for configuration 10

7.0 Results and Conclusions

7.1 Results

A total of seven criticality calculations were performed using the Monte Carlo computer code, KENO-IV, involving four geometric configurations and four fuel enrichments. Table 8 summarizes the results of the seven KENO-IV problems, listing the nominal neutron multiplication factor, K_{eff}, the standard deviation based on the number of neutron histories tracked by the code and the total uncertainty, U, as defined in Section 4.5.

Note in Table 8 that since the K_{eff} for Configuration 6 with fuel at 4.5 w/o was greater than 0.95, problems were run with lower enrichments (1.0 and 2.0 w/o U^{235}) in order to determine the equivalent enrichment (assuming credit for burnup) that would meet the criticality criterion.

Figure 11 graphically presents the KENO-IV results for Configuration 6 as a function of U^{235} enrichment.

For Configuration 10, one case was analyzed for a low U^{235} enrichment; namely, 1.6 w/o. The "curve" drawn on Figure 11 for Configuration 10 assumed the same shape as was observed for Configuration 6. It was necessary to run one low enrichment case for Configuration 10, since the "fresh" fuel case (4.5 w/o U^{235}) exceeded the criterion of 0.95.

7.2 Conclusions

Criticality is not a problem for the reference spent fuel waste package stored in a borehole in a vadose zone tuff geology as long as the fuel rods are maintained in the tight packed configuration for either dry or totally flooded conditions. The neutron multiplication factor, K_{eff}, for the canister fully loaded with fuel rods enriched to 4.5 w/o U^{235} under dry conditions (i.e., Configuration 1) is 0.3712 $\pm$ .0145. If the borehole, canister, and container

TABLE 8: RESULTS OF KENO-IV ANALYSES

CONFIGURATION*	FUEL ENRICHMENT (W/O U^{235})	NUMBER OF NEUTRON HISTORIES	K_{eff}	ONE STANDARD DEVIATION	U**
1	4.5	12980	0.37115	.00285	.0145
2	4.5	9735	0.68516	.00554	.0173
6	4.5	21240	1.17871	.00477	.0164
6	2.0	17405	0.99832	.00501	.0210
6	1.0	14750	0.78807	.00333	.0196
10	4.5	48085	1.16006	.00308	.0147
10	1.6	38350	0.95169	.00279	.0192

* See Figures 6 through 9 for geometric models of Configurations 1,2, 6, and 10, respectively.
** Total Uncertainty.

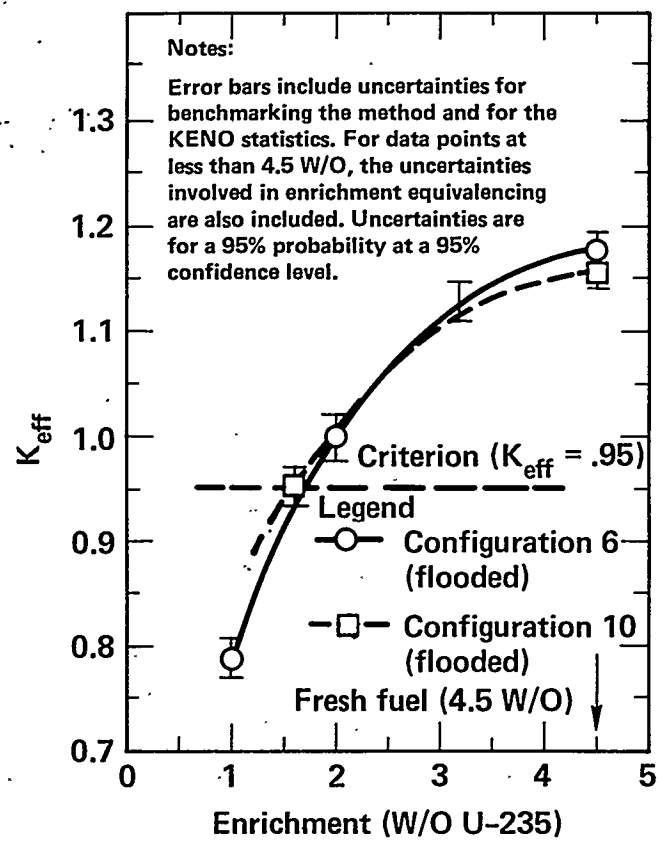

Fig. 11. K_{eff} versus fuel enrichment for deteriorated storage conditions

are flooded and the tuff is fully saturated with water (i.e., Configuration 2) the neutron multiplication factor, K_{eff}, is increased to 0.6852 $\pm$ .0173.

Configurations 6 and 10 represent severely deteriorated conditions of the waste package. If the fuel rods have an enrichment of unirradiated fuel (i.e., 4.5 w/o U^{235}) either configuration is supercritical. K_{eff} was computed to be 1.1787 $\pm$ .0164 for Configuration 6 and 1.1601 $\pm$ .0147 for Configuration 10.

However, in actual practice, it is highly unlikely that fresh fuel rods would be stored as waste and the actual waste rods would have an equivalent U^{235} enrichment of much less than the reference value of 4.5 w/o. From Figure 11, assuming a criterion of K_{eff} 0.95 with a 95% probability at a 95% confidence level, it can be seen that the equivalent U^{235} enrichment must be $\leq$1.6 w/o for Configuration 6 conditions and $\leq$1.4 w/o for Configuration 10.

Specific reactivity equivalencing calculations are needed to define the acceptable combinations of initial enrichments and burnup for the configurations. However, it is expected that these calculations will demonstrate that fuel which is acceptable for storage will also be acceptable for disposal from a criticality safety point of view. This conclusion is based on the following: 1. The acceptable zero burnup enrichments for these configurations are similar to that shown in Figure 6; 2. The Figure 6 results can be considered typical for spent fuel storage arrangements; 3. These results are consistent with the fact that fuel assemblies normally are depleted to 1 to 1-1/2 w/o U^{235}; and 4. Previous work has shown only small variations in the shape of the constant reactivity contour with different types of modules and different storage rack designs.

Furthermore, if credit is permitted for the fissile inventory depletion, assuming that the fuel can be shown to have been "burned up" to an equivalent enrichment of U^{235} of about 1.4 w/o or less, it is reasonable to believe that the storage package would be subcritical under any postulated condition.

8.0 Recommendations for Further Analysis

This evaluation represents an initial assessment of the criticality potential associated with the disposal of spent fuel in a tuff geology. Additional calculations should be performed to verify and extend the conclusions of this analysis. In the short-term, four areas should be addressed. The first need is to perform reactivity equivalencing calculations for the spent fuel configurations. These should include a range of geometries from the nominal to the fuel powder configuration to determine the variability of the equivalent zero burnup enrichment as a function of the geometry. Second, the uncertainties associated with the reactivity of the plutonium and due to irradiation of the fuel need to be better defined. Third, worst case configurations need to be identified and evaluated (e.g., define the worst case pitch for a configuration similar to Case 6, define a worst case realistic powder porosity for Configuration 10). Fourth, there is a need to determine the sensitivity of the results of these evaluations to the choice of parameters (e.g. fuel type, assembly manufacturer, assembly size, etc.)

Acknowledgments

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