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ADVANCED NUCLEAR FUEL CYCLE EFFECTS ON THE TREATMENT OF UNCERTAINTY IN THE LONG-TERM ASSESSMENT OF GEOLOGIC DISPOSAL SYSTEMS - EBS INPUT

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Disclaimer

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Acronyms

ABR	Advanced Breeder Reactor
BWR	Boiling Water Reactor
DOE	U.S. Department of Energy
EBS	Engineered Barrier System
EC	Electro-Chemical HLW waste form
FCT	Fuel Cycle Technology
FY	Fiscal Year
GWd	Gigawatt days
HLW	High-Level nuclear Waste
IM	Information Management
LA	License Application
LLNL	Lawrence Livermore National Laboratory
LWR	Light Water Reactor
MOX	Mixed Oxide Fuel
MTHM	Metric Tons of Heavy Metal
NE	DOE, Office of Nuclear Energy
NFC	Nuclear Fuel Cycle
ORNL	Oak Ridge National Laboratory
PWR	Pressurized Water Reactor
R&D	Research and Development
SFR	Sodium Fast Reactor
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory
TRU	Transuranic
TSPA	Total System Performance Assessment
UFD	Used Fuel Disposition
UOX	Uranium Oxide Fuel
WP	Waste Package
YMP	Yucca Mountain Project

1. Introduction

The Used Fuel Disposition (UFD) Campaign within the Department of Energy's Office of Nuclear Energy (DOE-NE) Fuel Cycle Technology (FCT) program has been tasked with investigating the disposal of the nation's spent nuclear fuel (SNF) and high-level nuclear waste (HLW) for a range of potential waste forms and geologic environments.

The planning, construction, and operation of a nuclear disposal facility is a long-term process that involves engineered barriers that are tailored to both the geologic environment and the waste forms being emplaced. The UFD Campaign is considering a range of fuel cycles that in turn produce a range of waste forms. The UFD Campaign is also considering a range of geologic media. These ranges could be thought of as adding uncertainty to what the disposal facility design will ultimately be; however, it may be preferable to thinking about the ranges as adding flexibility to design of a disposal facility. For example, as the overall DOE-NE program and industrial actions result in the fuel cycles that will produce waste to be disposed, and the characteristics of those wastes become clear, the disposal program retains flexibility in both the choice of geologic environment and the specific repository design. Of course, other factors also play a major role, including local and State-level acceptance of the specific site that provides the geologic environment.

In contrast, the Yucca Mountain Project (YMP) repository license application (LA) is based on waste forms from an open fuel cycle (PWR and BWR assemblies from an open fuel cycle). These waste forms were about 90% of the total waste, and they were the determining waste form in developing the engineered barrier system (EBS) design for the Yucca Mountain Repository design. About 10% of the repository capacity was reserved for waste from a full recycle fuel cycle in which some actinides were extracted for weapons use, and the remaining fission products and some minor actinides were encapsulated in borosilicate glass. Because the heat load of the glass was much less than the PWR and BWR assemblies, the glass waste form was able to be co-disposed with the open cycle waste, by interspersing glass waste packages among the spent fuel assembly waste packages. In addition, the Yucca Mountain repository was designed to include some research reactor spent fuel and naval reactor spent fuel, within the envelope that was set using the commercial reactor assemblies as the design basis waste form.

This milestone report supports Sandia National Laboratory milestone M2FT-12SN0814052, and is intended to be a chapter in that milestone report. The independent technical review of this LLNL milestone was performed at LLNL and is documented in the electronic Information Management (IM) system at LLNL.

1.1 Objective

The objective of this work is to investigate what aspects of quantifying, characterizing, and representing the uncertainty associated with the engineered barrier are affected by implementing different advanced nuclear fuel cycles (e.g., partitioning and transmutation scenarios) together with corresponding designs and thermal constraints.

1.2 Approach

This report chapter approaches the objective of studying EBS uncertainty in two ways. One aspect of the study is to look at the performance (with associated uncertainties) of

repositories in various geologic media (including oxidizing and reducing environments), and in particular for various waste forms that would be produced by open, modified open, and closed fuel cycles. The other aspect of the study is to continue the trade-off analyses for a variety of repository designs, waste forms and geologic media. The following sections are in pairs (1.2.1 and 1.2.2, approach; 2, fuel cycle analysis; and 3, thermal design analysis) associated with these two aspects of the study. Section 4 summarizes both aspects of the study.

The UFD Campaign has developed a research and development (R&D) roadmap for use as an evaluation and prioritization tool for R&D opportunities that could be pursued by the campaign (FCRD 2011). The R&D roadmap is organized according to features, events and processes (FEPs) that pertain to a variety of geologic disposal scenarios. A multi-laboratory team evaluated both the R&D roadmap and FEPs during 2010 and 2011. FEPs were used in the YMP LA as well as for many international repository programs, with a screening of FEPs into the total systems performance assessment (TSPA). Some FEPs are excluded from the TSPA based on low probability, low consequence, or because the governing regulation has prescribed how an aspect of performance is to be modeled. A significant portion of the FEPs (and the subsequently roadmap) relate to the properties, behavior and performance of the EBS and radionuclides in the EBS, as well as uncertainties in them. This report discusses aspects of the EBS pertinent to those FEPs and Roadmap sections.

1.2.1 Influence of Fuel Cycle on Performance Uncertainty

The study of the influence of the fuel cycle on the EBS uncertainty begins with a discussion of the radionuclide inventory of three representative fuel cycles (one open, one modified open and one closed). Then, repository performance for an open fuel cycle in oxidizing and reducing environments is reviewed. The influence of model inputs on the repository performance is then discussed. Finally, inferences are drawn about what uncertainties and input parameters may not be applicable for the three fuel cycles.

1.2.2 Thermal Aspects of Design

In this report chapter, the process of developing a repository layout for a specific waste form and geologic medium is addressed. The multiple tradeoffs among the four key design parameters of *storage time, drift/borehole spacing, waste package spacing and waste package size (capacity*) are explored. Two additional design parameters are *geologic medium* and *waste form*. In turn, the *fuel cycle* that produces the waste forms can be thought of as a seventh parameter. The parameter, *medium*, includes the effects on the engineered barrier system design and the thermal limits potentially driven by the thermal conductivity of the engineered and natural barriers. Ultimately, both the overall cost of building a repository and the overall performance can be assessed as a function of these seven parameters. For example, the cost equation would be in terms of the first four parameters, with the other three parameters constraining those four. The equation could be of the form

$$C = f\left(\; t_{Store}, D_{SP}, WP_{SP}, \frac{1}{Cap_{WP}} \right)$$

Or, perhaps more explicitly,

$$C = \sum_{1}^{4} c_i u_i^{n_i}$$

where the constants c_i and exponents n_i are greater than zero. Because each of the equation parameters has uncertainty (at least until the design is frozen), there is a consequent uncertainty in the overall cost. Perhaps more importantly, the constants and exponents have uncertainties as well, even after the design is frozen, and some of the uncertainties are beyond the designer's control (such as the prevailing interest rate).

In the first equation, t_{Store} is the surface storage time, D_{SP} is the drift spacing, WP_{SP} is the waste package spacing, and Cap_{WP} is the waste package capacity. The parameters not shown in the equation (but see below) are *Med* which is the geologic medium hosting the repository, T_{Lim} which are the thermal limit(s) of the engineered material and/or natural barrier material surrounding the waste package, P_{WF} which is the thermal power of the waste form in one waste package at the time of emplacement, and *Cycle* which represents the fuel cycle strategy chosen (namely open, modified or closed).

The four parameters are listed as directly or inversely related to the cost, based on first order relationships. For example, the longer the surface storage time, the higher the cost of that pre-disposal activity associated with the repository. However, it should be noted that varying the surface storage time also affects some of the other parameters, with their cost effects being captured by those parameters; the net effect of longer surface storage time could very well decrease the total system cost. A wider drift/borehole spacing and a wider waste package spacing increases the layout size and hence the cost. A larger waste package capacity results in fewer waste packages (albeit of a larger size) and the number of waste packages contributes more to the overall cost than the slightly higher unit cost of a waste package (and associated EBS components).

The effects on cost of the geologic medium, the temperature limits, the waste form thermal power, and the fuel cycle are captured in the other terms. The effects of the geologic medium are on the overall design (e.g., a granite repository likely requires a bentonite buffer), which affects the unit cost of the waste package and associated EBS components. The temperature limit(s) are inversely related to the cost because a higher temperature limit permits either a smaller layout or less storage time. The thermal power of the waste form in a single waste package (of a given size) at the time of emplacement (after a given storage time) is determined by the waste form composition, and affects the layout. A waste form composition that produces higher heat per unit mass than some nominal waste form requires some combination of longer storage time, smaller waste package capacity, wider waste package spacing, and wider drift/borehole spacing. Finally, the fuel cycle directly affects the waste form composition.

A similar discussion could be constructed for the effects of the parameters on repository performance. Ultimately, uncertainties in fundamental process models such as these conceptual designs are passed upward through intermediate-level system models such as Goldsim to full TSPA models (NAS 2011). Once cost and performance models have adequate maturity, an optimization can determine the lowest cost repository that meets performance requirements, with appropriate consideration of uncertainties in both the cost and performance models. This report chapter advances the discussion, incrementally, toward that goal.

The FY11 report (LLNL 2011, SNL 2011) used three fuel cycles, six waste forms, and four geologic media (with associated designs and layout parameters, and thermal limits). The

report explored the tradeoff of the other two variables: waste package capacity and storage time. This report chapter continues the exploration, including a range of layout parameters (drift/borehole spacing, waste package spacing) and uncertainties in thermal limits and EBS and geologic medium thermal properties.

2. Fuel Cycle Analysis

The Fuel Cycle Options (FCO) Campaign is currently studying a number of Open, Modified Open, and Closed Fuel Cycle options. The FCO Campaign combines the prior Systems Analyses and Systems Engineering Campaigns within the DOE Office of Nuclear Energy. In FY11, the UFD Campaign selected one fuel cycle of each type, as representations for use in repository studies. The three fuel cycles are the following:

- The once-through (Open) Cycle allows for the direct disposal of high-burnup (60 GWd/MTHM burnup) uranium oxide (UOX) spent nuclear fuel (SNF) from Gen-III reactors and earlier LWRs
- The Modified Open Cycle includes reprocessing of LWR UOX (51 GWd/MTHM burnup) to produce mixed oxide (MOX) fuel that is subsequently used once (50 GWd/MTHM burnup), generating a MOX SNF package from the MOX reactor and co-extraction high level waste in the form of borosilicate glass from the UOX reactor. This cycle includes irradiation of MOX fuel from the Pu-disposition program (nominally 500 MTHM). While not seen as a significant long-term fuel cycle, the Modified Open Cycle with MOX fuel was considered because MOX fuel currently exists.
- The example Closed Fuel Cycle investigated in FY11 includes reprocessing of LWR UOX (51 GWd/MTHM burnup) to produce U-TRU metal fuel for an advanced burner reactor (ABR, which is a Sodium Fast Reactor, SFR, with 99.6 GWd/MTHM burnup) with a conversion ratio of 0.75 and repeated recycling of the TRU elements in the ABR fuel. This Closed Fuel Cycle generates "new-extraction" borosilicate high-level waste glass from the UOX reactor, and the ABR reactor fuel recycling produces electrochemical (EC) separation ceramic (for most of the fission products), as well as electrochemical separation metal. The EC metal includes elements that are more electrochemically noble than uranium, including hardware and some metallic fission products.

Section 2.1 summarizes the inventory, and the uncertainty thereof, for the three fuel cycles, as well as comparison information from the Yucca Mountain License Application and from the Swedish repository design. Section 2.2 summarizes repository performance for an Open Fuel Cycle in oxidizing and reducing environments. Section 2.3 summarizes the influence of model inputs on repository performance, drawing inferences about what uncertainties and input parameters may be less applicable for advanced fuel cycles.

