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Modeling Status and Needs For Temperature Calculations Within Spent Fuel Disposal Containers

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EXECUTIVE SUMMARY

Many processes relevant to long term performance of a spent fuel waste package are sensitive to the temperature within the container and of its shell, e.g., cladding degradation, the release of ^{14}C from spent fuel, UO_2 oxidation, evaporation of moisture within the container, the likely location where wetting will occur, etc. With most processes overprediction of the temperature causes a conservative prediction of the performance. For some processes, however, this is not true. For example, overprediction in temperature leads to an overprediction of the time at which water can exist in liquid form in a waste container. For these reasons, reliable waste package temperature calculations are an important concern from a performance assessment and a licensing point of view.

Waste package temperatures depend on both internal factors, such as internal geometry, material properties, and heat loading, and on external factors, such as host rock properties and areal heat loading of the entire repository.

The primary objective of this report is to present the findings of a literature review of work pertinent to predicting *intact* waste package internal temperatures under spent fuel isolation conditions. Therefore, it is assumed that a repository scale thermal analysis has been conducted and that the exterior temperature of the waste package is known. The problem then reduces to one determined by the waste package and its properties.

Secondary objectives of this report are to identify key parameters and methodologies for performing the thermal analysis within intact waste containers, and identify sources of uncertainty in these calculations.

Based on information supplied in the latest version of the Yucca Mountain Site Characterization Plan (SCP), three basic categories of spent fuel arrangements within the disposal containers are envisioned: a) spent fuel consolidated at the repository; b) spent fuel consolidated away from the repository in a 2:1 ratio; and c) unconsolidated spent fuel assemblies. There exist conceptual designs for each of these categories. The leading design contemplates the disposal of fuel consolidated at the repository site with argon as the backfill gas.

With reference to Figure ES-1, the container for spent fuel consolidated at the repository implements an internal structure with six compartments. Within each compartment, the fuel rods occupy approximately 50% of the volume available. The rods are free to move within each compartment during handling and emplacement operations. Thus, it is unlikely that the precise geometry will be known after emplacement. For horizontal emplacement, the rods will distribute themselves under the force of gravity and it is likely that there will be large gaps

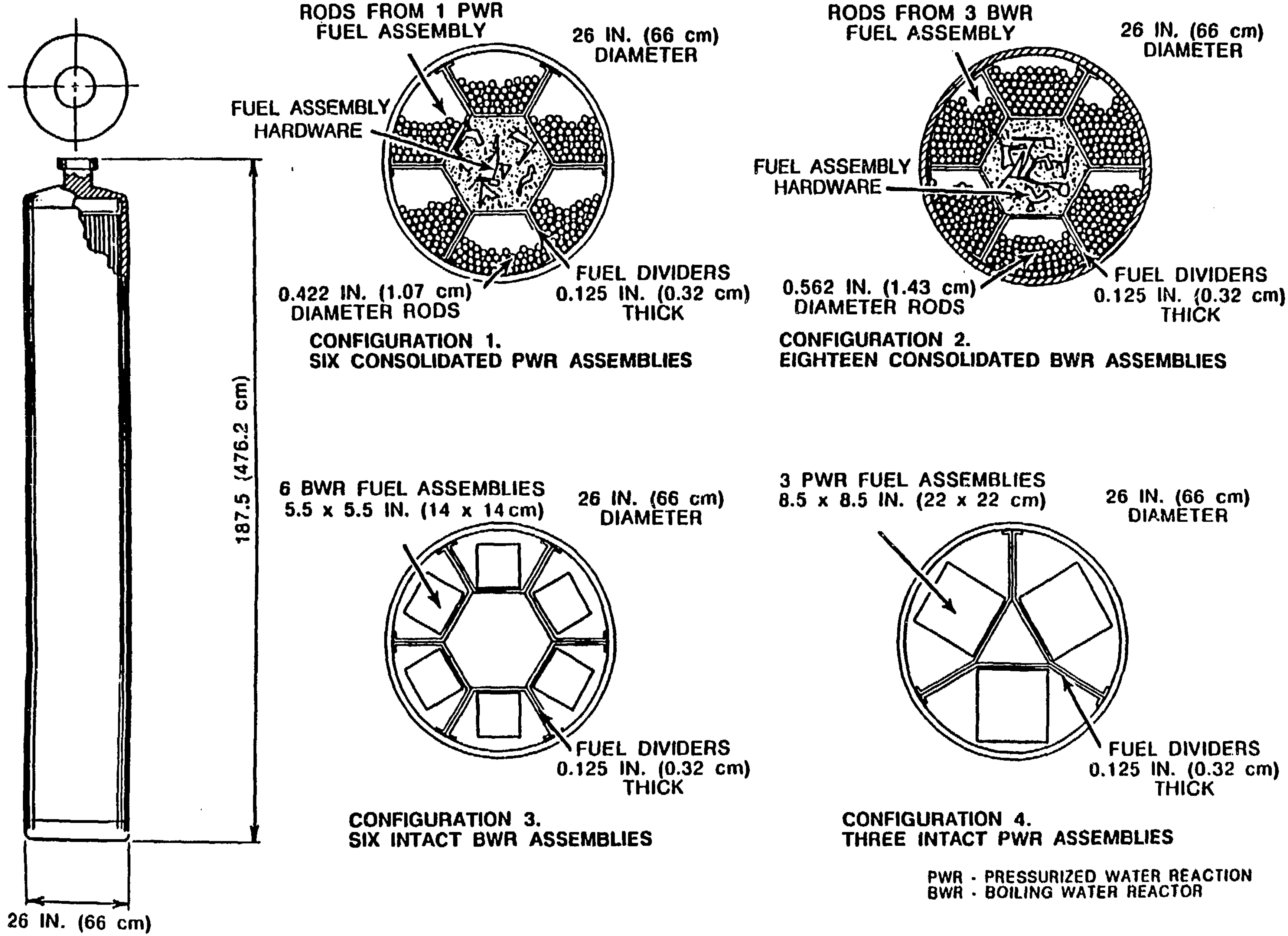

Figure ES-1 Yucca Mountain Project reference spent fuel container design (adapted from DOE, 1988).

around the container. For vertical emplacement (the reference emplacement strategy), the final location and shape of the gas gaps is not well defined.

For preconsolidated or intact spent fuel assemblies the rods are not free to move. Thus, the internal geometry in the container is more accurately known.

The waste package thermal history presented in the SCP dates back to 1984 and is for a consolidated spent fuel design that is no longer under consideration. In the original analysis, the main objective was to demonstrate that peak temperatures did not exceed design limits. However, certain assumptions may have prevented this objective from being met. In that analysis the waste package was modeled in two-dimensions as a semi-infinite cylinder. Thus, there were no axial variations in temperature. The heat generation rate was the average for the spent fuel. The consolidated fuel region was homogenized and the gaps around the fuel pins were ignored. Also, helium was the fill gas (argon, a gas with much less favorable heat transfer properties, is the present reference fill gas). Given the same boundary conditions, these assumptions are likely to produce non-conservative predictions of the temperature profile within the container.

Review of spent fuel dry storage and shipping cask systems indicates that there are many similarities between these systems and containers planned for use in geologic disposal of spent fuel. Experiments and thermal analyses have been performed for single and multi-assembly dry storage systems containing both consolidated and unconsolidated fuel. Many of the lessons learned from these experiments and analyses are applicable to spent fuel disposal containers. In particular, the following can be deduced:

a) To accurately predict temperatures within the spent fuel container requires precise knowledge of the geometry and, in particular, of the exact locations of gas gaps. Internal geometry is the most important cause of uncertainty in internal waste package temperature predictions. The internal geometry determines the dominant heat transfer mechanism, with consolidated geometries dominated by conduction and unconsolidated geometries influenced more by radiation heat transfer. Eccentricities within the container can also have a significant influence on temperature.

b) The fill gas plays an important role in determining the temperature rise across the container. This is particularly true for consolidated fuel rods, where conduction is the major heat transfer mechanism.

c) Upon consolidation of the fuel rods it is unlikely that there will be perfect contact along the rods. Ignoring rod-to-rod contact when performing the heat transfer calculations leads to only a slight overprediction of peak temperatures as compared to experimental data.

d) In the literature, a number of different methods exist to predict temperatures within dry storage systems. These range from simple semi-empirical expressions with correlation coefficients based on experimental data to three-dimensional numerical simulations of the thermal-hydraulic performance of the system. The choice of which method is best depends on the problem under study and the level of accuracy desired. Simpler models may be adequate for preliminary screening and sensitivity analysis. More elaborate models may be necessary for design basis calculations. The simpler approaches usually require symmetry or simple geometries and would require modification before they could be used for spent fuel disposal concepts. In most cases, modification would require new experiments to obtain data for the empirical models. The three-dimensional thermal-hydraulic simulations are the most accurate approaches for predicting waste package temperatures. Given a well characterized problem and a suitable experimental data base, these methods are capable of predicting temperature rises within dry storage systems to within 10%. However, due to the poorly defined geometry in the reference design case and the expense in operating and using these codes, it is not clear that their use is justified under all circumstances.

e) Axial variations in temperature can be substantial. Axially, the peak temperature was often more than 20% greater than the average. The axial variation in temperature depends on geometry, fill gas, and heat generation rate. For vertical emplacement, the interplay among these factors also causes the maximum temperature to be reached at a location above the midplane of the container, especially for gases with poorer heat transfer properties (Figure ES-2). Axial variations in temperature are important then in order to determine the peak and the average temperature within a container. The latter parameters are important for estimating the gas gap pressures in fuel rods, the partial pressure of oxidized ^{14}C within intact and partly failed containers, the oxidation rates of UO_2, and the rate of degradation of the cladding according to various processes.