2.1 Inventory for Three Fuel Cycles

The UFD Campaign has obtained radionuclide inventory data for a number of waste forms resulting from multiple fuel cycles. The Systems Analysis Campaign (currently the FCO Campaign) developed these data using reactor neutronics and isotope generation software. The most recent summary of these data is in the Inventory Report by Carter (2011), and

more detailed data are in large spreadsheet files available from the authors of the Inventory Report. Those detailed data spreadsheets were used to develop Table 1.

Table 1 Radionuclide Inventory in Three Fuel Cycles,

Radionuclide	YMP LA SAR	Open Cycle	Open Cycle	Modified Open Cycle		Closed Fuel Cycle		
	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr	Grams per Fuel Cycle GWe-yr
	YMP Commercial SNF	40 GWd/MT UOX	60 GWd/MT UOX	50 GWd/MT MOX	COEX Glass PWR 51&5	NUEX Glass PWR 51&5	E-Chem Zeolite FR Metal 0.75	E-Chem Metal FR Metal 0.75
227Ac	7.290E-06	6.351E-07	8.153E-07	2.505E-08	0.000E+00	0.000E+00	0.000E+00	0.000E+00
241Am	2.414E+04	3.573E+03	2.679E+03	3.671E+03	4.638E+04	0.000E+00	0.000E+00	0.000E+00
243Am	3.660E+03	3.841E+03	5.007E+03	4.187E+03	2.100E+04	0.000E+00	0.000E+00	0.000E+00
14C	3.985E+00	8.626E+00	8.406E+00	8.358E-05	2.145E-03	1.683E-03	0.000E+00	0.000E+00
36Cl	9.534E+00	9.733E+00	9.251E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
245Cm	5.165E+01	6.562E+01	1.764E+02	2.802E+02	6.052E+02	0.000E+00	0.000E+00	0.000E+00
135Cs	1.287E+04	1.345E+04	1.423E+04	1.956E+03	6.980E+04	4.363E+04	2.309E+04	1.054E+04
137Cs	1.741E+04	3.847E+04	3.769E+04	3.869E+03	1.711E+05	1.070E+05	1.935E+04	8.833E+03
129I	5.106E+03	5.975E+03	5.780E+03	7.367E+02	0.000E+00	0.000E+00	4.259E+03	1.944E+03
237Np	1.349E+04	1.895E+04	2.210E+04	1.832E+03	6.573E+04	0.000E+00	0.000E+00	0.000E+00
231Pa	2.707E-02	1.472E-02	1.612E-02	9.113E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00
210Pb	0.000E+00	2.492E-09	5.834E-09	9.807E-11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
238Pu	4.486E+03	7.179E+03	1.131E+04	6.874E+03	1.947E+01	1.273E+01	0.000E+00	0.000E+00
239Pu	1.275E+05	1.770E+05	1.369E+05	7.046E+04	3.905E+02	2.553E+02	0.000E+00	0.000E+00
240Pu	6.051E+04	7.032E+04	7.382E+04	5.167E+04	1.853E+02	1.211E+02	0.000E+00	0.000E+00
241Pu	7.851E+03	3.966E+04	2.812E+04	2.793E+04	8.772E+01	5.735E+01	0.000E+00	0.000E+00
242Pu	1.558E+04	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
226Ra	0.000E+00	1.616E-06	1.970E-06	6.782E-08	0.000E+00	0.000E+00	0.000E+00	0.000E+00
228Ra	0.000E+00	1.045E-12	1.620E-12	1.069E-13	0.000E+00	0.000E+00	0.000E+00	0.000E+00
79Se	1.237E+02	1.959E+02	1.934E+02	1.589E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00
126Sn	1.367E+03	9.249E+02	9.212E+02	1.189E+02	4.526E+03	1.367E+03	0.000E+00	0.000E+00
90Sr	7.349E+03	1.701E+04	1.633E+04	8.676E+02	7.403E+04	4.916E+03	4.375E+03	1.998E+03
99Tc	2.228E+04	2.534E+04	2.358E+04	2.364E+03	1.211E+05	9.419E+04	0.000E+00	0.000E+00
229Th	0.000E+00	3.639E-05	9.867E-05	1.183E-06	2.946E-04	2.311E-04	0.000E+00	0.000E+00
230Th	4.486E-01	6.576E-02	5.448E-02	3.513E-03	5.401E-01	4.237E-01	0.000E+00	0.000E+00
232Th	0.000E+00	1.296E-02	1.557E-02	1.232E-03	1.320E-01	1.036E-01	0.000E+00	0.000E+00
232U	3.011E-02	3.127E-02	5.365E-02	6.237E-04	2.095E-05	1.651E-05	0.000E+00	0.000E+00
233U	1.700E-01	5.435E-02	4.880E-02	7.160E-03	6.906E-05	5.442E-05	0.000E+00	0.000E+00
234U	5.165E+03	5.076E+03	3.341E+03	4.497E+02	3.893E+00	3.068E+00	0.000E+00	0.000E+00
235U	1.848E+05	2.322E+05	9.908E+04	8.644E+03	1.619E+02	1.276E+02	0.000E+00	0.000E+00
236U	1.133E+05	1.302E+05	1.150E+05	1.062E+04	1.208E+02	9.517E+01	0.000E+00	0.000E+00
238U	2.308E+07	2.583E+07	1.680E+07	1.817E+06	1.949E+04	1.535E+04	0.000E+00	0.000E+00
	2.371E+07	**2.662E+07**	**1.739E+07**	**2.014E+06**	**5.948E+05**	**2.671E+05**	**5.107E+04**	**2.332E+04**

Notes for Table 1 are in the Text Box on the next page

The radionuclides in Table 1 are those screened into the TSPA for Yucca Mountain, and similar lists can be found in design studies for repositories in other countries. The totals at the bottom of each column are a good starting point for considering the inventories of the representative Closed Fuel Cycle, the representative Modified Open Cycle, and three Open Cycles (YMP, OC_40, and OC_60; only the latter is included in the UFD Campaign thermal studies documented in this report and other UFD Campaign reports). From left to right in the table:

- The YM (burnup 38, see DOE 2008, Section 2.3.7.4.2.1) total inventory per unit reactor energy production is about 11% less than the Inventory Report total for the Open Cycle with burnup 40. This could be due to different assumptions, including the averaging of inventories across multiple reactor types and burnups in Yucca Mountain's numbers.
- The Open Cycle with burnup 60 has 65% of the inventory of the burnup 40 open cycle. This is mainly due to the large reduction in U-238, which appears to be

proportional to the burnup. The authors of this report will consult with the Inventory Report authors to verify that this is the expected behavior of U238 in low-enrichment LWRs.

- The MOX total (which is consolidated, for convenience, in Table 2) is reasonable considering that the Modified Open Cycle has 0.1089 MT_MOX per MT_LWR. The co-extraction glass total is much less than the inventory of the radionuclides in the UOX that was reprocessed into the glass because the reprocessing removes most of the actinides, including a large amount of the U-238.
- The Closed Fuel Cycle new-extraction glass total is less than the co-extraction glass total in the Modified Open Cycle because the Closed Fuel Cycle has more of its power generated in ABRs (which have 0.6142 MT_ABR per MT_LWR).

A careful examination of Table 1 reveals key differences between the waste inventories. For example, YMP includes radium 226 and 228 in its list of radionuclides, but the inventory of these radioisotopes in-grows over time, from decay of higher actinides that are also included in the inventory (DOE 2008, Section 2.3.7.4.1.2). In the YMP column, there is no initial inventory of these radium isotopes, but in the other UOX and MOX spent fuel columns in the inventory report, there is an initial inventory. The authors of this report will consult with the Inventory Report authors in FY12 to better understand the differences between YMP and the FCO Campaign in development of initial inventories of radium.

Iodine is not included in the co-extraction and new-extraction waste glass from LWRs because it is separated from other radionuclides during the reprocessing (captured on silver mordenite and grouted into 55 gallon drums) and is not listed in the table (Carter 2011, Section 8.4). Strontium-90 inventories across the table also are non-intuitive (consider the co-extraction glass in the Modified Open Cycle has almost five times the inventory of the Open Cycle which has higher burnup and is the only reactor in the fuel cycle) . Such differences are a matter for further discussion and collaboration between LLNL and SRNL during FY12.

The next two subsections discuss which radionuclides are most significant to long-term performance of the repository and which uncertainties are most significant to the overall uncertainty in that performance. Notwithstanding the inventory details, such as those discussed above, that remain to be verified, the information in the two tables is adequate to consider how changes in inventory across candidate fuel cycle options could affect overall repository performance and could affect the amount of research and site or engineered materials characterization necessary to limit the uncertainty in repository performance.

Notes for Tables 3-1 and 3-2:

1. The YMP data column is from DOE 2008, Table 2.3.7-3, which is at 23 yr after removal from the reactor flux (DOE 2008, Section 2.3.7.4.1.2).

2. The other data columns are from Carter 2011 and its associated spreadsheets; the time column at 23 yr was used.

3. For LWR waste (UOX in the Open Cycle, co-extraction glass in the Modified Open Cycle, and new-extraction glass in the Closed Fuel Cycle), the source values, in g/MT_LWR, were divided by GWe.yr_FC/MT_LWR to obtain grams per unit of fuel cycle energy.

4. For other waste (MOX in the Modified Open Cycle and EC-Ceramic and EC-Metal in the Closed Fuel Cycle, the source values, in g/MT_Reactor, were divided by GWe.yr_FC/MT_LWR, and multiplied by MT_Reactor/MT_LWR, to obtain grams per unit of fuel cycle energy.

5. For Yucca Mountain (38 GWt.d/MT burnup) and for the UOX with burnup 40, the source values, in g/MT_LWR_BU were divided by GWe.yr_FC_60/MT_LWR_60, and also divided by BU/60, to obtain grams per unit of fuel cycle energy. This process uses the facts that the burnup ratio is the same as the fuel cycle energy ratio, and that the MT_Reactor loading is independent of burnup.

6. For the Open Cycle with burnup 38 GWt.d/MT, the fuel cycle energy is 38 * 0.33 thermal efficiency * yr/d = 0.0542 GWe.yr/MT_LWR.

7. For the Modified Open Cycle, the UOX reactor (with co-extraction glass waste) contribution to the fuel cycle energy is 51 GWt.d/MT_LWR * 0.33 thermal efficiency * yr/d = 0.0461 GWe.yr/MT_LWR. The MOX reactor contribution is 50 GWt.d/MT_MOX * 0.33 thermal efficiency * yr/d = 0.0452 GWe.yr/MT_MOX.

8. For the Closed Fuel Cycle, the UOX reactor (with new-extraction glass waste) contribution to the fuel cycle energy is 51 GWt.d/MT_LWR * 0.33 thermal efficiency * yr/d = 0.0461 GWe.yr/MT_LWR. The ABR contribution is 99.6 GWt.d/MT_MOX * 0.4 thermal efficiency * yr/d = 0.1091 GWe.yr/MT_ABR.

9. To obtain the fuel cycle energy, the overall burnup and efficiency are calculated. The overall burnup is the sum of the products of the reactor burnup ($GWt.d_i/MT_i$) and the fuel ratio (MT_i/MT_LWR), which then has the units of GWt.d_FC/MT_LWR. The weighted efficiency is the ratio of the sum of the products of the reactor burnup times fuel ratio times efficiency, all divided by the overall burnup already calculated. The numerator is the fuel cycle electrical energy per MT_LWR, and the denominator is the thermal energy.

10. For the Modified Open Cycle, the fuel ratio is 0.1089 MT_MOX/MT_LWR, the overall burnup is 56.445 GWt.d/MT_LWR, and the overall efficiency is 0.33. Using these values, the fuel cycle energy is 0.051 GWe.yr/MT_LWR.

11. For the Closed Fuel Cycle, the fuel ratio is 0.6142 MT_ABR/MT_LWR, the overall burnup is 112.2 GWt.d/MT_LWR, and the overall efficiency is 0.368. Using these values, the fuel cycle energy is 0.113 GWe.yr/MT_LWR.

12. For Table 3-2, the contributions of the multiple waste forms in the Modified Open Cycle and the Closed Fuel Cycle (in Table 3-1) are summed. This is valid because the contributions in Table 3-1 have been normalized to the Fuel Cycle Energy Production using the procedure outlined above.

Table 2 Combined waste forms for each fuel cycle compared to the YMP LA SAR after 23 years of decay

Radionuclide	YMP LA SAR	Open Cycle	Modified Open Cycle	Closed Fuel Cycle
	Grams per Fuel Cycle GWe-yr	Grams per MTHM	Grams per MTHM	Grams per MTHM
	YMP Commercial SNF	UOX LWR	UOX LWR, MOX LWR	UOX LWR, ABR
227Ac	7.290E-06	8.153E-07	2.505E-08	0.000E+00
241Am	2.414E+04	2.679E+03	5.005E+04	0.000E+00
243Am	3.660E+03	5.007E+03	2.519E+04	0.000E+00
14C	3.985E+00	8.406E+00	2.229E-03	1.683E-03
36Cl	9.534E+00	9.251E+00	0.000E+00	0.000E+00
245Cm	5.165E+01	1.764E+02	8.853E+02	0.000E+00
135Cs	1.287E+04	1.423E+04	7.175E+04	7.726E+04
137Cs	1.741E+04	3.769E+04	1.750E+05	1.351E+05
129I	5.106E+03	5.780E+03	7.367E+02	6.203E+03
237Np	1.349E+04	2.210E+04	6.756E+04	0.000E+00
231Pa	2.707E-02	1.612E-02	9.113E-04	0.000E+00
210Pb	0.000E+00	5.834E-09	9.807E-11	0.000E+00
238Pu	4.486E+03	1.131E+04	6.893E+03	1.273E+01
239Pu	1.275E+05	1.369E+05	7.086E+04	2.553E+02
240Pu	6.051E+04	7.382E+04	5.186E+04	1.211E+02
241Pu	7.851E+03	2.812E+04	2.802E+04	5.735E+01
242Pu	1.558E+04	0.000E+00	0.000E+00	0.000E+00
226Ra	0.000E+00	1.970E-06	6.782E-08	0.000E+00
228Ra	0.000E+00	1.620E-12	1.069E-13	0.000E+00
79Se	1.237E+02	1.934E+02	1.589E+01	0.000E+00
126Sn	1.367E+03	9.212E+02	4.645E+03	1.367E+03
90Sr	7.349E+03	1.633E+04	7.489E+04	1.129E+04
99Tc	2.228E+04	2.358E+04	1.235E+05	9.419E+04
229Th	0.000E+00	9.867E-05	2.958E-04	2.311E-04
230Th	4.486E-01	5.448E-02	5.436E-01	4.237E-01
232Th	0.000E+00	1.557E-02	1.333E-01	1.036E-01
232U	3.011E-02	5.365E-02	6.447E-04	1.651E-05
233U	1.700E-01	4.880E-02	7.229E-03	5.442E-05
234U	5.165E+03	3.341E+03	4.536E+02	3.068E+00
235U	1.848E+05	9.908E+04	8.806E+03	1.276E+02
236U	1.133E+05	1.150E+05	1.074E+04	9.517E+01
238U	2.308E+07	1.680E+07	1.837E+06	1.535E+04
	2.371E+07	**1.739E+07**	**2.609E+06**	**3.415E+05**

Notes for Table 2 are in the Text Box on the previous page

2.2 Performance in Oxidizing and Reducing Environments

Swift (2010) reviewed performance assessments of geologic repository designs in several countries, with emphasis on the influence of the waste form and repository environments. This subsection summarizes that report.

Figure 2-1 shows the radionuclides that drive the performance of the Yucca Mountain design, which is in unsaturated tuff, an oxidizing environment. Actinides have relatively higher solubility in oxidizing environments, and three actinides dominate the long-term dose. Removing these radionuclides from the waste stream, using an advanced fuel cycle that repeatedly recycles them through the flux in advanced reactors, could limit their contribution to the small leakage fraction inherent in any reprocessing facility. The highest

non-actinide contributor at very long times (~ 800 ky) is I-129, which is about 10% of the total. Note that the inventory of this radionuclide in Table 1 is underestimated for the Modified Open Cycle and the Closed Fuel Cycle, because the table does not include the getter material used to capture gaseous iodine during reprocessing of the UOX into glass; a full accounting of iodine will have similar totals of this isotope per unit of fuel cycle energy. At earlier times, Tc-99 will also be a significant contributor, and will have similar inventories in the various fuel cycles.

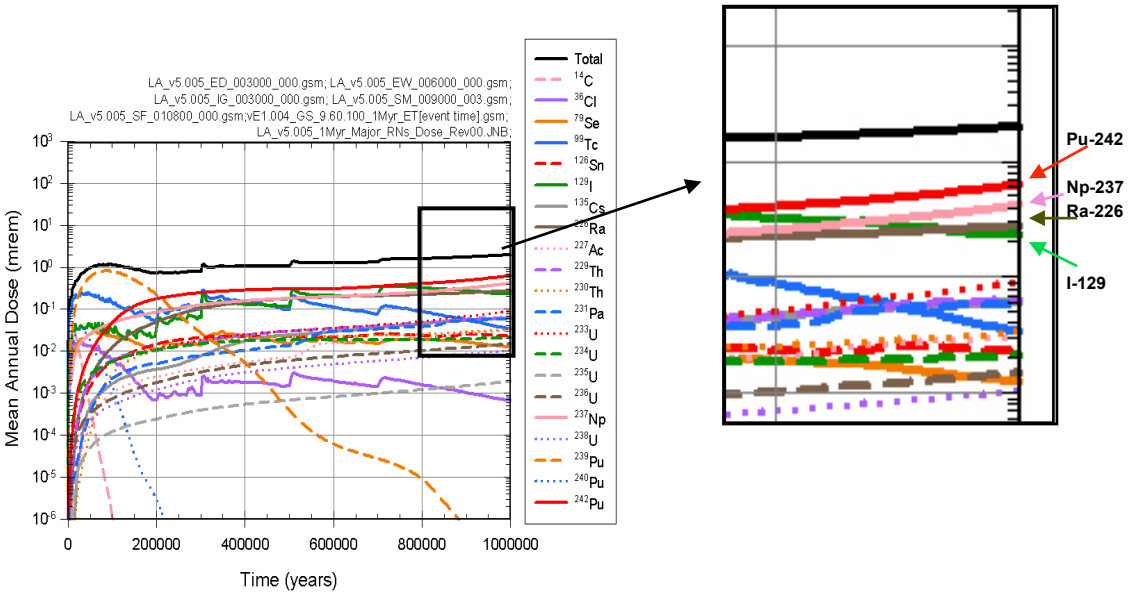

Figure 2-1 Performance of the Yucca Mountain repository. The expanded view at the right shows the key radionuclides at very long times (800 ky – 1 My) (Swift 2010)

In contrast, Figure 2-2 shows the performance of a clay repository, a reducing environment, with high-level-waste glass as the waste form. Actinides have limited mobility in both the repository environment and the surrounding geosphere, and the performance is dominated by I-129, Cl-36, and Se-79. These dominating radionuclides are fission products that are not recycled multiple times through reactor neutron fluxes in advanced fuel cycles. Iodine was discussed above. The other two dominating radionuclides are shown as zero in both the glass and electrochemical waste streams in Table 1 (for the Modified Open Cycle and the Closed Fuel Cycle); discussions with the Inventory Report authors will determine in what waste form these radionuclides are accounted. Further, Cl-36 is shown as zero for MOX in Table 1; which is counterintuitive. These issues will be resolved by discussions between LLNL and SRNL later in FY12.

Swift (2010) also shows the performance of a granite repository with spent nuclear fuel as the waste form. I-129 and Ra-226 dominate the performance. Ra-226 is a decay product of U-234 and Th-230, and is more mobile in reducing environments than its parent actinides. In clay settings that are dominated by diffusive transport, Ra-226 (half-life ~1600 yr) decays before reaching the biosphere. In the granite repository performance assessment, rapid transport by advection in fractures moved the Ra-226 to the biosphere in a short enough time that it dominated the dose rate after about 50 ky. This radionuclide

In summary, an advanced fuel cycle has the potential to improve long term performance by about a factor of 10 (reduce the dose rate to 10%) compared to the Open Cycle, for repositories in oxidizing environments, such as the unsaturated tuff at Yucca Mountain. However, for repositories in reducing environments, the actinides that are largely removed from the advanced fuel cycle waste forms are largely immobile, and the advanced fuel cycle has only a minor effect on long-term repository performance.

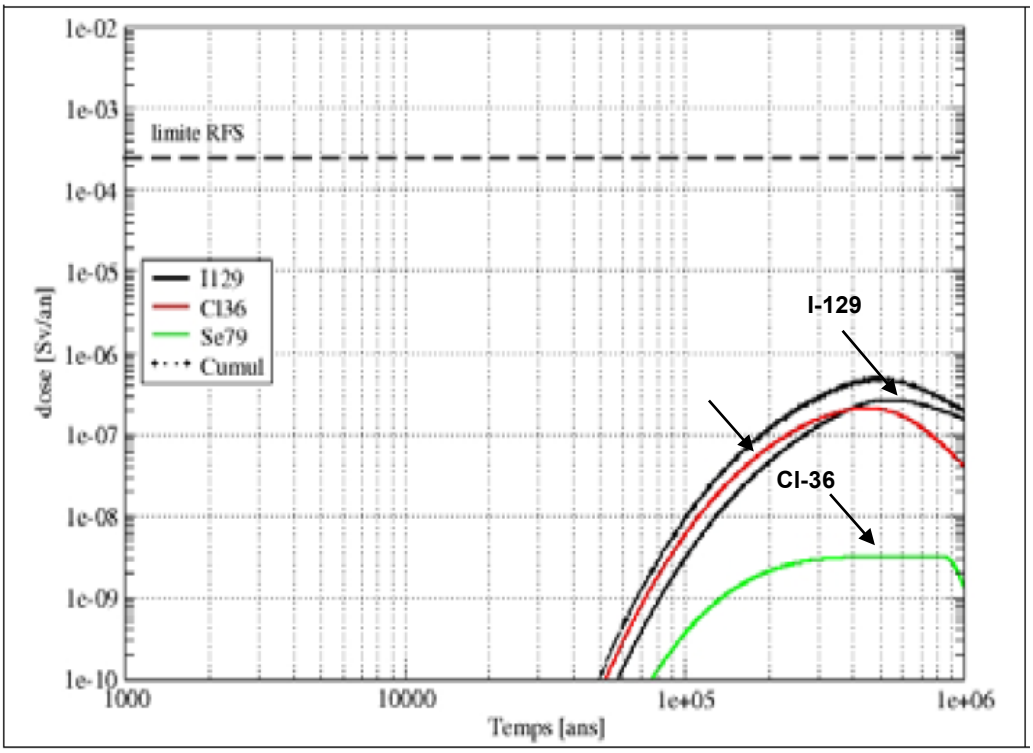

Figure 2-2 Performance of a clay repository with a HLW glass waste form (Swift 2010)

2.3 Dependence of Repository Performance on Uncertain Inputs to the Total System Performance Assessments

In the YM TSPA (SNL 2008), the top-ranking uncertainty importance parameters for the nominal scenario relate to the residual stress threshold for the Alloy-22 waste package outer barrier and the temperature dependence of the Alloy-22 waste package outer barrier general corrosion rate. While the primary cause of the residual stress is from seismic ground motion, it is also considered that rock-fall and drift collapse would contribute to residual stress. For the temperature dependence, higher temperatures result in earlier, higher general corrosion rates during the thermal period, while the cooler periods yield lower long-term corrosion rates. Other uncertainties relating to the nominal case and early failure included scale factor used to incorporate uncertainty into the stress intensity factor for closure-lid weld, host rock thermal conductivity level, stress corrosion cracking growth rate exponent, and concentration of irreversibly attached plutonium on stable glass/waste form colloids. Aleatory uncertainties identified are those relating to the time and location of general corrosion failures of each type of waste package.