The thermal analyses performed in the past that calculate waste package temperatures are inadequate for designs presented in the SCP. It is suggested that the previous analyses be updated for each of the proposed disposal configurations. The new analyses should also consider non-uniform temperatures around the borehole as a boundary condition. For vertical emplacement, the borehole will be

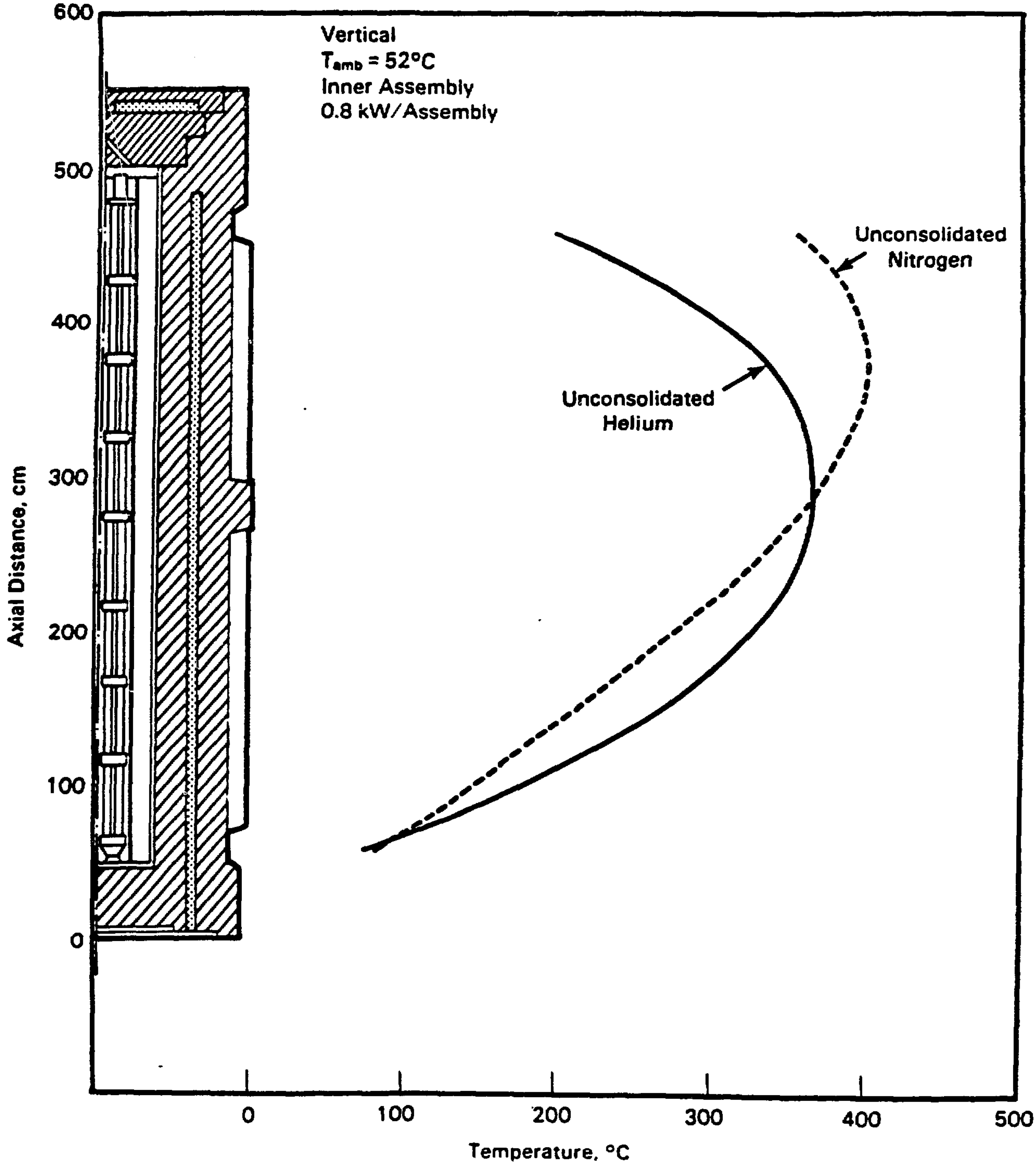

Figure ES-2 Predicted axial temperature profile predictions for unconsolidated fuel in nitrogen and helium in a CASTOR-1C dry storage cask [Rector, 1986].

cooler at the top and bottom as compared to the middle. This is due to the axially non-uniform heat generation rate within the container, to heat convection within the air gap between the borehole and the container, and to the better contact of the container with the host rock at the bottom of the borehole. This non-uniform temperature around the container will be largest during the first few hundred years when the heat generation rates are at their highest.

For containers with fuel rods consolidated at the repository, lack of a well defined geometry poses a large problem in accurate determination of internal temperatures. Sensitivity analysis for a range of geometries should be performed to determine the worst possible case.

The geometry is better defined for the preconsolidated or intact assembly designs (Configurations 3 and 4 of Figure ES-1). However, these still need to be analyzed. This need may increase in importance in view of the apparent shift in emphasis away from consolidation. The influence of eccentricities within the container should be examined through a sensitivity analysis.

A potential benefit of performing detailed thermal analysis of the waste packages is the possibility of obtaining correlations for the time-dependent temperature profile for use in system codes. The correlations could be developed as a function of different disposal configurations and external boundary temperatures.

Consideration should also be given to modeling heat transfer in breached containers. Important processes such as Zircaloy and spent fuel oxidation, wetting of the fuel, etc., will occur after breach. Breached containers will have a different gas environment and will no longer be a closed system.

Experimental results from dry storage systems provided insight into heat transfer mechanisms and provided confidence in analytical modeling results. Consideration should be given to performing similar experiments for waste container systems. In addition to increasing confidence in the modeling, the experiments could be designed to determine simple, empirical correlations which could be used for heat transfer analysis.

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1. INTRODUCTION

The Brookhaven National Laboratory (BNL) Waste Materials and Environment Modeling (WMEM) Program has been assigned the task of helping the DOE formulate and certify analytical tools needed to support and/or strengthen the Waste Package Licensing strategy. One objective of the WMEM program is to perform qualitative and quantitative analyses of processes related to the internal waste package environment, e.g., temperature, radiolysis effects, presence of moisture, etc.

Many processes relevant to long term performance of a spent fuel waste package are sensitive to the temperature within the container and of its shell, e.g., cladding degradation, ^{14}C release from spent fuel assemblies, UO_2 oxidation, evaporation of moisture within the container, the likely location where wetting would occur, etc. With most processes overprediction of the temperature causes a conservative prediction of the performance. For some processes, however, this is not true. For example, overprediction in temperature leads to an overprediction of the time at which water can exist in liquid form in a partially failed container. For these reasons, reliable waste package temperature calculations are an important concern from a performance assessment and a licensing point of view.

Waste package temperatures depend on internal factors, such as internal geometry, material properties, and heat loading, and also on external factors such as host rock properties and areal heat loading of the entire repository.

The most common approach to account for the coupling between repository and waste package temperatures involves splitting the problem into two separate calculations. First, a repository thermal analysis treating the waste package as a point, line, or areal source of heat is performed. Then, the results from this analysis are used to obtain the temperature at the exterior boundary of the waste package. This boundary temperature is used for a more detailed calculation of the waste package internal temperature.

The primary objective of this report is to present the findings of a literature review of work pertinent to predicting *intact* waste package internal temperatures under spent fuel isolation conditions. Therefore, it is assumed that a repository scale thermal analysis has been conducted and the exterior temperature of the waste package is known. Thus, the problem reduces to one determined by the waste package and its properties.

Secondary objectives of this report are to identify key parameters and methodologies for performing the thermal analysis within intact waste containers, and identify sources of uncertainty in these calculations.

Although not included in this report, consideration should be given to modeling temperatures in breached containers. Upon breach, the internal gas environment will change from argon to air and heat transfer out of the container may occur by convection. These changes are expected to make small changes in the internal temperatures but may make large changes in UO_2 oxidation rates, radiolysis rates, and ^{14}C release rates from activated metals.

To place the problem in perspective conceptual waste package designs and design temperature limits are reviewed in Chapter 2. Chapter 3 reviews thermal analyses performed for spent fuel waste package designs proposed for the Yucca Mountain site. Chapter 4 reviews thermal analyses performed for dry storage and multi-assembly shipping casks. Chapter 5 discusses areas that may lead to uncertainties in the temperature predictions. Finally Chapter 6 presents conclusions and recommendations for future work.

2. CONCEPTUAL WASTE PACKAGE DESIGNS AND DESIGN REQUIREMENTS

2.1 Design Requirements

Although there is no direct regulatory requirement on waste package internal temperature, a maximum spent fuel cladding temperature of 350 °C is a design requirement [DOE, 1988]. This value was chosen to limit the degradation of the cladding.

2.2 Conceptual Designs

Currently a number of design concepts have been developed for spent fuel waste packages. They are presented in the DOE's Yucca Mountain Site Characterization Plan [DOE, 1988]. Spent fuel may be received at the repository in three forms. The majority are expected to be in the form of intact assemblies that contain undamaged fuel rods. The second form is fuel that has been preconsolidated at the reactors or at another facility. In this case, the rods are consolidated in a 2:1 ratio and placed into a canister. The canister with the consolidated assemblies has dimensions almost identical to the unconsolidated assembly. The third form that is expected is fuel that is structurally damaged to the extent that the fuel assemblies must be placed in a canister to contain the particulate fuel materials. Although no reference dimensions have been established for failed fuel assemblies it is assumed that the canisters will be only slightly larger than the assemblies that they contain. Thus all assemblies will have approximately the same dimensions. This will allow similar container designs for all three categories of spent fuel.

The reference form for disposal of spent fuel is fuel rods that are removed from intact assemblies and consolidated at the repository [DOE, 1988][1]. However, the option of disposing of intact spent fuel assemblies as they are received is retained in the reference design because it may not be possible to consolidate assemblies with failed fuel. Further, fuel with high burnup or short cooling times may require disposal as intact assemblies to prevent temperature limits from being exceeded.