For early-failure scenarios, aleatory uncertainties in the TSPA related to the number of early-failed waste packages, the number of early-failed drip shields, the type of waste

package under each early-failed drip shield, and the location of each early-failed drip shield. More specifically, for early failure of the drip-shield, the uncertainty is dominated by the probability for undetected defects in drip shields. Other notable (although less prominent) uncertainties relating to drip-shield early failure were:

- uncertainty factor to account for small-scale heterogeneity in fracture permeability
- logarithm of the mean fracture permeability in lithophysal rock units
- variable for determining infiltration conditions (10^{th}, 30^{th}, 50^{th}, 90^{th} percentile infiltration scenario)
- groundwater biosphere dose conversion factor for Tc-99 in modern interglacial climate
- van Genuchten capillary strength parameter in lithophysal rock units
- logarithm of the colloid retardation factor in alluvium
- logarithm of the scale factor used to characterize uncertainty in groundwater specific discharge, and
- scale factor used to characterize uncertainty in plutonium solubility at an ionic strength below 1 molal.

For early failure of the waste package, the uncertainty is dominated by the probability of undetected defects in the waste package. Other lesser uncertainties relating to waste package early failure include:

- groundwater biosphere dose conversion factor for Tc-99 in modern interglacial climate
- groundwater biosphere dose conversion factor for C-14 in modern interglacial climate
- scale factor used to characterize uncertainty in radionuclide content of DOE SNF
- variable for determining infiltration conditions (10^{th}, 30^{th}, 50^{th}, 90^{th} percentile infiltration scenario
- selector variable for one of three host-rock thermal conductivity scenarios
- fracture aperture for Group 8 rock units
- pointer variable used to determine ionic strength for commercial SNF cell under vapor influx conditions
- logarithm of the scale factor used to characterize uncertainty in groundwater specific discharge
- logarithm of the mean fracture permeability in lithophysal rock units, and
- scale factor used to characterize the uncertainty in plutonium solubility at an ionic strength below 1 molal.

In addition to the probability of early failure of a single waste package and drip shield, other uncertainties that may be improved by further research relating to the EBS and the waste package include:

- EBS environment

    - thermal conductivity of surrounding host rock
    - ambient water composition
    - pCO_2, ionic strength, and pH of in-drift seepage water
    - water-rock interaction for seepage water
- waste package and drip shield degradation
    - corrosion rates of Alloy-22 and drip shield components
    - temperature and relative humidity at the drip shield and waste package
    - pH, NO_3^-, and Cl^- of crown seepage water
- EBS flow
    - drip shield and waste package flux splitting factors
    - representative subregion typical liquid saturation in the invert
    - representative subregion typical imbibition flux in the invert
    - representative subregion typical liquid saturation and flux through the EBS UZ interface
- EBS transport
    - steel corrosion rates
    - specific surface area of steel corrosion products
    - adsorption isotherm for water vapor sorption onto degraded waste form and steel corrosion products
    - density of radionuclide sorption sites in steel corrosion products.

Another example of uncertainty inputs to PA can be drawn from the Swedish repository investigations (SKB TR06-09). A variety of data were used in the illustration of uncertainty due to lack of knowledge and spatial variability. The key uncertainties relate primarily to:

- the number of failed canisters
- the canister defect sizes
- fuel dissolution rate concentration limits
- buffer porosities, diffusivities and sorption coefficients
- backfill diffusivity and sorption coefficients
- rock porosities, diffusivities and sorption coefficients
- hydrogeological data related to flow and transport
- rock Peclet number
- maximum penetration depth in rock matrix
- biosphere landscape dose factor

Given the uncertainties identified in both the YM TSPA and the SKB investigations, the fuel cycle itself has little if any impact on the overall uncertainty. C-14 amounts relating to uncertainty are several orders of magnitude less in both the Modified Open and Closed Fuel

Cycles compared with both the YMP LA SAR and the Open Cycle. Similarly, Pu inventory is less in the Closed Fuel Cycle compared to the Open and Modified Open Cycles. Tc-99 amounts in the Closed Fuel Cycle are similar to those in the Open Cycle, while the concentration in the Modified Open Cycle is an order of magnitude higher. However, the uncertainties identified above associated with these radionuclides are minor when compared to those related to those associated with general corrosion, stress corrosion cracking, and early failure of the waste package and drip shield.

3. Thermal Design Analysis

Conceptual models of geologic repository designs and thermal load management have been (and continue to be) investigated (LLNL 2011, SNL 2011, SNL 2012). A combination of transient heat transfer analytical solutions for a finite line source, a series of point sources, and a series of parallel infinite line sources were combined with a quasi-steady-state multi-layered cylindrical solution to simulate the temperature response of a deep geologic radioactive waste repository with multi-layered natural and engineered barriers. This thermal model enables exploration of the relationships among the design parameters and of the effects of uncertainties.

Uncertainties exist in the characteristic properties of the EBS. Clearly, the geologic and engineered materials chosen relate directly to the design concept selected. Properties such as thermal conductivity and diffusivity, hydraulic conductivity and diffusivity and radionuclide sorption are specific to the material chosen for the EBS components, and are not directly affected by either the design concept itself, or the fuel cycle strategy. These uncertainties play a role in determining the design concept, including the dimensions, spacing, and choice and arrangement of materials.

Section 3.1 reviews the fuel cycles considered in the FY11 work and that continue to be considered in this report chapter. The section includes an evaluation of the thermal output of waste packages for one or more spent fuel assemblies or high-level waste canisters from the three fuel cycles, such that these waste packages all lie under the power history of a 4-assembly UOX SNF package (4-UOX) in clay and granite, or 12-assembly UOX SNF package (12-UOX) in salt (UOX is the dominant waste form in the open fuel cycle). Calculations of tradeoffs between storage time (aging) and layout parameters (drift/borehole spacing and waste package spacing) for the UOX WPs will then apply to the other five waste forms from the other two fuel cycles.

Section 3.2 discusses the thermal limits for clay, granite, and salt, as well as recent information of how those limits could be evolving in ongoing international studies.

Section 3.3 explores the tradeoffs between repository layout parameters (drift/borehole spacing and waste package spacing) and surface storage time.

Section 3.4 discusses the effect of thermal limit uncertainty on storage time, for each of the three geologic media (using one pair of drift/borehole and WP spacings for each medium).

Section 3.5 examines the effect of uncertainty in the bulk thermal conductivity of the EBS.

Section 3.6 discusses the effect of buffer thermal conductivity due to uncertainty in the buffer and container material design.

Section 3.7 studies the conceptual uncertainty of the EBS.

Section 3.8 considers the variety of materials used for waste package and EBS materials for each geologic media.

Section 3.9 explores the uncertainties associated with the transport of radionuclides in the EBS.

3.1 Nuclear Fuel Cycles Investigated in Engineered Barrier Studies

Three fuel cycles were investigated in the Repository Design / Thermal Load work performed during FY11 by SNL, LLNL, ORNL, and SRNL (SNL 2011, LLNL 2011). These fuel cycles, which are described above, in Section 2, produce six waste forms with significant thermal power levels.

The representative once-through fuel cycle produces UOX spent fuel assemblies. The thermal output from each waste type is shown in Figure 3-1.

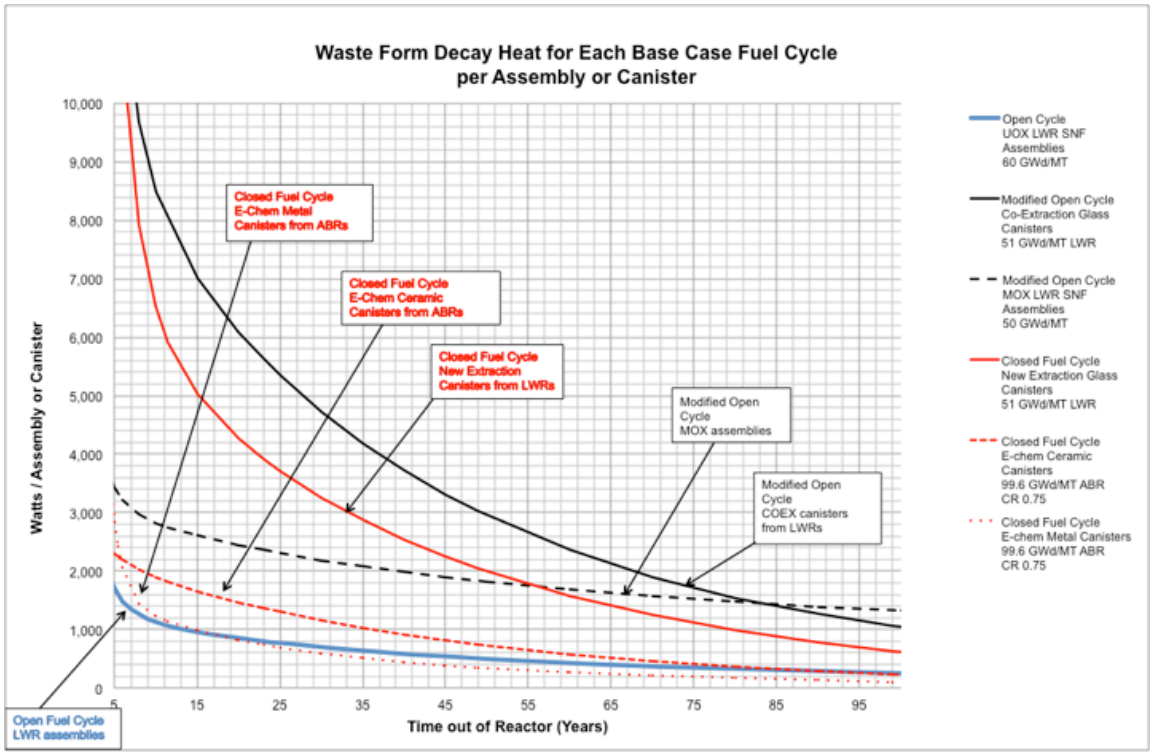

Figure 3-1 Decay heat curves for one assembly or one canister for UOX, MOX, co-extraction, new extraction, EC-ceramic, and EC-metal (LLNL 2011)

For granite and clay media, a waste package with four UOX spent fuel assemblies (4-UOX) was shown in FY11 to have reasonable surface storage times to remain within a thermal limit of 100°C (see Section 3.3 of this report for a review of the FY11 results). For salt, a waste package with twelve UOX spent fuel assemblies (12-UOX) was shown to have reasonable surface storage times to remain within a thermal limit of 200°C. Figure 3-2 shows the number of canisters of high-level waste, or assemblies of MOX, that have similar heat to the 12-UOX waste package. Table 1 provides examples of equivalent waste package power following 50 and 100 years of pre-emplacement storage time. Based on that similarity, parametric calculations for the UOX waste are applicable to the other five waste

forms from the modified open and closed fuel cycles studied in FY11. Note that MOX in clay and granite at 50 and 100 years falls just short of a 12-UOX package, but it is reasonable to imagine that aging for 105 years would (for example allow disposal of a 1-MOX package. Also, a reasonable-size EC-Ceramic or EC-Metal waste package will have much less heat than the other waste packages, and could be used between hotter waste packages as a thermal buffer, similar to the use of cooler HLW waste packages in the Yucca Mountain design.

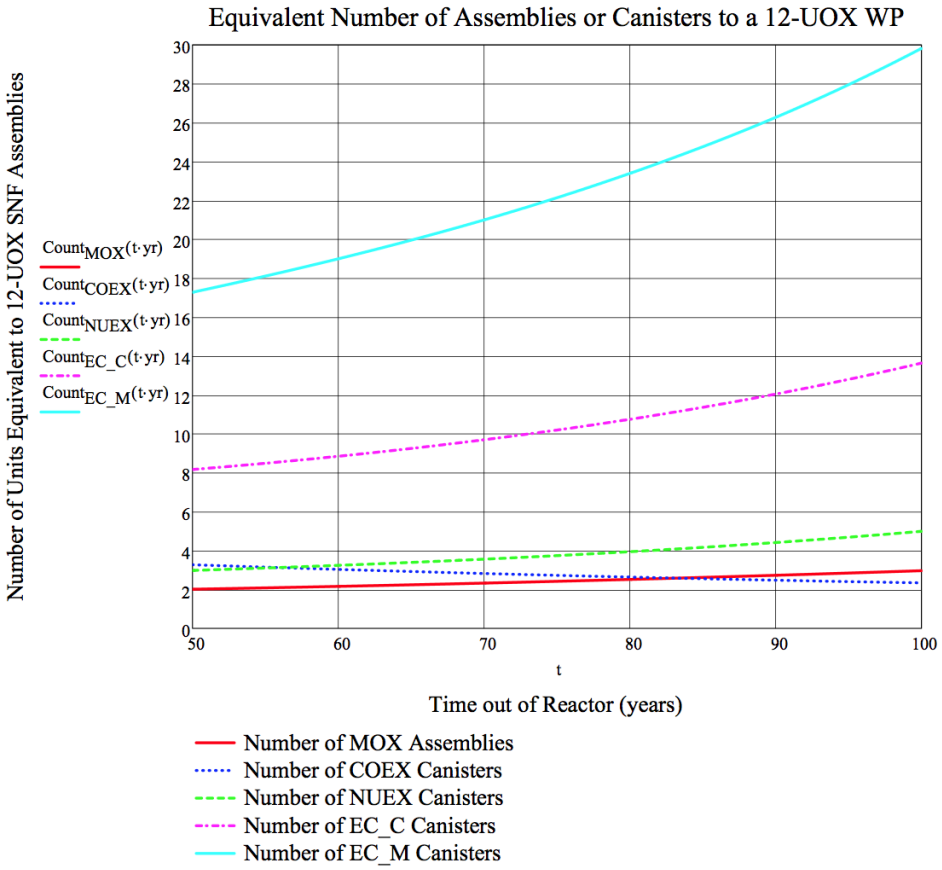

Figure 3-2 Number of waste packages for a variety of waste forms equivalent to a 12-UOX waste package that meet the thermal constraints of salt after pre-emplacement surface storage

Table 3 Maximum equivalent waste forms with thermal power less than a 12-UOX in salt or a 4-UOX in clay/granite

Waste Form	Salt (12-UOX)		Clay/Granite (4-UOX)	
Storage Time	50	100	50	100
MOX	2	2	0*	0*
COEX	3	2	1	0
NUEX	2	4	0	1
EC-C	8	13	2	4
EC-M	17	29	5	9

* MOX in clay/granite is 0.67 and 0.99 at 50 and 100 respectively.

** See Figure 3-2

3.2 Temperature Limits for Geologic Media and Engineered Barriers

Four geologic environments were considered in the FY11 Repository Design / Thermal Management work, namely granite, clay/shale, salt, and deep borehole. For each waste form and geologic environment combination, there are multiple options for a repository conceptual design. In FY11, an expert multidisciplinary panel, consisting of representatives from four National Laboratories and DOE/NE, with experience in US and international repository programs, selected basic input data to be analyzed for thermal load from a variety of waste streams, repository configurations, and material properties and thermal constraints.

The repository configurations selected were based on current international design concepts for both SNF and HLW deep geologic disposal systems in each of the host rock types. Unlike repository designs with large open tunnels and pre-closure ventilation (such as Yucca Mountain), all of the disposal concepts selected for the FY11 studies used enclosed emplacement modes, where the waste packages are in direct contact with encapsulating engineered or natural materials. The concepts of operation for the various alternatives are discussed elsewhere (SNL 2011). Example design concepts were considered for the various media for:

- Granite (crystalline rock) – from Sweden, Finland, and Japan
- Clay – from Belgium, France, and Switzerland
- Salt - from Germany and the US
- Deep Borehole – from Sweden and the US.

The following temperature limits were applied at the interface between the waste package surface and the EBS (or rock wall, depending on design):

- Granite: 100°C, based on a bentonite layer near the waste package surface

- Clay: 100°C, based on the host rock for the HLW waste forms, and on a bentonite layer for the UOX and MOX waste forms
- Salt: 200°C, based on the bulk salt properties
- A temperature limit for deep borehole remains to be determined.

These temperature limits are not final, and may be lower or higher than the limits that will eventually be used in license applications after site investigations and detailed design activities. Variations on clay buffer limits have been proposed, for example, limiting an outer portion of the buffer cross section to 125°C (NAGRA 2003). Recent discussion with Andra (personal communication February 2012) indicate that lower thermal constraints may be applicable in the case of clay, such as 90°C (or even 85°C) to protect against material property changes and to avoid two-phase flow complications. Conversely, there has been discussion with some Japanese scientists (personal communication, Intera, March 2012) that a higher limit (possibly 130°C) could be adopted after more research. For a salt repository, a thermal constraint of 250°C (50°C higher than the value used in the UFD Campaign FY11 studies) was adopted for the Deaf Smith County design concept (DOE 1986). Finally, for deep borehole disposal, the borehole size, rather than a potential thermal limit, will likely drive the repository design.

Again, while these thermal limits are subject to further investigation and may be eventually either lowered or raised, they provide a baseline from which we can perform sensitivity studies of other independent variables such as thermal conductivity, repository layout, waste package capacity, and surface storage time.

3.3 Tradeoffs of Drift/Borehole Spacing, Waste Package Spacing, Waste Package Capacity, and Waste Aging

The storage time required to meet the thermal limits of the EBS components for UOX and MOX in granite, clay and salt (for one set of drift/borehole and waste package spacings in each medium) are shown in Figure 3-3. The constraints are 100°C for clay or granite (with bentonite buffers), and 200°C in salt. The 100°C temperature constraint was chosen to limit alteration of clay in buffers, for example by illitization or cementation. Alteration generally involves dissolution, aqueous transport, and precipitation. For salt, which is a more ductile material, a higher target value of 200°C is used for the maximum temperature, to limit uncertainty in performance assessment. Additional thermal constraints for other materials, such as metal liners, may exist, but were not considered.

Based on these FY11 results (LLNL 2011), up to four assemblies of UOX SNF (4-UOX) can be emplaced in salt or granite with approximately 100 years of surface storage. A 12-assembly UOX waste package (12-UOX) requires around 50 years of surface storage for emplacement in salt. Similarly, for MOX (which is initially around three times as hot, but stays hot much longer than UOX assemblies), 4 assemblies can be disposed of in a salt repository after around 100 years of surface storage. In granite and clay repository concepts, a single assembly of MOX would require around 300 years of surface storage, for the repository layout parameters evaluated, to meet the thermal constraints assumed. (Current studies are investigating why one MOX assembly would not meet thermal limits in perhaps 150 yr, based on the heats discussed in Section 3.1.)

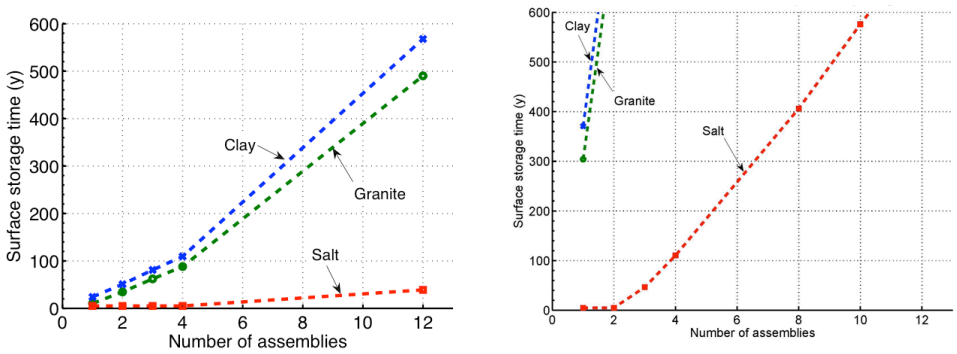

Figure 3-3 Surface storage time required for UOX and MOX assemblies to comply with temperature constraints of 100°C for clay or granite (with bentonite buffer), and 200°C in salt (LLNL 2011)

For the present study, the FY11 analysis was extended to a range of waste package spacing and drift spacing. Recall that the thermal model calculates the contributions to the transient temperature from a central waste package, a collection of axially spaced neighbor packages and from collection of laterally spaced lines of neighboring packages (for example, see Figure 3-4). Thus, detailed analysis of the contributions at a given set of drift/borehole and waste package spacings can point to whether either parameter can be changed with little effect on the peak temperature.

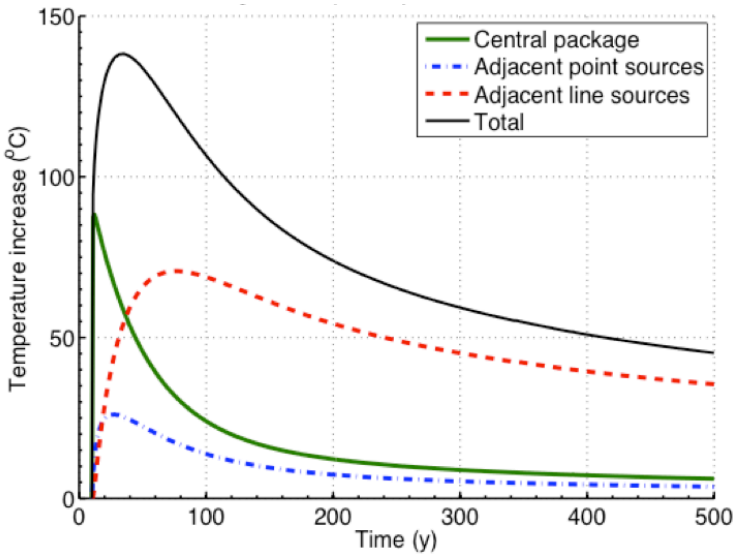

Figure 3-4 Contributions to the transient rock temperature at the calculation radius from the central package, adjacent point sources and adjacent line sources for 4 UOX assemblies per waste package in granite (LLNL 2011)

Results of varying waste package spacing and drift spacing are shown in Figure 3-5. The top left panel shows the waste package peak temperature in a granite repository for each increment in 4-UOX waste package spacing and drift spacing after 85 years of pre-emplacement surface storage. (Note that the analysis treats the space between vertical granite boreholes as the waste package spacing.) This is an informative figure given that it allows the assessment of combinations of spacing that do not exceed the thermal limit (in

this case 100°C). A more informative interpretation of the data is a 2D contour plot, shown in the lower panel of Figure 3-5. These results for waste packages stored for 85 years before emplacement allow the assessment of surface storage duration sensitivity (recall that FY11 studies found that 88 years of surface storage was needed for the pre-selected repository design in the thermal report). Examining the interface between the 90-100°C zone and the 100-110°C zone provides a clearer interpretation of the waste package spacing and drift spacing to maintain temperatures at or below the 100°C thermal limit. If it is determined that lower limits are required (for example 90°C), one simply needs to examine the interface between the 80-90°C and 90-100°C zones to select repository designs following 85 years of surface storage.