The containers for spent fuel will be 1 cm thick and have an internal structure to provide mechanical stability and facilitate loading operations. This structure is particularly important when loading spent fuel consolidated at the repository. Figure 2.1 which is taken from the Site Characterization Plan [DOE,

[1] This position may soon be changed as the DOE has recently indicated that rod consolidation studies "*...have not identified sufficient advantages for consolidation to warrant its use at present.*" [DOE, 1989]

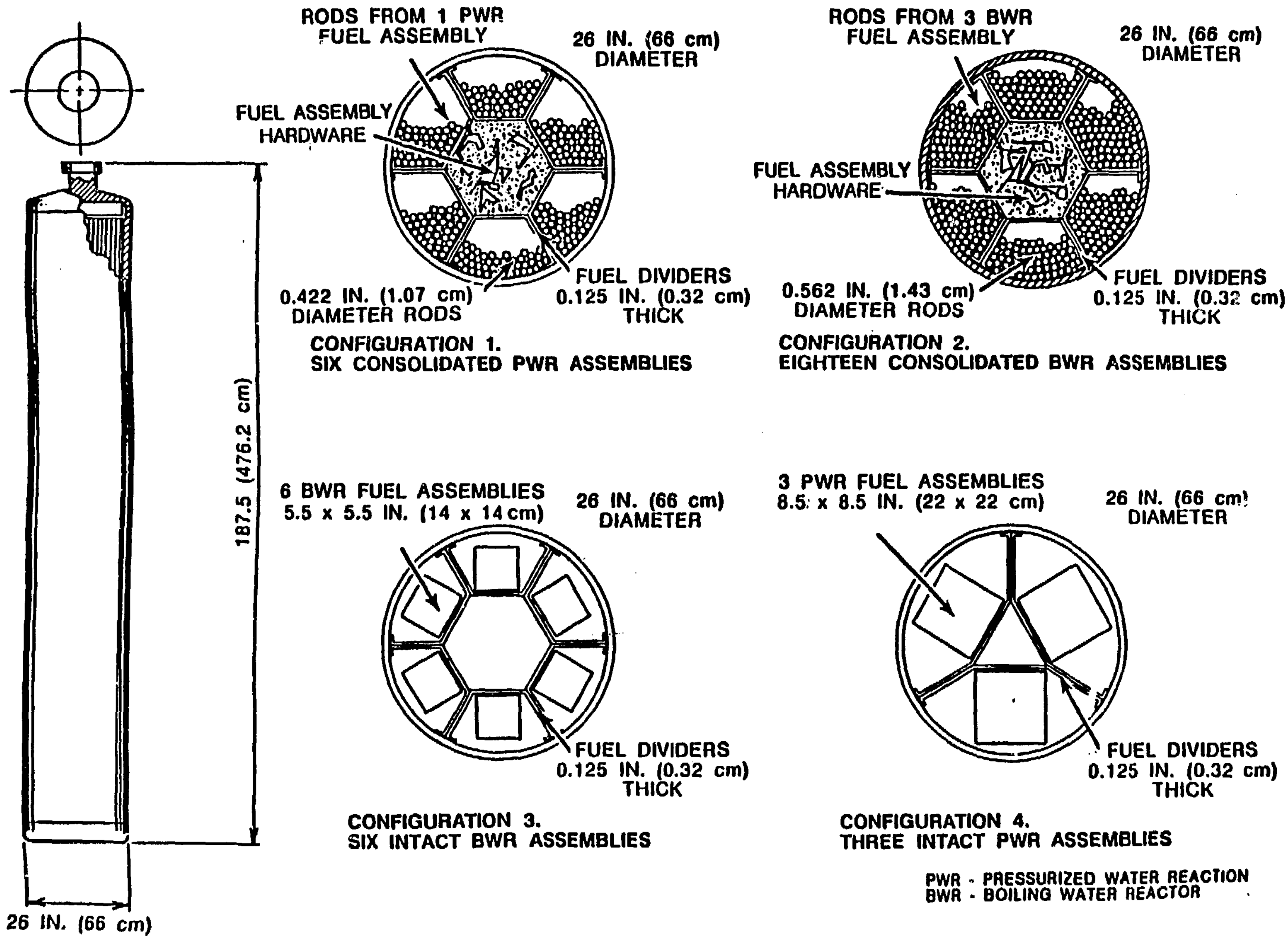


Figure 2.1 Yucca Mountain Project reference spent fuel container designs (adapted from DOE, 1988).

1988] presents the reference design for spent fuel containers. The reference design diameter is 66 cm. In all cases, the spent fuel containers will be backfilled with an inert gas. The current reference gas is argon [DOE, 1988].

The reference waste packages for consolidated fuel are designed to accommodate 6 PWR (configuration 1) or 18 BWR (configuration 2) assemblies. The fuel rods are placed in one of six sectors around the perimeter of the waste package. The central section is reserved for assembly nonfuel hardware resulting from the consolidation process. In configuration 1 and 2 the fuel rods are free to move under the force of gravity. This is the reason for the large gaps distributed around the container. For example, for a canister filled with fuel rods from six 15x15 PWR assemblies, approximately 49% of the available cross sectional area is occupied by the fuel (fuel would occupy 1218 out of 2466 cm^2). For the canister filled with fuel rods from eighteen 7x7 BWR assemblies, 57% of the available area is occupied by fuel (1411 out of 2466 cm^2). There are many different assembly configurations, i.e., 17x17 PWR, 8x8 BWR etc. Similar calculations for these different assemblies do not significantly alter the conclusion that fuel occupies approximately 1/2 of the void space.

Configuration 3 of Figure 2.1 is designed to accept 6 preconsolidated (2:1) BWR fuel assemblies or 6 intact assemblies. Configuration 4 of Figure 2.1 is designed to accept either 3 preconsolidated (2:1) PWR fuel assemblies or 3 intact assemblies.

Alternative designs discussed in the SCP are variations of the designs presented in configurations 3 and 4. They place entire assemblies inside the waste container and do not disassemble and consolidate the spent fuel. The major difference is that they place both PWR and BWR assemblies in a single container.

From Figure 2.1 it can be seen that accurate prediction of internal waste package temperatures for the consolidated spent fuel reference designs (configurations 1 and 2) requires knowledge of the heat transfer properties of consolidated spent fuel surrounded by a large gas gap. For horizontal emplacement the gas gap will have a distribution similar to that shown in Figure 2.1. This geometry is non-symmetric and any analysis will require considering at least 2-dimensions. For vertical emplacement the distribution of the gaps is ill-defined .

For configurations 3 and 4, heat transfer analysis will need to consider 2:1 consolidated fuel as well as intact assemblies surrounded by large regions containing the inert fill gas. Consolidated and failed fuel will be enclosed in a canister which is placed inside the container. Whereas unconsolidated unfailed assemblies may be placed directly into the container.

3. WASTE PACKAGE HEAT TRANSFER FOR THE YUCCA MOUNTAIN SITE

A number of studies on the temperature field in a high-level waste repository located at Yucca Mountain have been performed. However, very little work has been done on accurately calculating internal waste package temperatures. The primary objective of most of these studies has been to obtain temperatures in the near-field and far-field for performing mechanical stability analysis of the boreholes and the entire repository. The Site Characterization Plan Conceptual Design [MacDougall, 1987] reports several calculations to that effect. More sophisticated analyses have considered two phase flow and heat transfer through fractured porous media [Pruess, 1984; Pruess, 1988]. In each case the waste form is treated as a heat source and waste package internal temperatures are not calculated.

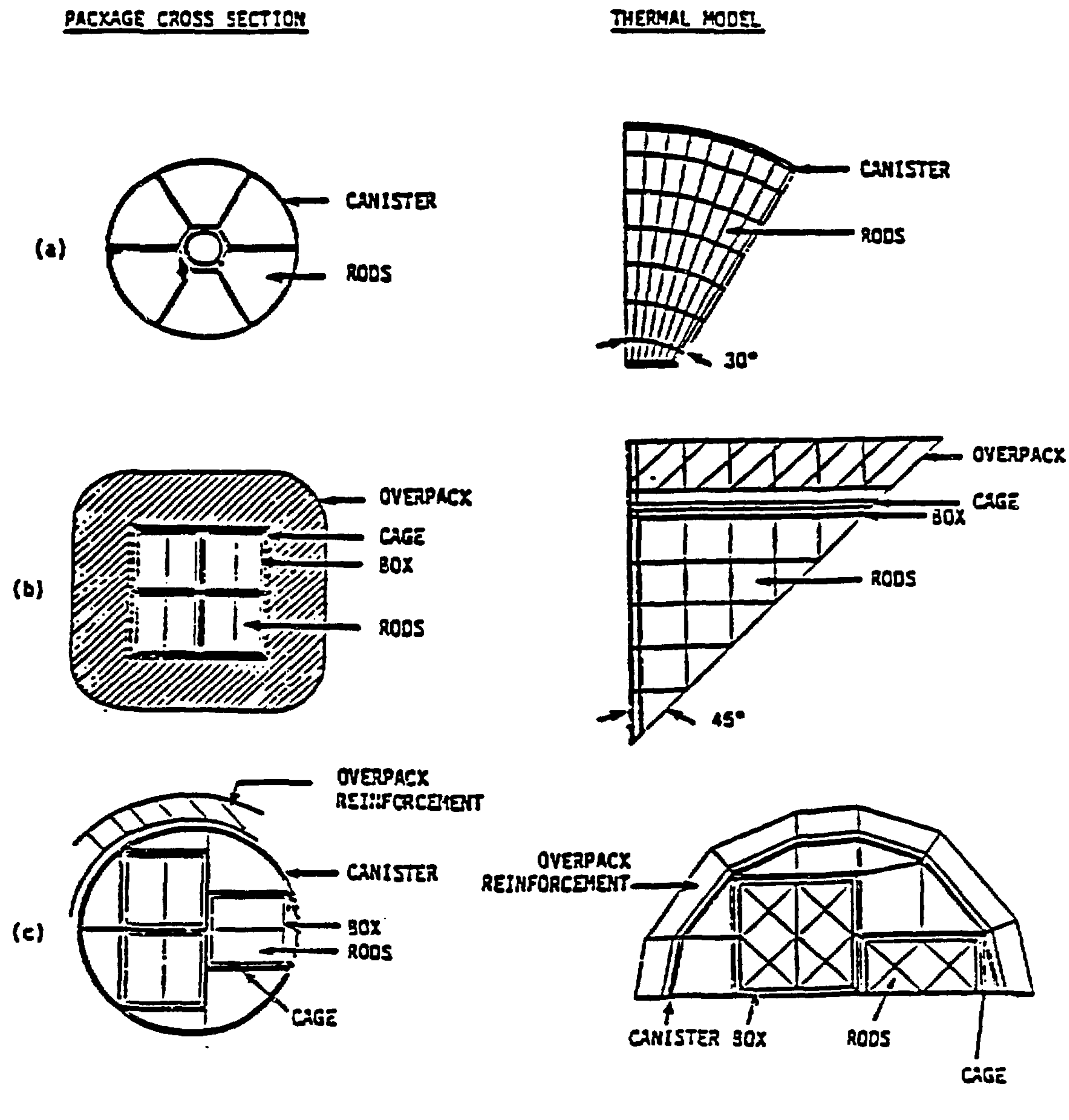
3.1 The 1983 Westinghouse Conceptual Design Study

Initial attempts at calculating waste package internal temperatures were performed by Westinghouse to support preliminary waste package designs [Schornhorst, 1983]. In these studies emphasis was placed on obtaining an upper bound on temperature to insure that design limits were not exceeded. Only consolidated geometries were considered due to the belief that this would lead to higher temperatures. We know now, however, that consolidation does not necessarily lead to higher temperatures. Internal temperatures are highly dependent on waste package internal geometry [See Chapter 4].

The Westinghouse design study modeled three different, consolidated spent fuel geometries: (Figure 3.1): a) fuel in six compartments in a circular container (similar to the current reference design but with a smaller container diameter); b) fuel in square boxes in a square container; and, c) fuel in square boxes in a circular container. Heat transfer through the container structure (internal dividers and boxes for holding the fuel) was modeled in each geometry. Outside of the boxes (but within the container), radiation and conduction heat transfer were modeled using the properties of air.

Maximum temperature rises were approximately 50 °C for the design similar to the current reference design, case a), to 90 °C for the square overpack design, case b). In all three cases, the internal structure provided an efficient means for heat transfer. Peak temperatures ranged from 345 °C for case a) to 375 for case c). At that time, the design temperature limit was 375 °C. Since then it has been reduced to 350 °C.

Figure 3.1 Internal waste package geometries used for thermal analyses in the Westinghouse study [Schornhorst, 1983].



In the Westinghouse approach, the spent fuel region was homogenized and treated as a single conducting medium. That is, all three modes of heat transfer (conduction, convection, and radiation) were modeled through the use of a single parameter called the effective thermal conductivity. The effective conductivity value was obtained using a correlation developed by Cox for thermal radiation heat transfer between parallel rods in a cylindrical geometry [Cox, 1977]. This ignored heat transfer by conduction and convection. Further, as applied by Westinghouse to spent fuel waste containers, the correlation assumes that the rods are consolidated to a pitch to diameter ratio of 1.0. For radiation heat transport, this implies lower heat transfer rates and therefore a lower effective conductivity.

Although waste package dimensions and internal geometry have changed since the Westinghouse design report [Schornhorst, 1983], the general approach to calculate temperatures has not. The effective conductivity approach based on the Cox correlation for radiation heat transport is still the approach most widely used to estimate waste package temperatures [Hockman, 1984; O'Neil, 1984; Johnson, 1988].

In contrast with the Cox correlation, the effective thermal conductivity of a spent fuel rod assembly has also been determined from experimental data in support of dry fuel storage studies [Mahini, 1989]. In this approach, temperature data from an unconsolidated assembly were used to obtain an estimate for the effective conductivity. Effective conductivities were determined for helium, air, and vacuum environments surrounding an unconsolidated single PWR assembly contained in a circular container [Westinghouse, 1982]. Conductivities were determined as a function of temperature through changing the temperature at the boundary of the container. These effective conductivities account for all three modes of heat transfer. It has been shown that radiation, conduction, and convection are all important for unconsolidated fuel assemblies in dry storage [Cuta, 1986; Rector, 1986a; Rector, 1986c; Lombardo, 1986a].

Although, this latter approach provides a simple method of calculating temperatures, the effective conductivities are likely to be meaningless for present spent fuel disposal concepts because of the different geometries, i.e., consolidated fuel, internal structure, multiple assemblies. This approach could be used only after conducting experiments using the designs chosen for final disposal.

3.2 NNWSI Studies of 1984

Two other reports present results of spent fuel waste package thermal calculations. In both reports, calculations were performed using the two-dimensional, finite element, heat conduction code TACO-2D and the spent fuel region was modeled using the Cox correlation to determine an effective conductivity.

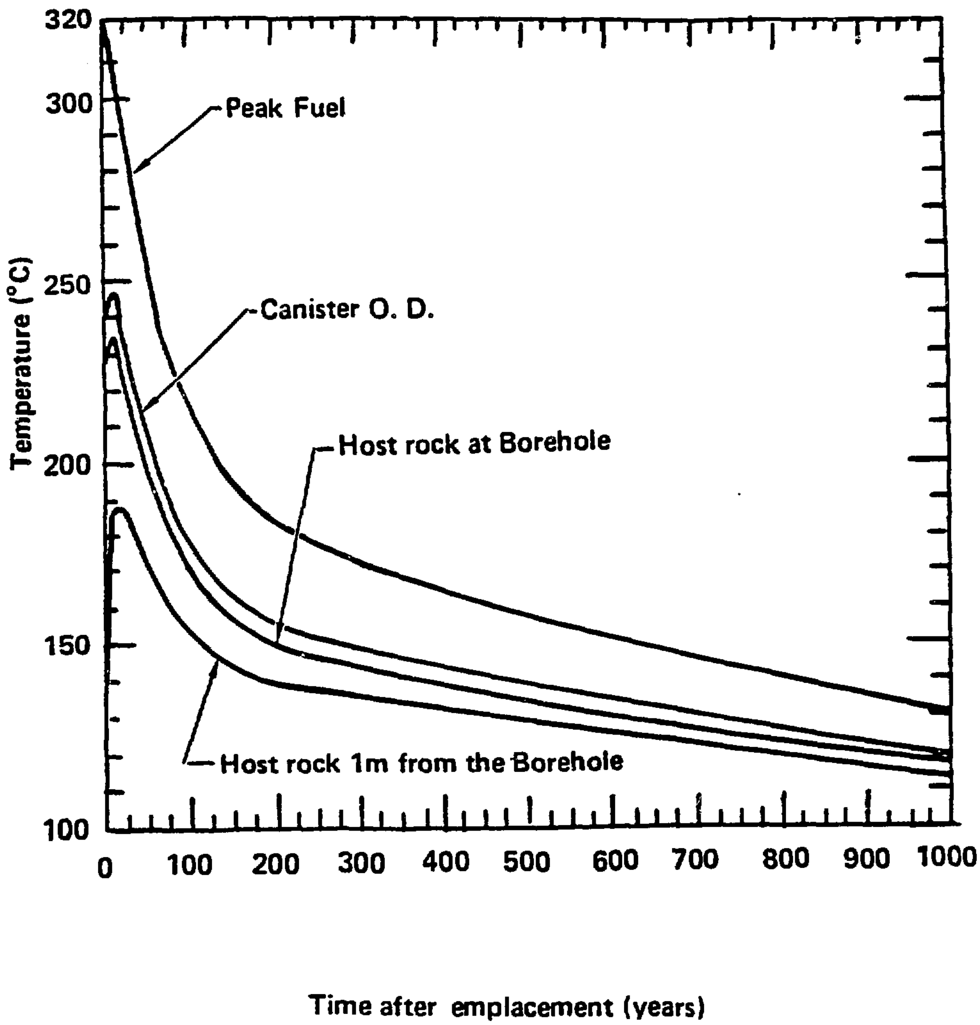
In the first report, temperature calculations were performed for 9 different horizontal and 2 vertical emplacement scenarios [O'Neal, 1984]. The different scenarios used package diameters ranging from 40 to 70 cm and different repository heat loadings. In all cases, the backfill gas within the container was helium.

For vertical emplacement, the waste package was 70 cm in diameter and contained three 2:1 preconsolidated boxes of spent fuel similar to drawing c) in Figure 3.1. This design is no longer being considered. However, these are the results presented in the SCP as a typical waste package thermal history Figure 3.2, [DOE, 1988].

For the horizontal emplacement scenarios the internal waste package geometry that was modeled is unclear. The text of this report states that the internal geometry was similar to that used in the vertical case, i.e., three 2:1 preconsolidated boxes of spent fuel. However, the effects of internal heat conducting fins were also considered in some cases. The use of internal fins is inconsistent with the description of the three boxes.

The second report presents the results of thermal calculations for 6 different horizontal emplacement scenarios for PWR spent fuel and 1 vertical emplacement scenario for BWR fuel [Hockman, 1984]. Spent fuel waste container diameters ranged from 45 - 50 cm for the PWR fuel and was 57 cm for the BWR fuel. The internal structure that was simulated was compartmentalized as in the current reference design, Figure 2.1. However, the number of compartments ranged from 6 to 24. Between the internal structure and the stainless steel container there was a 1.27 cm gap. This gap was assumed to be filled with air.

The results of this study [Hockman, 1984] indicate that the fins act as an effective path for heat transfer. Changing the design from no internal fins to six internal fins reduced peak temperatures by 70 °C.



WF............................PWR.SF

LPD..........................57.0

APD..........................48.4

10yr PWR-AVE.........3.3KW

^{C}Diam.......................0.7m

^{P}PKG........................5m

^{P}DRIFT...................46.86m

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Figure 3.2 Temperature histories, presented in the SCP, of waste package components for vertical emplacement (adapted from DOE, 1988)