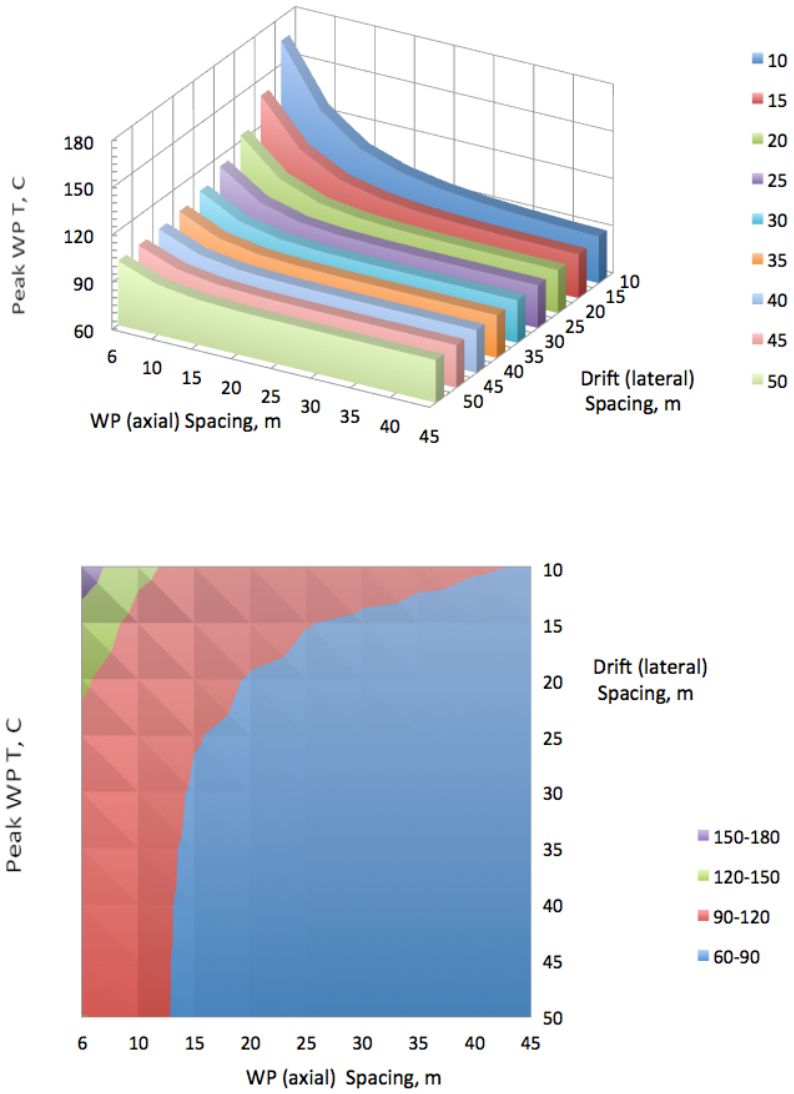

Figure 3-5 Granite repository design dimensions showing 4-UOX waste package spacing and drift spacing that maintain temperatures at or below 100°C at the waste package/bentonite buffer interface following 85 years of pre-emplacement surface storage

The results of multiple contour plots can be shown on one figure for the selected thermal limit (in this case 100°C). Figures 3-6, -7 and -8 show the results of a series of calculations for the three geologic media, the range of waste package and drift spacing, and a range of surface storage durations that meet the thermal limits of each medium. Figure 3-6 shows that in granite, large reductions in drift spacing (for large drift spacing) require only small increases in WP spacing to meet the thermal limit for a given surface storage duration. The base case (large black dot symbol, 88 years surface storage) was the design point used in the FY11 studies.

Drift (lateral) spacing must beat least a factor of three of the drift or borehole diameter, for mechanical stability. For granite, the factor of three applies to the vertical boreholes in the drift floor and the drifts themselves, and for clay it applies to the horizontal boreholes in the drift sides. Waste package spacing is center to center, and therefore the WP spacing is limited by the length of the waste package (~6 m). The results for clay (Figure 3-7) are somewhat similar to those for granite given that both designs are constrained by the thermal limits for clay EBS. Note that for salt cases (Figure 3-8), an age range of 20 years is shown; this should not be mistaken for a higher sensitivity when compared with clay and granite with a 10-year age range shown in Figures 3-6 and 3-7.

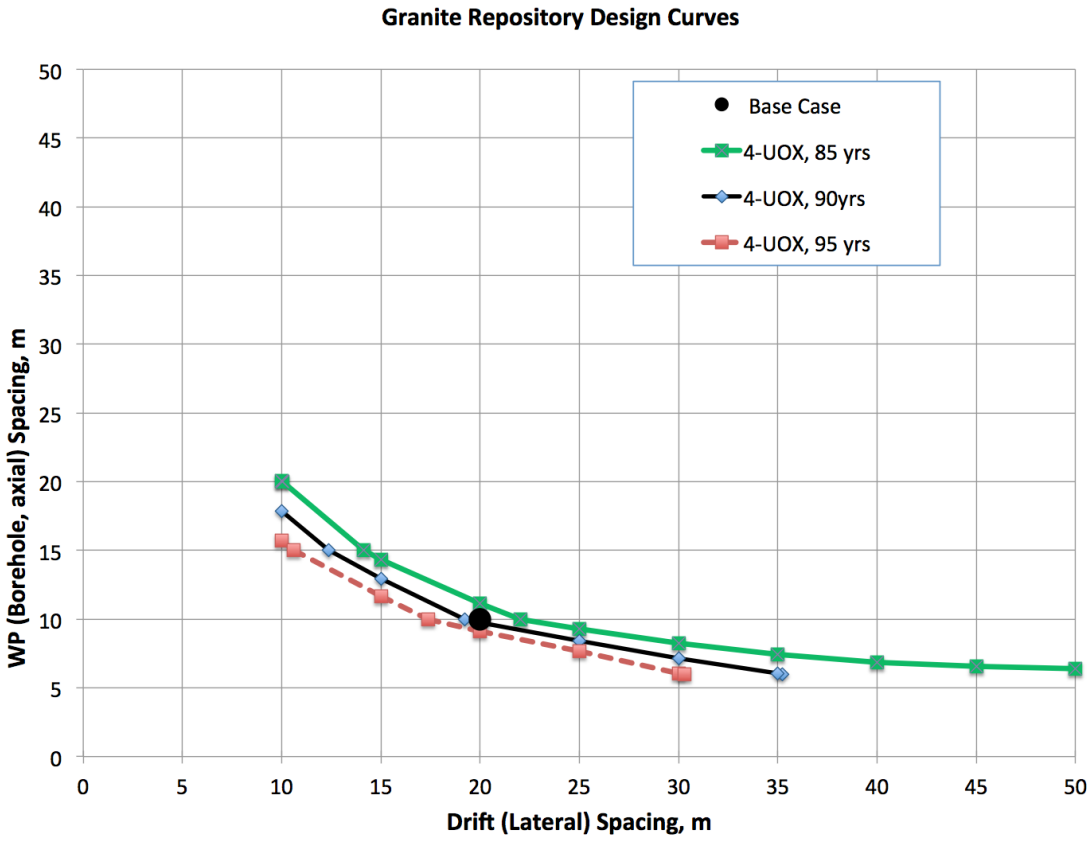

Figure 3-6 Granite repository design curve showing 4-UOX waste package and drift spacings that maintain temperatures at or below 100°C at the waste package/bentonite buffer interface following 85, 88 (base case), 90 and 95 years of pre-emplacement surface storage

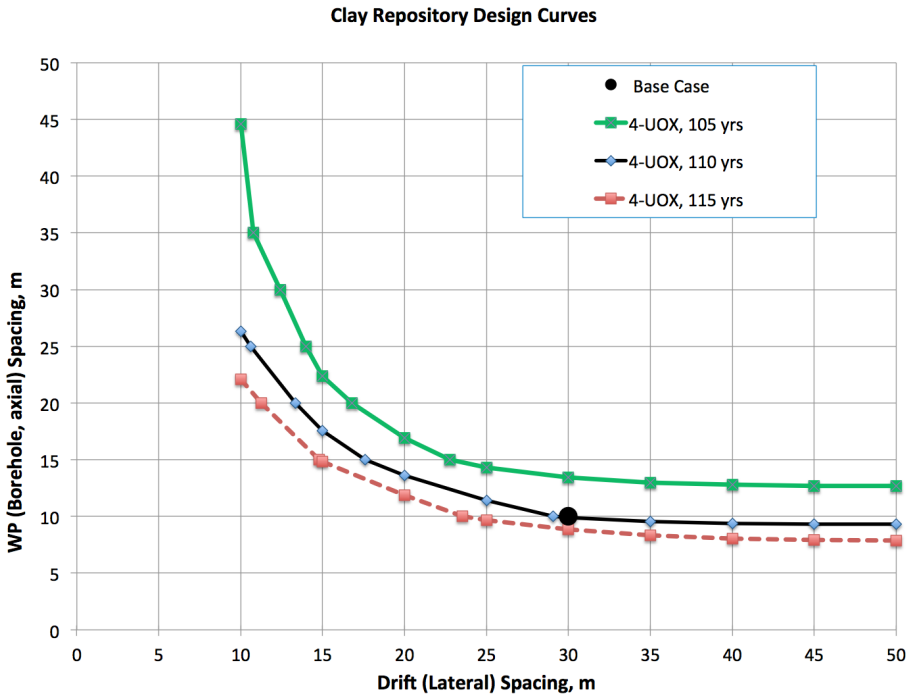

Figure 3-7 Clay repository design curve showing 4-UOX waste package and drift spacings that maintain temperatures at or below 100°C at the waste package/clay interface following 105, 109 (base case), 110 and 115 years of pre-emplacement surface storage

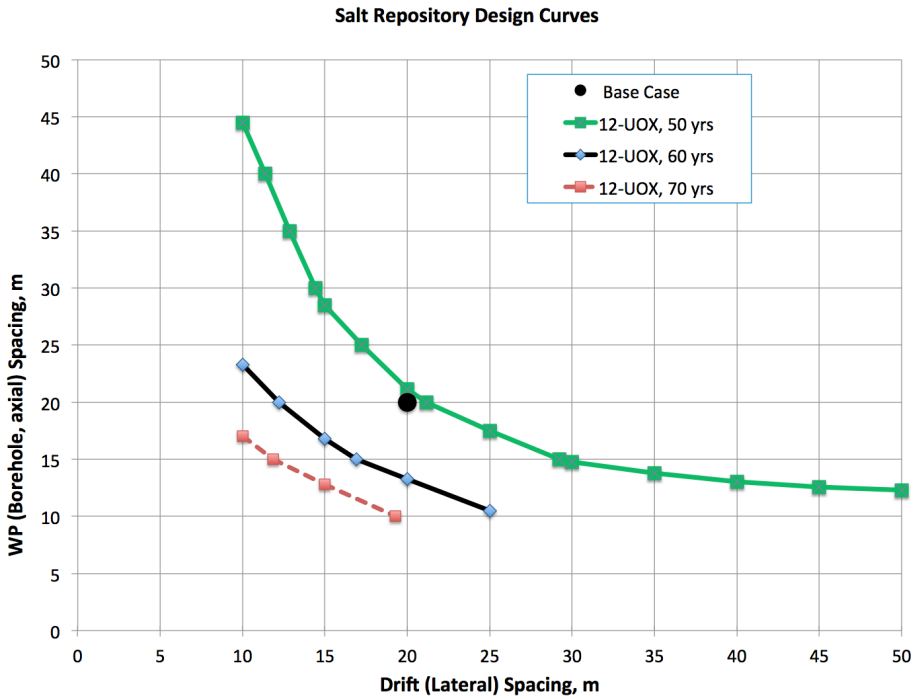

Figure 3-8 Salt repository design curve showing 12-UOX waste package and drift spacings that maintain temperatures at or below 200°C at the waste package/salt interface following 50, 60 and 70 years of pre-emplacement surface storage with a base case of K_{th} at 200°C

3.4 Design Sensitivity to Near Field and EBS Thermal Properties

The storage time is driven largely by the material properties and thermal constraints of the engineered and natural barriers; therefore, the effects of relaxing the thermal constraints were investigated. It is again important to note that these thermal constraints are preliminary, and subject to change based on site-specific data and further studies. As discussed in Section 3.2, variations on clay buffer limits have been proposed, for example, limiting an outer portion of the buffer cross section to 125°C (NAGRA 2003). Furthermore, for a salt repository, a thermal constraint of 250°C was adopted for the Deaf Smith County design concept (DOE 1986).

Figure 3-9, from the FY11 work, shows the sensitivity of required surface aging times of UOX and MOX waste packages to variations in the thermal constraints for granite and clay (100°C, 125°C and 150°C), and salt (200°C, 225°C, and 250°C). The results show that for UOX in granite and clay, significantly shorter surface storage times are needed if the thermal constraints can be relaxed by just 25 – 50°C. Alternatively, higher capacity waste packages could be disposed of in some cases without significantly increasing the surface storage time. Because of the relatively high thermal conductivity of salt coupled with the much higher initial temperature constraint, the impact in salt is not as great as that observed in clay and granite. For MOX waste packages in granite and clay, the effect is negligible simply because no more than one assembly can be disposed of after even 300 years of surface storage, even with the relaxed thermal constraints. For MOX in salt, relaxing the thermal constraints by 25 or 50°C may allow larger capacity waste packages or shorter pre-emplacement storage times to be used.