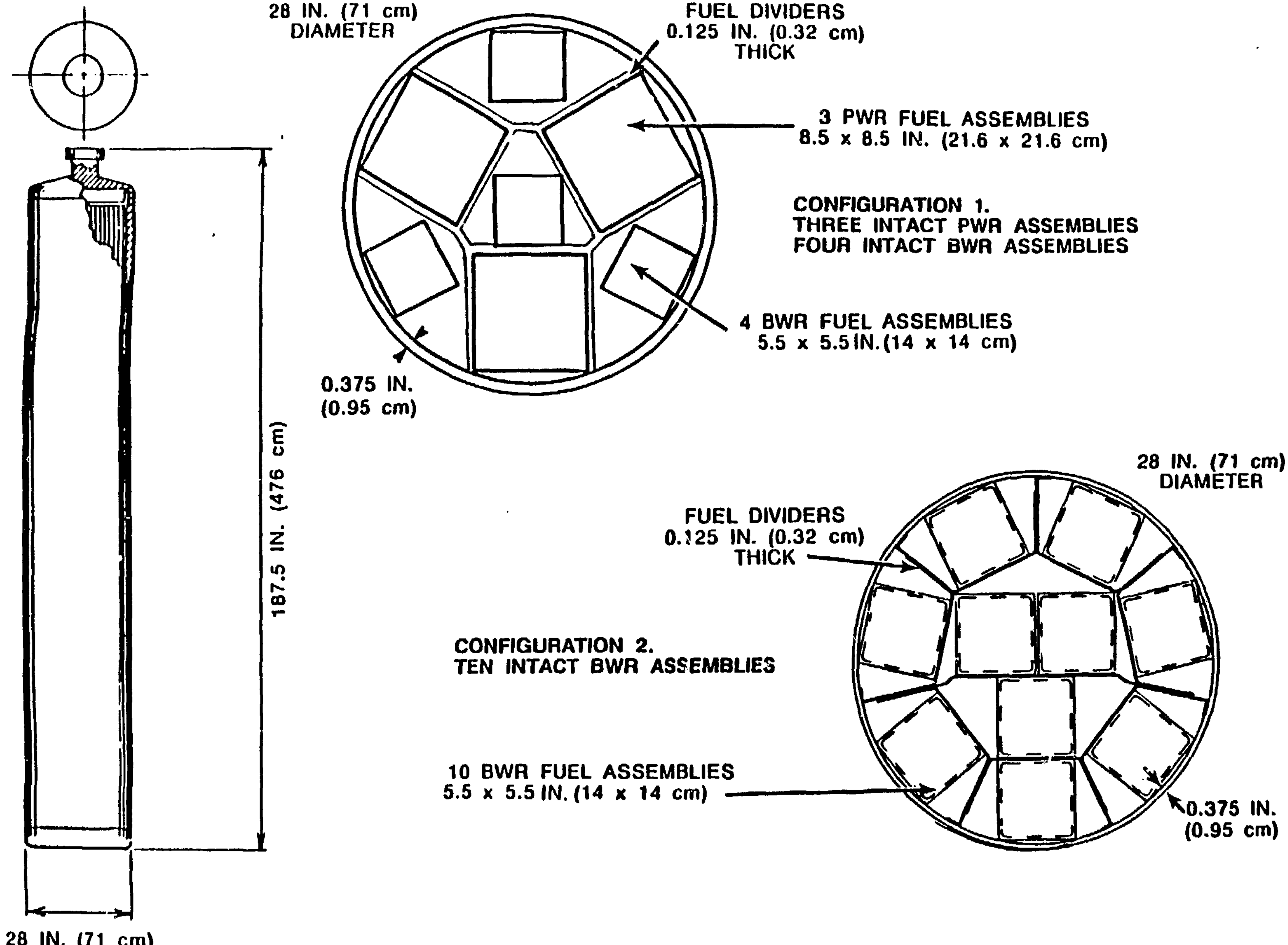

Figure 3.3 Yucca Mountain Project alternate spent fuel container designs (adapted from DOE, 1988).

3.3 LLNL Study of 1988

Recently, internal waste package temperature calculations have been performed for vertical emplacement of a 71 cm outside diameter waste package containing 3 consolidated 2:1 PWR fuel packages and 4 consolidated 2:1 BWR fuel packages [Johnson, 1988]. The internal package geometry was almost identical to the alternative concepts presented in the SCP, Figure 3.3, with the exception that the geometry of the support structure was slightly different. Another difference between the two designs is that in the SCP use of unconsolidated fuel was envisioned. For consolidated fuel, the package power is 4.7 kW for 10 year old spent fuel. This is twice as great as the package power mentioned in the SCP for unconsolidated fuel and is greater than the 3.3 kW package power for the SCP reference design.

In these studies, the computer code TACO-3D was used to perform a repository scale thermal analysis. From this the borehole wall temperature was determined as a function of time. This served as input to the internal waste package analysis which was conducted with the computer code TACO-2D. In these calculations, the areal power density was 80 kW/acre and no credit was taken for ventilation of the main drifts or evaporation of the pore water.

Internal waste package temperatures were calculated using an effective conductivity for the consolidated spent fuel regions and assuming that the gas region around the fuel was a vacuum or air. In most test cases, the effective conductivity approach based on the Cox correlation was used. This only accounts for radiation heat transfer between parallel cylinders in cylindrical geometry. In some cases, the effective conductivity was estimated from Cuta's numerical simulations[2] of fuel rods in a square geometry with constant boundary temperatures [Cuta, 1984]. The internal fuel rod temperature profile was predicted using the computer code COBRA-SFS. It was not obtained experimentally as stated by Johnson [Johnson, 1988]. In the report by Cuta, a number of test cases were simulated. It is not clear which of these cases was used by Johnson to obtain the effective conductivity of the fuel bundle. Therefore, the values relevance to the consolidated system modeled by Johnson is unclear.

The sensitivity of internal temperature to a number of different conditions relevant to spent fuel disposal was also analyzed. The analyses examined the response in predicted temperature profiles to a) different container materials, SS-304, 70/30 Cupro-nickel, and Incoloy 825; b) the presence of 0.05 m of bentonite packing between the outer edge of the container and the borehole wall; c) a change of the emissivity of the internal structure from 0.8, the historically used value, to 0.5,

2 In Cuta's study the internal fuel rod temperature was not obtained from experimental studies, as suggested by Johnson [Johnson, 1988], but it was predicted using the COBRA-SFS code.

a value believed to be more realistic; and d) different power levels, representative of 5 and 10 year old spent fuel.

For an Incoloy 825 container with a surface emissivity of 0.5, 10 year old spent fuel, air as the backfill gas, and no bentonite packing, the peak temperature was 336 °C in the PWR fuel and 334 °C in the BWR fuel. The peak occurred at 3.5 years after emplacement. The author considered this case as the best estimate. Cases with bentonite backfill or 5 year old fuel had higher peak temperatures. In fact, for the low conductivity bentonite backfill and for 5 year old spent fuel had higher peak temperatures, ranging from 341 to 411 °C.

The temperatures calculated in this report were based on the average power density in the spent fuel and average material properties i.e., the study did not take into account the axial power generation rate and the presence of a large empty space on top of the fuel bundles. It was estimated that temperatures may vary by 11 - 33 °C around this average. This is a rather large range of values when compared to the total ΔT across the spent fuel.

This report recommended a number of improvements that should be made to the heat transfer analysis. They include:

a) Establish an accurate value for the effective conductivity of the spent fuel region for all possible packing configurations. Determine the relationship between the actual peak temperature and that predicted by the homogenized model.

b) Model convection around the spent fuel assemblies within the container. These analyses modeled conduction and radiation. However, their is evidence that convection can be important for vertical emplacement [Cuta, 1984]. This may be particularly important considering the large gaps around the spent fuel containers in the hybrid design as compared to the gaps in the study by Cuta.

c) Determine the emissivity of the borehole wall, i.e. tuff. A value of 1.0 was used in this study.

d) Determine the thermal conductivity of potential backfill materials more accurately.

e) Using the best available model, perform a three-dimensional analysis of the container including axial power variation, internal geometry, etc.

f) Perform a transient three-dimensional analysis of various combinations of emplacement history.

g) Perform a more accurate analysis of the drift tunnels including the effects of ventilation.

3.4 Discussion

The four studies discussed in the previous section are the best available studies on internal waste package temperature. However, these studies do not accurately reproduce the thermal performance of current designs for a number of reasons including:

a) None of the studies considered internal waste package geometries identical to the consolidated reference design (configurations 1 and 2 of Figure 3.1), nor are there any studies that remotely resemble the two unconsolidated reference designs (configurations 3 and 4 of Figure 2.1). The study by Johnson [Johnson, 1988] did accurately model the geometry of the alternate hybrid design referenced in the SCP (configuration 1 of Figure 3.3).

b) The peak fuel temperature profile reported in the SCP is not applicable to the present reference designs of Figure 2.1. In particular, the possibility of large gas gaps around the consolidated fuel were not considered. Preliminary calculations show that a 1.25 cm annular gap around the entire edge of the spent fuel region could lead to a temperature rise of between 30 - 100 °C depending on the emissivity of the materials.

c) All of the studies homogenized the spent fuel region and used an effective conductivity approach. This approach considered only radiation heat transport. Conduction and convection were not modeled in the spent fuel region. The latter have been shown to be important in certain cases [See Chapter 4].

d) None of the studies considered argon as the fill gas. Argon has a lower thermal conductivity than helium or air and therefore its use leads to comparatively higher temperatures. In one study for a dry shipping cask system [Tanaka, 1985], use of argon as compared to helium as the fill gas caused the temperature rise to increase by almost 40%.

e) None of the studies considered unconsolidated spent fuel. Depending on geometry and backfill gas, peak temperatures can be higher for an unconsolidated geometry as compared to a consolidated geometry in dry systems. Lower temperatures have been found to occur for consolidated systems using a high conductivity gas, such as helium, as compared to an unconsolidated system with the same geometry [Cuta, 1984; Rector, 1986a].

f) None of the studies considered axial variations in temperature. In dry storage systems, there is a substantial axial variation in temperature along the length of a fuel rod. The amount of variation depends on the fill gas, internal geometry, and axial heat rate in the fuel rods. In dry storage systems, the peak temperature rise was often more than 20% greater than the mean temperature rise (see Figures 4.1 and 4.2 in section 4.1.4) [Rector, 1986]. Similar results should be expected for spent fuel disposal systems.

Axial temperature variations may be important in determining cladding degradation due to creep, ^{14}C release from activated metals, and potential flooding of a breached container or borehole. Cladding degradation is a function of the gas pressure within the rods which depends on the average (not the peak) temperature of the gap gas. ^{14}C release depends strongly on temperature and axially non-uniform release rates can be expected. Similarly, flooding could occur at the bottom of the borehole or container even if the peak temperature is above the boiling temperature.

4. THERMAL ANALYSIS OF SPENT FUEL DRY STORAGE SYSTEMS

Dry storage of spent fuel is receiving widespread attention as a means of relieving pool storage limitations at operating nuclear power plants. Also, spent fuel shipping casks are often dry systems. These dry systems present many similarities with the waste package disposal concepts. Spent fuel assemblies are placed in a cask and, generally, the cask is backfilled with an inert atmosphere. The assemblies can be in the form as used during power generation or they can be consolidated in a 2:1 ratio.

As part of the analysis of dry storage systems, experiments have been conducted for single PWR and BWR assemblies, consolidated PWR and BWR assemblies, and multiple assemblies in a storage cask. These experiments have included various backfill gasses (helium, air, nitrogen) and vacuum as well as various orientations (horizontal and vertical) and power levels. To complement the experiments, thermal-hydraulic analyses have been performed.

Thermal-hydraulic analyses of spent fuel assemblies have ranged from simplified calculations in which the assembly is treated as a homogeneous medium to detailed three-dimensional calculations including the processes of conduction, convection and thermal radiation.

4.1 Review of Dry Storage System Thermal Methodologies and Analysis

Design and licensing of spent fuel storage and shipping casks requires an analysis of the cask's thermal performance. To verify the accuracy of computer codes used for these analyses, a standard thermal problem set has been developed [Glass, 1988]. This problem set consists of a set of six two-dimensional thermal problems which have either known analytical solutions or experimental data. These problems have been solved by a number of computer codes. A report by Glass [Glass, 1988] provides the problems and corresponding analytical solutions or experimental data. This problem set is useful for benchmarking of computer codes. However, because of the different size, fuel rod geometry, and external environment as compared to spent fuel disposed of as high level waste these problems are not directly applicable to the thermal problems of high level waste disposal.

In addition, the NRC has sponsored work related to predicting thermal performance of dry storage casks, shipping casks, and spent fuel assemblies. This has resulted in the development of two computer models, SFHA and HTAS2. SFHA (Spent Fuel Heating Analysis) predicts temperatures within single assemblies while HTAS2 performs a similar task for multi-assembly dry storage casks.

The DOE and EPRI have also sponsored dry storage thermal analysis programs. Most of the experimental work previously mentioned has been funded through these two agencies. Analytical work has focused on attempting to reproduce experimental results using either one of the computer codes COBRA-SFS or HYDRA-II.

4.1.1 The SFHA Code

The SFHA code [Fisher, 1985; Fisher, 1989] is used to model heat transfer within consolidated or unconsolidated assemblies. SFHA is applicable to square or hexagonal fuel rod distribution geometries and uses a generalization of the Wooton-Epstein semi-empirical correlation [Wooton, 1963] for radiation heat transport in a 17 x 17 PWR fuel bundle. The generalization accounts for radiation, conduction, and convection heat transfer. This correlation has been specialized for helium and air environments through use of experimental data.

SFHA has been benchmarked against experimental data for simulated PWR rods in a vacuum environment, unconsolidated spent PWR fuel rods in air, vacuum, and helium environments, and simulated consolidated BWR rods in air, vacuum, and helium environments. Results for predicted peak temperatures were always within 12 °C of the experimentally measured value. However, the percentage error in predicted temperature rise was as large as 30% for unconsolidated rods and 75% for consolidated rods. The largest percentage errors occurred when helium was the backfill gas and the actual temperature rise was smallest. Also, the accuracy of the predictions decreased away from the center of the assembly where peak temperatures occurred.

For unconsolidated or 2:1 consolidated fuel assemblies disposed of as high-level waste under an argon atmosphere, this approach would require further experimental work to obtain the proper correlation coefficients. For consolidated assemblies and the current design, this approach could not be used directly because of the lack of symmetry and lack of square or hexagonal rod geometries. Modification of this approach to account for geometries similar to the proposed HLW consolidated geometries would be possible only if experimental data were available to determine the correlation coefficients.

4.1.2 The HTAS2 Code

HTAS2 is a transient three-dimensional analysis computer code used to predict maximum fuel pin temperatures in shipping casks under accident conditions [Wendel, 1989]. HTAS2 is the system driver module which calls upon two separate computer codes to perform the analysis. First, HTAS2 calls WHOCAM (WHOle CAsk Model) to calculate the temperature field within the cask using a lumped parameter model. In this calculation each assembly is treated as a single computational cell. From this, the hottest assembly is identified and the computer code HEATING version 6.1, (HEATING-6), is used to perform a detailed 2-D thermal analysis. As configured, HEATING-6 can model only square fuel rod geometries.

HEATING-6 is a two-dimensional finite difference code capable of modeling conduction and radiation heat transfer. For simplicity, the fuel pins and gas gaps are modeled in rectangular geometry. Radiation view factors are calculated automatically by the HTAS2 driver.

The HTAS2 approach is a compromise between the semi-empirical approaches based on the Wooton-Epstein correlation and three-dimensional thermal-hydraulic analysis.

This approach may be useful for thermal analysis of unconsolidated assemblies disposed of as HLW, (designs 3 and 4 of Figure 2.1). Currently, the requirement for square arrays of fuel pins prohibits HTAS2's use for 2:1 consolidated assemblies although, with minor modifications, it may be applicable to this geometry. This approach is not useful for the reference consolidated geometries due to the lack of symmetry and lack of square arrangement of the fuel rods.

4.1.3 The COBRA-SFS and HYDRA-II codes

Two computer codes, COBRA-SFS [Rector, 1986b] and HYDRA-II [McCann, 1987a], have been used extensively to perform thermal-hydraulic analyses of dry storage spent fuel systems. Both codes are recognized as state-of-the-art codes capable of providing a best estimate of fuel temperature in dry storage systems. Both codes use a finite-difference formulation to solve the mass, momentum, and energy conservation equations in three dimensions to determine pressure, temperature, and velocity fields. Both codes consider convection, fluid-fluid conduction, solid-solid conduction, and surface-to-surface thermal radiation. HYDRA-II is a fully three-dimensional hydrothermal computer program. COBRA-SFS uses the steady-state subchannel formulation used by its predecessors in the COBRA family of codes. In the subchannel approach, the problem is divided into a number of flow channels that are interconnected by means of thermal conduction and diversion crossflow paths.

Both COBRA-SFS and HYDRA-II have been used to predict temperatures in single unconsolidated spent fuel assemblies, 2:1 consolidated spent fuel assemblies, and both unconsolidated and consolidated multi-assembly dry storage casks. In these analyses the following factors have been considered: fuel orientation (horizontal and vertical); backfill gas (helium, nitrogen, air, and vacuum); and different power levels. Analyses have been performed for actual spent fuel and for simulated fuel. Tables 4.1 and 4.2 provide a summary of the analyses performed by COBRA-SFS and HYDRA-II, respectively. These tables show that COBRA-SFS has been used on 12 and HYDRA-II on 7 different dry storage systems over a range of conditions.

Table 4.1 Dry Spent Fuel Storage Thermal Analyses Performed by COBRA-SFS

Assembly Config.	Fuel Rod* Config.	Backfill Gas	Reference
	Unconsolidated Single Assemblies		
Single	An PWR	He/Air	Cuta, 1984
Single	Exp Sim BWR	He/Air/Vac	Cuta, 1986
Single	Exp PWR	He/Air/Vac	Lombardo, 1986a
	Consolidated Single Assemblies		
Single	An. PWR	He/Air	Cuta, 1984
Single	Exp Sim BWR	He/Air/Vac	Cuta, 1986
	Unconsolidated Multi-assembly Shipping Casks		
Castor 1-C	Exp 16 BWR	He/N	Lombardo, 1986b
REA 2023	Exp 52 BWR	He/N/Vac	Lombardo, 1986b
TN-24P	Exp 24 PWR	He/N/Vac	Lombardo, 1986b
MC-10	Exp 24 PWR	He/N/Vac	McKinnon, 1987
	Consolidated Multi-assembly Shipping Casks		
Castor 1-C	An BWR	He/N	Rector, 1986a
REA 2023	Sim BWR	He/N	Rector, 1986a
TN-24P	Exp PWR	He/N/Vac	McKinnon, 1989

*Under the column titled Fuel Rod Config. the information supplied tells if the thermal analysis was compared to Experimental data on spent fuel or Simulated (electrically heated rods) fuel or if the problem was entirely an Analytic exercise. For example, Exp BWR implies that experiments with BWR fuel were performed and are used as a basis for comparison; Exp Sim BWR implies that experiments were conducted on simulated BWR rods; and An BWR implies that the thermal analyses were performed but there was no experiment performed.

Both COBRA-SFS and HYDRA-II are capable of providing fairly accurate estimates of the temperature within a dry storage system. In most instances temperature predictions were within 10% of the data. In all cases where there were data, pre- and post-look thermal analyses were performed. Post-look analyses were performed with the intent of improving the modeling for future use. COBRA-SFS has recently been submitted to the NRC for approval as a dry storage licensing code.

Table 4.2 Dry Spent Fuel Storage Thermal Analyses Performed by HYDRA-II

Assembly Config.	Fuel Rod* Config.	Backfill Gas	Reference
	Unconsolidated Single Assemblies		
Single	Exp Sim. PWR	He/Air	McCann, 1986
Single	Exp PWR	He/Air/Vac	McCann, 1986
Single	Exp Sim. BWR	He/Air	McCann, 1988
	Consolidated Single Assemblies		
Single	Exp Sim. BWR	He/Air	McCann, 1988
	Unconsolidated Multi-assembly Shipping Casks		
Castor 1-C	Exp BWR	He/N	McCann, 1987b
REA 2023	Exp BWR	He/N/Vac	Wheeler, 1986
Castor V/21	Exp PWR	He/N/Vac	McCann, 1987b

*Under the column titled Fuel Rod Config. the information supplied tells if the thermal analysis was compared to Experimental data on spent fuel or Simulated (electrically heated rods) fuel. For example, Exp BWR implies that experiments with BWR fuel were performed and are used as a basis for comparison; and Exp Sim BWR implies that experiments were conducted on simulated BWR rods.

4.1.4 Major Results and Findings

As a result of the experiments and thermal analyses performed on dry storage and shipping cask systems a number of important conclusions can be reached. The major findings of these studies are as follows:

Unconsolidated Assemblies

a) For unconsolidated geometries radiation is an important heat transfer mode. Conduction is important for a high conductivity fill gas, while convection becomes important as the conductivity of the fill gas decreases. In particular, it has been experimentally shown that if nitrogen is the fill gas, convection is an important heat transfer mode [McKinnon, 1987]. For helium, conduction and radiation are generally the primary modes of heat transport. However, convection can be important for a horizontal orientation [Neumann, 1985; Nitsche, 1986; McKinnon, 1987; McKinnon, 1989].

b) Sensitivity studies done to determine the influence of emissivity on heat transfer showed that emissivity is an important parameter in unconsolidated assemblies.

Consolidated Geometries

c) As compared to unconsolidated rod geometries, 2:1 consolidated geometries provide an easier heat transfer problem because the rods are so close that convection and radiation are drastically reduced. Radiation is reduced due to rod shadowing, while convection is hindered by the close packing of the rods. Thus, the consolidated rods act as a lumped heat source with a relatively flat temperature profile with conduction as the primary mode of heat transfer. For a high conductivity fill gas (e.g., helium) the enhanced conduction and reduced radiation essentially cancel each other out and the peak temperatures for the two cases do not differ sensibly [Rector, 1986a, McCann, 1988]. In fact, for some geometries with helium as the backfill gas, the consolidated fuel case can have lower temperatures than the unconsolidated case [Cuta, 1984; Rector, 1986a] For a lower conductivity fill gas (nitrogen, or air), the reduction in the effectiveness of both radiation and convection heat transfer is not fully compensated by the increased conduction. Thus, peak temperatures increase [Rector, 1986a]. However, they do not increase in proportion to the power increase associated with 2:1 consolidation.

d) The thermal conductivity of the fill gas has a significant effect on rod temperatures. The peak temperature rise across a simulated consolidated

BWR fuel assembly in helium was approximately 0.4 times that in air [McCann, 1988]. The emissivity of the fuel rods and containers is relatively unimportant due to the reduced radiation heat transfer.

e) The assumed geometric arrangement of the rods has a significant effect on the predicted temperature drop from the centerline to the edge of a container. Geometrical factors include the exact location of the rods within the container, the effects of rods contacting other rods, rods located axisymmetrically within the container, and rods contacting the container walls. In one study [Cuta, 1984], the overall temperature drop changed by more than 40% between cases with the most conservative and most optimistic geometric assumptions for both air and helium backfill gas.

f) Contact conductances within a consolidated assembly, even with the rods touching is low enough that an assumption of zero contact conductance results in calculated temperatures that are only slightly higher than measured data [Cuta, 1986]. The predicted temperature rise across an assembly increased by 20% if the rod-to-rod gap increased from 0.0 (perfect contact) to 0.01 inches [McCann, 1988].