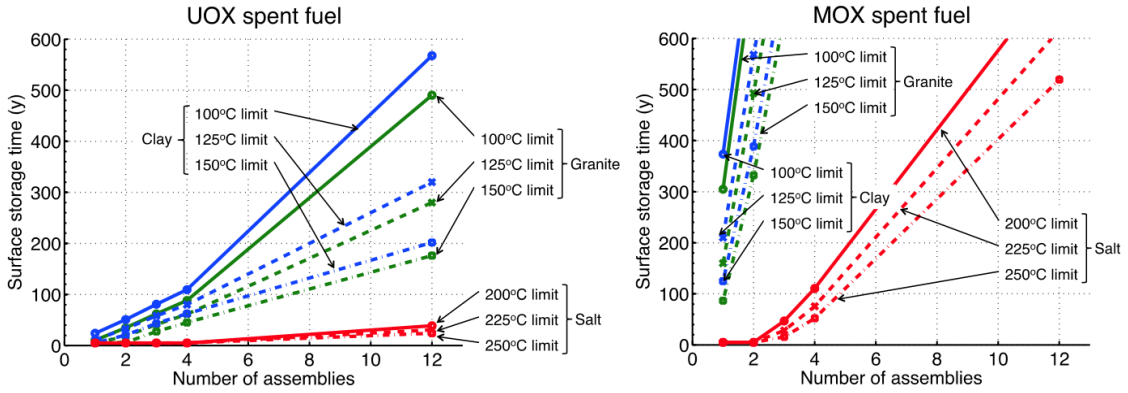

Figure 3-9. Surface Storage Time Required for Compliance with Temperature Constraints of 100°C, 125°C, or 150°C for Clay or Granite (with Bentonite buffers) and 200°C, 225°C, or 250°C for Salt (Greenberg 2012)

Figure 3-10 shows the same information for 4-UOX and 12-UOX waste packages. The results show that allowing the temperature of the EBS layer to be 50°C higher than the base case results in only about half of the required pre-emplacement storage time for granite, clay, and salt. For salt, the figure also shows the effect of evaluating salt thermal properties at 200°C rather than 100°C in the EBS region (out to about 3 m). In some cases, the EBS material may be designed to withstand higher temperatures, while in other cases, a segment of the EBS layer may be deemed to be sacrificial provided the mechanical properties do not change considerably.

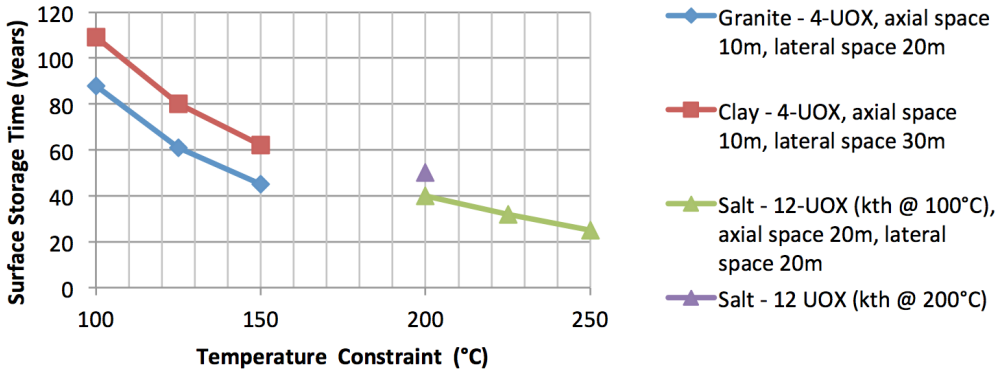

Figure 3-10 Surface storage requirements as a function of relaxed thermal constraints for granite (bentonite buffer), clay and salt compared to base case

3.5 Bulk Thermal Conductivity of the Geologic Medium

Prior calculations have used a nominal thermal conductivity (and associated thermal diffusivity) of the geologic medium. Uncertainty ranges have been collected for each medium. As a first step in evaluating the effects of these property uncertainties, the thermal calculations were repeated over a ±20%, range of conductivity for the base case drift/borehole and waste package spacing. Figure 3-11 shows the sensitivity of the surface storage time to the thermal conductivity uncertainty. For clay and granite, a 20% change in conductivity results in about a 10% change in surface storage time. For salt, there is less sensitivity, with a 20% change in conductivity resulting in about a 5% change in surface storage time.

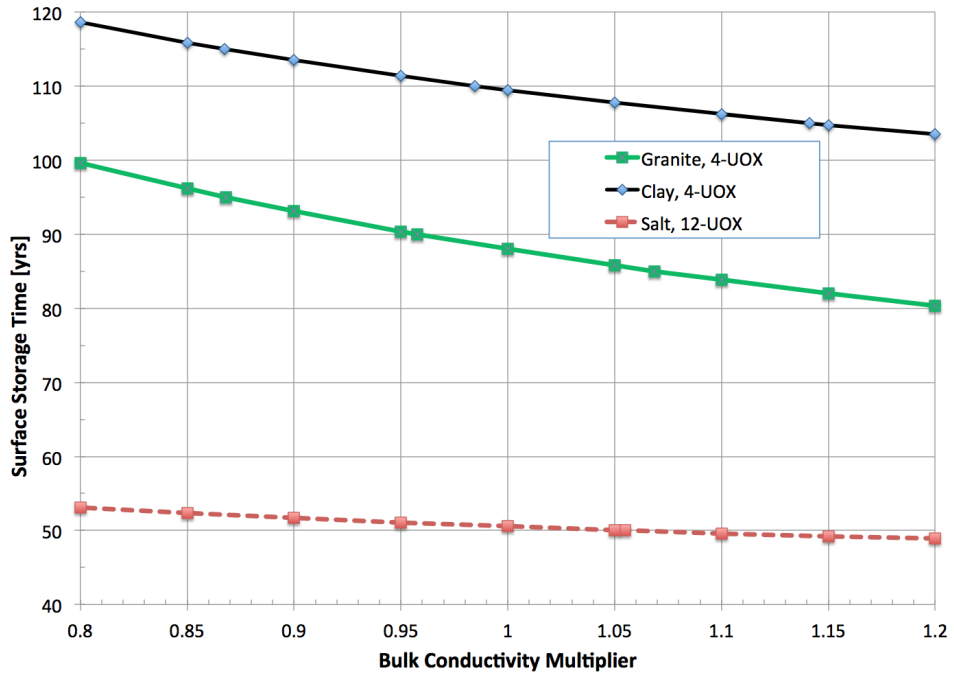

Figure 3-11 Effect of multiplying the bulk thermal conductivity for granite, clay and salt repositories on the storage time required to meet the thermal constraints of the EBS

3.6 Buffer Thermal Conductivity

Work performed in FY12 (Greenberg 2012) investigated the effect of bentonite thermal conductivity on the required surface storage of a variety of waste package capacities while maintaining temperatures at or below the thermal limit of bentonite in granite and clay repositories (Figure 3-12). The results show the effect on required surface storage time for UOX and MOX in granite and clay repositories due to changing the thermal conductivity of the buffer layer of the EBS from 0.6 W/m-K for a homogeneous bentonite buffer, to 2.0 W/m-K for a modified bentonite buffer that contains sand and graphite (Beziat 1992). Analysis of the clay repository also needs to account for the temperature limit of the bulk clay, if the EBS buffer conductivity improves sufficiently.

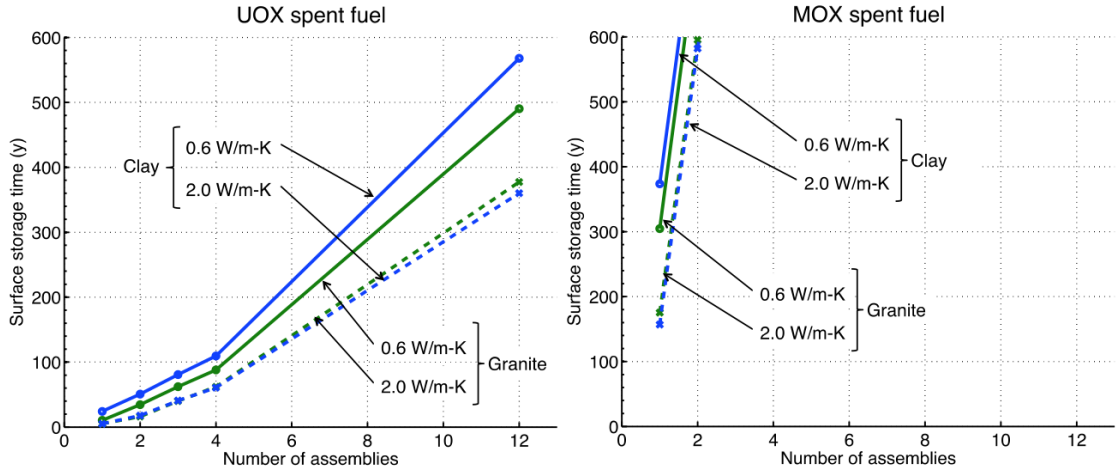

Figure 3-12 Effect of changing the thermal conductivity of the bentonite buffer layer in the repository designs for granite and clay (Greenberg 2012)

In the present study, temperatures have been calculated as a function of the location within the bentonite buffer. Figure 3-13 shows the temperature across the buffer thickness for a 4-UOX clay repository with 50 years of surface storage time (about half that required for the entire bentonite buffer to remain below the 100°C limit). The temperature profiles are shown at the bounding times after emplacement (55 years when the temperature of the inner surface of the bentonite peaks, and 88 years when the temperature of the interface between the rock wall and bentonite reaches a maximum). The figure shows the temperature profiles for a homogeneous bentonite buffer with 0.6 W/m-K thermal conductivity and for a composite bentonite-sand-graphite buffer with higher thermal conductivity of 2.0 W/m-K. Most of the homogeneous buffer exceeds the temperature limit during this peak temperature time period, while most of the composite buffer remains below the temperature limit.

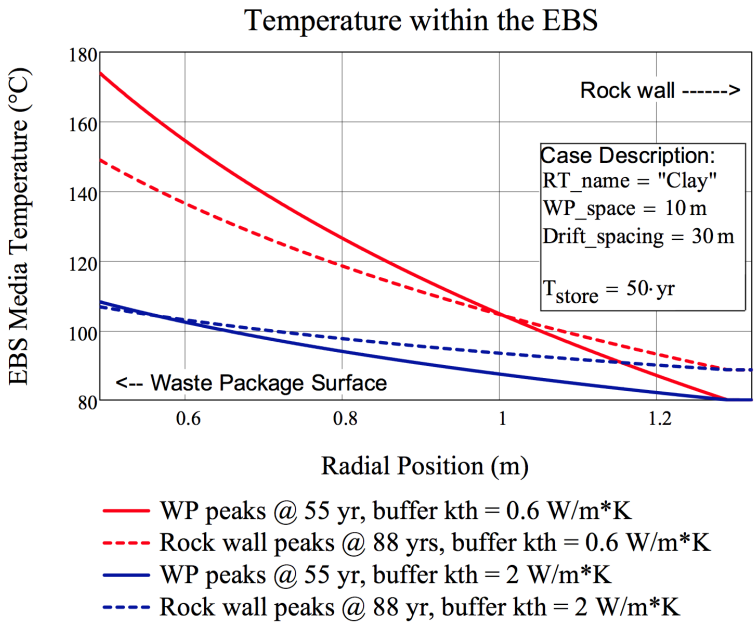

Figure 3-13 Temperature gradient within a bentonite and modified bentonite EBS layer within a clay repository at 55 and 88 years after emplacement

Similar results are seen in Figure 3-14 for a 4-UOX granite repository with 60 years of surface storage (about 2/3 of that required for the entire bentonite buffer to remain below the 100°C limit). The figure shows the temperature profiles in the bentonite at 65 years (time of WP peak temperature) and 87 years (time of rock wall peak temperature).