General

g) Two cases arose in which the computer codes did not accurately predict temperatures within the fuel assemblies. In the first case, the cause of the poor prediction was found to be due to use of an inaccurate estimate for the axial heat profile. The axial heat profile used to model the heat transfer was much different than the experimentally measured profile. The axial heat profile was predicted using ORIGEN2 and standard plant operating procedures. However, for this particular assembly there was an unusually long coast down from full power which caused the axial heat profile to change [Rector, 1986a]. In the second case, temperatures within the fuel assembly were substantially overpredicted due to improper choice of the internal cask geometry [Wheeler, 1986]. In modeling the heat transfer between the assembly and the storage canister, a gap was placed between the two. Although, as designed, this gap exists at room temperature, as the system temperature increased, the gap width decreased markedly and thereby lowered the thermal resistance. Correcting for this in the post-look analysis improved the temperature prediction.

h) For multi-assembly storage casks, gaps between the spent fuel and the cask are important to overall heat transfer performance [Tanaka, 1985; Nitsche, 1986]. In one case, approximately 65% of the temperature rise occurred across this gap [McKinnon, 1987]. In another case, temperature differences between 20 and 100 °C occurred across this gap. The lower temperature difference occurring for helium which indicates the importance of conduction across-the gaps [McKinnon, 1989].

i) For both consolidated and unconsolidated geometries axial variations in temperature are substantial, [Cuta, 1984; Rector, 1986; McCann, 1987]. Figures 4.1 and 4.2 [adapted from Rector, 1986] display axial temperature profiles for two different spent fuel shipping casks with either helium or nitrogen as the fill gas. In these figures, the peak temperature rise across the system is often more than 20% greater than the mean temperature rise. Axial temperature variations depend primarily on system geometry, fill gas, and axial power generation rate. Axial temperature variations tend to be greater when convection is an important heat transfer mode, i.e., unconsolidated systems with a low conductivity fill gas. This is indicated in Figures 4.1 and 4.2 when nitrogen is the fill gas, peak temperatures occur closer to the top of the cask than when helium is the gas.

4.2 Conclusions

A number of computer codes have been developed to predict temperatures within spent fuel dry storage systems. They range in sophistication from simple codes, such as SFHA, that are based on semi-empirical expressions that run on a personal computer to a code, such as COBRA-SFS, that models the thermal-hydraulic behavior of the system in three dimensions by solving the mass, momentum, and energy balance equations.

As the degree of modeling sophistication increases, so does the accuracy of the predictions. COBRA-SFS and HYDRA-II are state-of-the-art codes which have been shown to be capable of predicting the temperature rise within dry spent fuel storage systems with a high degree of accuracy (10%) provided that the problem is well defined, i.e. system geometry, fuel rod geometry, decay heat level, material properties etc. are well characterized. However, this accuracy does have a cost. Both of these codes require large input decks to specify the geometry and material properties. Gaining the knowledge needed to define a problem and develop an input deck is not a trivial task. In addition, computer costs will be high. For example, problem execution time for COBRA-SFS typically requires several minutes of CPU time on a CRAY supercomputer.

In comparison to spent fuel waste disposal, the analyses of dry storage and shipping cask systems offers many similarities. They both consider consolidated and unconsolidated spent fuel stored in an inert gas medium surrounded by a container. Many of the conceptual lessons learned will be applicable to the high-level disposal situation. In particular, the work done on dry storage systems indicates that the

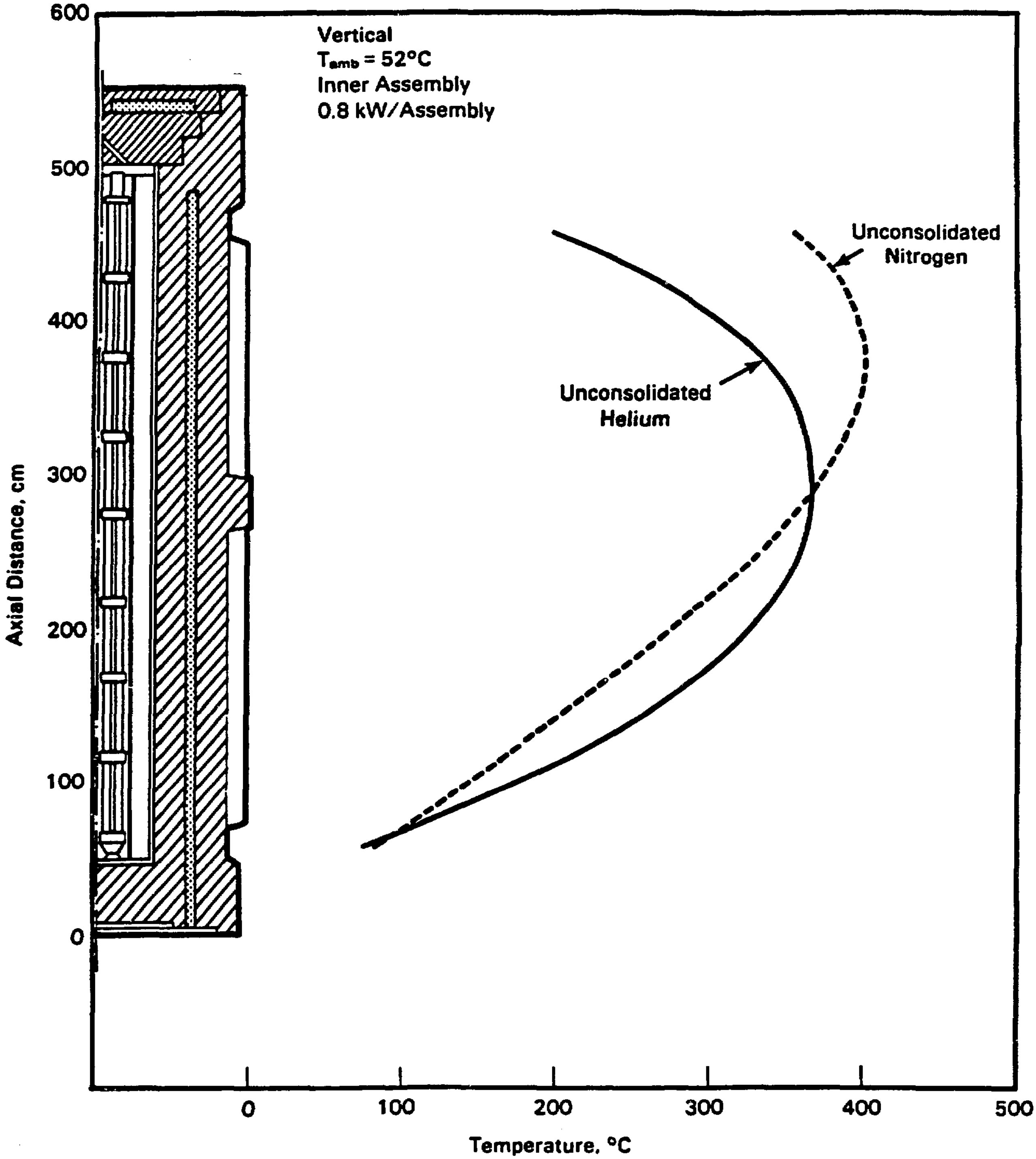

Figure 4.1 Axial temperature profile predictions for unconsolidated fuel in nitrogen and helium in a CASTOR-1C dry storage cask. [Rector, 1986]

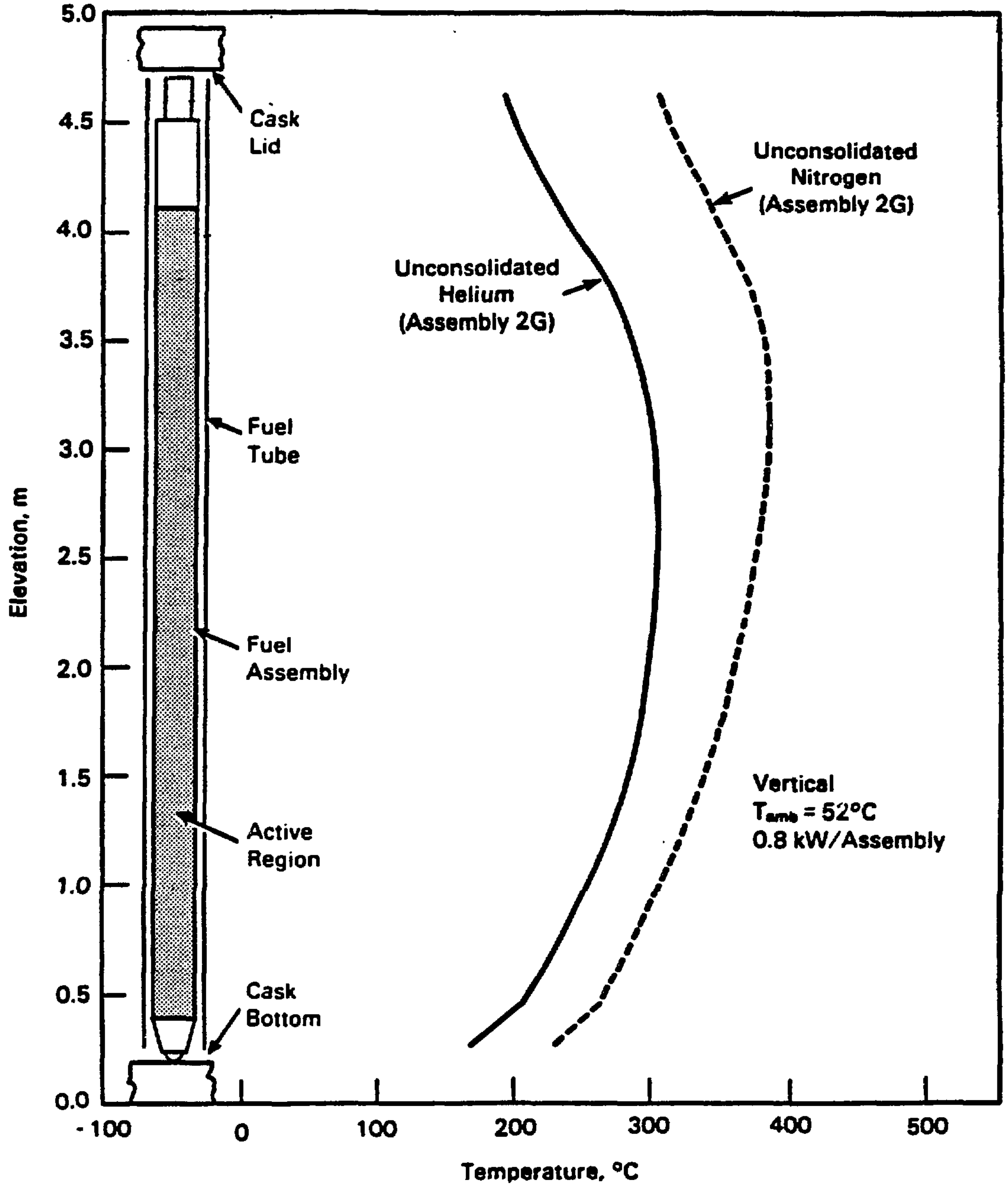

Figure 4.2 Axial temperature profile predictions for unconsolidated fuel in nitrogen and helium in a REA 2023 dry storage cask [Rector, 1986].

internal geometry of the waste package will be a critical factor in determining thermal performance. For example, changing from unconsolidated to consolidated geometries not only changes the temperatures, it also changes the dominant heat transfer mechanism. Further, small gaps around the assemblies have been shown to have important thermal resistance.

However, there are many differences that will require further investigation. The most important being the geometry within the proposed designs for spent fuel waste packages is much different than in any dry storage system. At this time, it is not clear that the consolidated fuel rod geometry within a spent fuel container will be defined with enough accuracy to justify use of the three-dimensional thermal-hydraulic computer codes. For unconsolidated or 2:1 preconsolidated assemblies the geometry is known well enough to analyze the thermal performance using either COBRA-SFS or HYDRA-II.

5. MODELING UNCERTAINTIES

As a result of the studies conducted on modeling of dry spent fuel shipping and storage systems a number of modeling uncertainties have been identified. These uncertainties will also be important for spent fuel waste packages. There are three broad categories of uncertainties:

a) Basic information that is application-specific and measurable (e.g. container dimensions, heat generation rates, ambient conditions);

b) Generic information such as property values and heat transfer correlations;

c) Uncertainties in the model itself. These include choice of the appropriate model and decisions on how to achieve the best match between predictions and data with a given model (e.g. choice of computational mesh size; computer code solution algorithms; and correlations).

Specific examples of these uncertainties follow:

a) Precise knowledge of the geometry is critical to accurate temperature predictions. This includes dimensional tolerances which may be particularly important when they influence small gaps with large thermal resistances, and eccentricities such as the placement of the fuel rods or fuel assembly within the container cavity.

b) The total heat generation rate and the axial heat profile of spent fuel assemblies have a direct effect on predicted cladding temperatures. For highest accuracy, the preferred approach is to determine these values experimentally as opposed to calculating them using ORIGEN2. However, this may not be practical for the scale of the repository.

c) Uncertainty in property values. This is most important for the emissivity of materials in unconsolidated geometries. For example, the emissivity of clean cladding may be as low as 0.3. For cladding covered with crud, it may be higher than 0.9. Typically it is assumed that a value of 0.8 is representative for spent fuel cladding [Lombardo, 1986b]. In practice, the emissivity may vary from rod to rod and axially along a rod. Predicted temperature results using a value of 0.8 have proved to be reasonable when compared with data [Cuta, 1986; Lombardo,1986b; McCann, 1988; McKinnon, 1987]. However, other values for emissivity have been successfully used in matching data [Fischer, 1989].

d) Difficulty in determining the boundary condition. This may be particularly true for high level waste disposal where the boundary condition will depend on the thermal properties of the host rock as well as the areal power density.

e) Discretization uncertainties. These can be eliminated by taking a sufficiently large number of mesh points. However, this may lead to unacceptable computer costs. Rector [Rector, 1989] presents results from a detailed analysis of the effects of mesh spacing for multi-assembly casks.

f) Modeling uncertainties. For example, the choice of a two-dimensional simulation as opposed to three-dimensional or the choice of one heat transfer correlation over another.

6. CONCLUSIONS

Based on information supplied in the latest version of the Yucca Mountain Site Characterization Plan [DOE, 1988], three basic categories of spent fuel arrangements within the disposal containers are envisioned: a) spent fuel consolidated at the repository; b) spent fuel consolidated away from the repository in a 2:1 ratio (preconsolidated); and c) unconsolidated spent fuel assemblies. There is a reference design for each of these categories.

The container for spent fuel consolidated at the repository will have an internal structure that has six compartments. Within each compartment, the fuel rods will occupy approximately 50% of the volume available. The fuel rods are free to move within each compartment during handling and emplacement operations. Thus, it is unlikely that the precise geometry will be known after emplacement. For horizontal emplacement, the rods will distribute themselves under the force of gravity and it is likely that there will be large gaps around the container. For vertical emplacement, the final location and shape of the gas gaps is not clear.

For preconsolidated or intact spent fuel assemblies the rods are not free to move. Thus, the internal geometry in the container is more accurately known.

The thermal profile presented in the SCP dates back to 1984 [O'Neal, 1984] and is for a design that is no longer under consideration. The main objective of O'Neal's study was to demonstrate that peak temperatures did not exceed design limits. In the original analysis the waste package was modeled in two-dimensions as a semi-infinite cylinder. Thus, there were no axial variations in temperature. The heat generation rate was the average for the spent fuel. The consolidated fuel region was homogenized and the gaps around the fuel pins that will form were ignored. Also, helium was the fill gas (argon, a gas with much less favorable heat transfer properties, is the present reference design fill gas). Given the same boundary conditions, these assumptions are likely to produce non-conservative predictions of the temperature profile within the container.

Review of spent fuel dry storage and shipping cask systems indicates that there are many similarities between these systems and containers planned for use in geologic disposal of spent fuel. Experiments and thermal analyses have been performed for single and multi-assembly dry storage systems containing both consolidated and unconsolidated fuel. Many of the lessons learned from these experiments and analyses are applicable to spent fuel disposal containers. In particular, the following can be deduced:

a) To accurately predict temperatures within the spent fuel container requires precise knowledge of the geometry and, in particular, of the exact locations of gas gaps. Internal geometry is the most important cause of uncertainty in internal waste package temperature predictions. The internal geometry determines the dominant heat transfer mechanism, with consolidated geometries dominated by conduction and unconsolidated geometries influenced more by radiation heat transfer. Eccentricities within the container can also have a significant influence on temperature.

b) The fill gas plays an important role in determining the temperature rise across the container. This is particularly true for consolidated fuel rods where conduction is the major heat transfer mechanism.

c) Upon consolidation of the fuel rods it is unlikely that there will be perfect contact along the rods. Ignoring any possible contact in performing the heat transfer calculations leads to only a slight overprediction of peak temperatures as compared to experimental data.

d) In the literature, a number of different methods exist to predict temperatures within dry storage systems. These range from simple semi-empirical expressions with correlation coefficients based on experimental data to three-dimensional numerical simulations of the thermal-hydraulic performance of the system. The choice of which method is best depends on the problem under study and the level of accuracy desired. Simpler models may be adequate for preliminary screening and sensitivity analysis. More elaborate models may be necessary for design basis calculations. The simpler approaches usually require symmetry or simple geometries and would require modification before these methods could be adapted to spent fuel disposal systems. In most cases, modification would require new experiments to obtain data for the models. The three-dimensional thermal-hydraulic simulations are the most accurate approaches for predicting waste package temperatures. Given a well characterized problem, these methods are capable of predicting temperature rises within dry storage systems to within 10%. However, due to the poorly defined geometry in the present reference design case and the expense in operating and using these codes, it is not clear that their use is justified under all circumstances.

e) Axial variations in temperature can be substantial. Axially, the peak temperature was often more than 20% greater than the average. The axial variation in temperature is a function of geometry, fill gas, and heat generation rates. For vertical emplacement, the interplay among these factors also causes the maximum temperature to be achieved at a location above the midplane of the container, especially for gases with poorer heat transfer properties. Axial variations in temperature are important then in order to determine the peak and average temperatures within a container.

The latter are important parameters for estimating gas gap pressures in the fuel rods, the partial pressure of oxidized ^{14}C within intact and partly failed containers, and the oxidation rates of UO_2 and cladding.

Recommendations for Future Work

The thermal analyses performed in the past that calculate waste package temperatures are inadequate for designs presented in the SCP. None of the available analyses takes into account the geometries found in the reference designs of Figure 2.1; none considers unconsolidated spent fuel; none utilizes the thermal properties of argon, the reference fill gas; and none consider axial variations in the temperature profile.

It is suggested that the previous analyses be updated. The new analyses should also consider non-uniform temperatures around the borehole as a boundary condition. For vertical emplacement, the borehole will be cooler at the top and bottom as compared to the middle. This is due to the axially non-uniform heat generation rate within the container, to heat convection within the air gap between the borehole and the container, and to the better contact of the container with the host rock at the bottom of the borehole. This non-uniform temperature around the container will be largest during the first few hundred years when the heat generation rates are at their highest.

For containers with fuel rods consolidated at the repository, lack of a well defined geometry poses a large problem in accurate determination of internal temperatures. Sensitivity analysis for a range of geometries should be performed to determine the worst possible case.

Although the geometry is better defined for the preconsolidated or intact spent fuel assemblies, these still need to be analyzed. The influence of eccentricities within the container should be examined through a sensitivity analysis.

A potential benefit of performing detailed thermal analysis of the waste packages is the possibility of obtaining correlations for the time-dependent temperature profile for use in system codes. The correlations could be developed as a function of different disposal configurations and external boundary temperatures.

Consideration should also be given to modeling heat transfer in breached containers. Important processes such as Zircaloy, spent fuel, and ^{14}C oxidation, wetting of the fuel, etc., will occur after breach. Breached containers will have a different gas environment and will no longer be a closed system.

Experimental results from dry storage systems provided insight into heat transfer mechanisms and provided confidence in analytical modeling results. Consideration should be given to performing similar experiments for waste container systems. In addition to increasing confidence in the modeling, the experiments could be designed to determine simple, empirical correlations which could be used for heat transfer analysis.

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