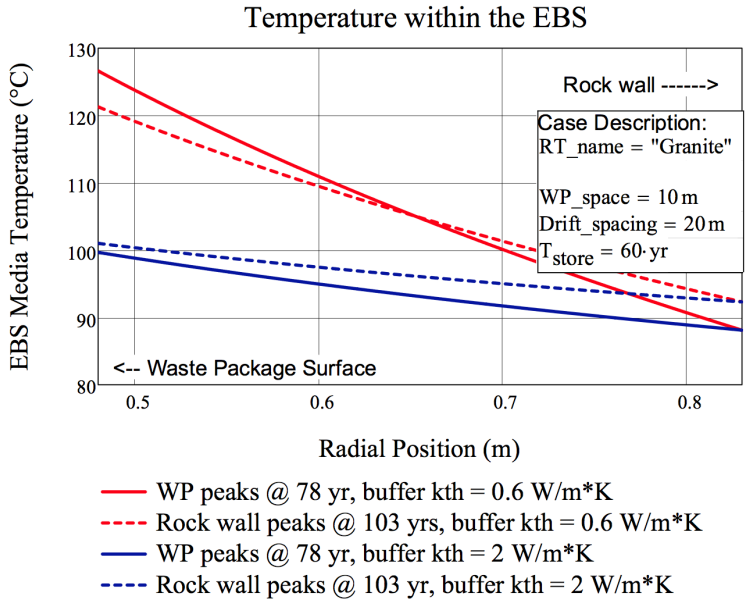

Figure 3-14 Temperature gradient within a bentonite and modified bentonite EBS layer within a granite repository at 65 and 87 years after emplacement

These calculations allow the evaluation of a sacrificial layer of clay material that (provided the mechanical properties of the clay do not change significantly) may be allowed to exceed the usual thermal limit.

Figure 3-15 extends the clay analysis to all times between 50 and 100 years (which includes the two peak times in Figure 3-13). The figure shows the fraction of the buffer (left axis) and the thickness (radial distance, right axis) that exceed the temperature constraint. For the homogeneous and composite buffers, at least 20% and 60%, respectively, of the buffer thickness are always below the temperature limit. Similar data are shown for granite (Figure 3-16).

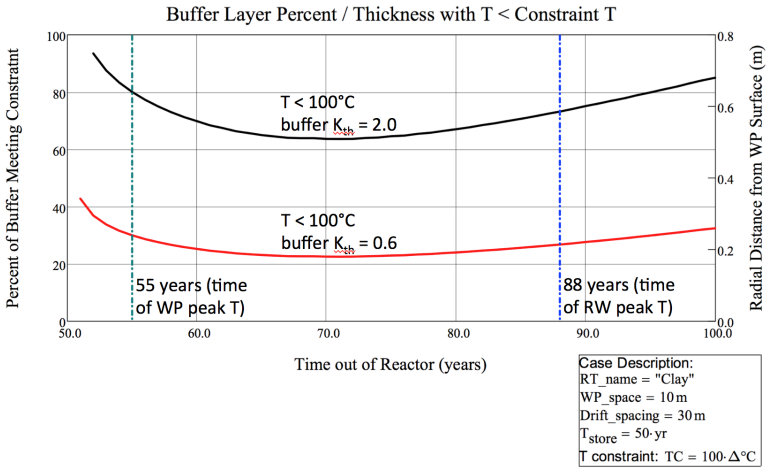

Figure 3-15 Fraction of the buffer and thickness of the buffer that exceed the bentonite temperature constraint during the time of peak temperatures, for a 4-UOX clay repository with 50 years of pre-emplacement storage, for homogeneous and composite buffer materials

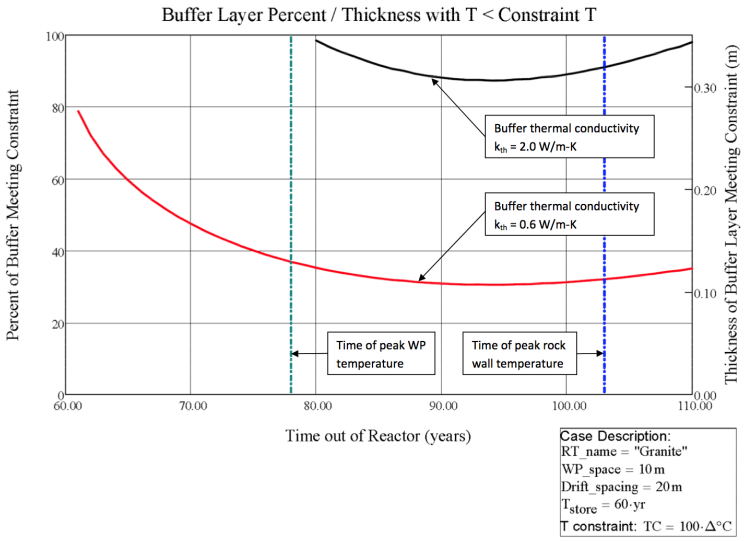

Figure 3-16 Fraction of the buffer and thickness of the buffer that exceed the bentonite temperature constraint during the time of peak temperatures, for a 4-UOX granite repository with 60 years of pre-emplacement storage, for homogeneous and composite buffer materials

3.7 Conceptual Model Uncertainties Associated with Buffers and Container Materials

Open and enclosed modes are being described in more detail and considered elsewhere in the UFD Campaign (SNL 2012). Open modes are repository designs that maintain in-drift ventilation after emplacement and closure, to allow heat removal by convection. Even if powered ventilation stops, chimney effects provide moderate natural ventilation. Examples of open mode emplacement concepts include clay without backfill, the YMP LA in tuff, and alluvium. In some cases, compartmentalization measures may be needed to limit preferential water flow, and drip-shields may be used to protect waste packages from dripping water and from rock fall.

Closed modes are those that place EBS materials or rock next to the waste package such that no significant airflow is possible. The discussions in Sections 3.3 through 3.6 are for closed mode concepts. Emplacement drifts and boreholes may be closed due to installation of buffer/backfill material at emplacement, or due to plastic deformation of the host rock into radial gaps after emplacement. Examples of enclosed modes include the generic salt repository, crystalline rock with buffer (KBS-3), and clay with backfill installed. Hybrid designs are also possible in which a buffer/backfill is used to enclose the waste package, but the access drifts are ventilated until they naturally collapse at some time well after the peak temperature pulse.

While the inclusion of EBS materials (e.g. bentonite clay in a granite repository) can be restrictive to the temperature constraints, and can increase both cost and construction time compared to an open mode, the material may also add significant performance. EBS materials can limit and chemically condition water contacting the waste package, and can retard transport of radionuclides from failed waste packages into the geologic medium.

3.8 Longevity of Engineered Barriers

In the Repository Design / Thermal Load investigations, we assumed the following EBS materials:

- For a granite repository, the waste package would use copper and steel for SNF and carbon steel for HLW package; both types of waste packages would be surrounded with a bentonite buffer
- For a clay repository, the waste package would use carbon steel and the borehole would be lined with steel. For SNF, a bentonite buffer in a carbon steel envelope would surround the waste package, within the steel liner
- For a salt repository, the waste package would use carbon steel, and the waste package would be emplaced on the floor at the rear of an excavated alcove. The waste package would be covered with a crushed salt backfill (that has seven times lower thermal conductivity than intact salt). The waste package would be in good contact with the floor and back wall, under the crushed salt, to enhance heat transfer. The crushed salt backfill is expected to consolidate into intact salt in a relatively short time (perhaps five years), as the alcove slowly collapses.
- For a deep borehole repository, the waste package would use carbon steel, with a "backfill" of water between the waste package and the steel drill casing liner. Due to diameter constraints, the SNF waste package would be limited to one PWR assembly, with the rods consolidated (removed from the spacer grids). For HLW,

smaller diameter canisters, compared to the standard sizes for the other candidate repository media, will be required. Many waste packages would be stacked in each deep borehole..

Depending on the repository design (open or enclosed mode, saturated or unsaturated), the environmental conditions experienced by each EBS material will vary greatly. For example, for a clay repository, a bentonite buffer will limit the flow of water to the waste package, but once the water reaches the waste package, the carbon steel is likely to degrade quickly. Alternatively, for a salt repository, water is largely excluded from the system, and carbon steel waste packages are expected to maintain integrity for a long period of time.

3.9 EBS Transport

Radionuclides interact with EBS materials within the degraded waste package and within the emplacement drifts/boreholes. Radionuclides can be dissolved from the waste form, precipitated into secondary phases (which have different solubilities than the waste forms), adsorbed onto colloids, and move as dissolved ions or on colloids into the EBS materials outside the waste package and then into the geologic medium. Sorption and dispersion processes retard the transport and spread the plume, diluting it. These processes depend on the redox and pH environments in these various regions.

Specific processes and parameters to be considered in transport models include radionuclide speciation/sorption, redox chemistry, microbial activity, temperature, clay hydration, in-EBS water chemistry, and colloid-facilitated transport under a wide range of physical and chemical conditions (e.g., various disposal environments).

A number of experiments are ongoing within the UFD Campaign that address transport in the EBS and the geologic medium. For example, FY11 experiments at LLNL examined the interaction of plutonium with clay (montmorillonite) and goethite (a steel corrosion product) at 25°C and 80°C. In FY12, LLNL is continuing this work, focusing on a mechanistic understanding of plutonium interactions with clay and other representative minerals.

4. Summary

The key uncertainties identified in both the YMP LA and the Swedish repository design are are not impacted by the chosen fuel cycle (Open, Modified Open Or Closed). Improvement of lesser *uncertainties* relating to Tc-99, C-14 and plutonium would not significantly benefit performance of one fuel cycle vs. the others. Instead, key uncertainties are associated with host rock and EBS properties, and with waste form and waste package degradation (excluding seismic and igneous scenarios).

Conceptual models of repository designs for granite, clay and salt media have been investigated with respect to fuel cycle, pre-emplacement storage time, WP spacing, drift/borehole spacing, thermal limits for EBS materials, buffer thermal conductivity, and WP capacity. Temperature limits for granite and clay were assumed to be 100°C, and 200°C for salt.

The six waste forms for three fuel cycles were compared, with UOX being selected as the most prevalent current waste form and as one that can act as a surrogate for the others in thermal calculations. The storage time required for UOX and MOX waste packages with a

variety of capacities were evaluated based on not exceeding the thermal limit for each geologic medium (and associated EBS materials).

Variation in repository design allowed the calculation of waste package and drift spacing combinations that meet the thermal constraints for each EBS material and each geologic medium. Typically, at drift spacings less than 20 m, and for a given surface storage time, the required WP spacing is highly sensitive to small changes in drift spacing. For designs with drift spacings above 20 m, the WP spacing showed little sensitivity to changes in drift spacing, for a given surface storage time. The thermal model used tracks the time-dependent contributions of a single waste package, axial neighbors (separated by the waste package spacing), and lateral neighbors (separated by the drift/borehole spacing); thus, it is straightforward to determine the effect of changing one of the spacing parameters on the peak temperature.

The thermal constraints may be subject to change (either higher or lower) as material properties are further investigated. Higher capacity waste packages or shorter pre-emplacement storage times can be achieved by raising the thermal constraints of such EBS materials by just 25 or 50°C. Required storage times for a clay and granite repository were more sensitivity to changes in the bulk thermal conductivity than was the storage time for a salt repository.

EBS layers may be modified such that thermal properties are advantageous to higher thermal loads, such as by adding sand and graphite to bentonite. Additionally, sacrificial regions of the EBS material could allow higher temperatures nearer the waste package surface, provided overall mechanical properties of the bentonite buffer are not compromised. Calculations have been performed to assess the thickness of a sacrificial region in bentonite and modified bentonite in both granite and clay geologic media.

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