OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

1. QA: QA

Complete Only Applicable Items

2. ☑ Analysis — Check all that apply

Type of Analysis:
- ☐ Engineering
- ☑ Performance Assessment
- ☐ Scientific

Intended Use of Analysis:
- ☐ Input to Calculation
- ☐ Input to another Analysis or Model
- ☑ Input to Technical Document
- ☐ Input to other Technical Products

Describe use:
Input to SR REV 01 and to the LA

3. ☐ Model — Check all that apply

Type of Model:
- ☐ Conceptual Model
- ☐ Abstraction Model
- ☐ Mathematical Model
- ☐ System Model
- ☐ Process Model

Intended Use of Model:
- ☐ Input to Calculation
- ☐ Input to another Model or Analysis
- ☐ Input to Technical Document
- ☐ Input to other Technical Products

Describe use:

4. Title:
Performance Assessment and Sensitivity Analyses of Disposal of Plutonium as Can-in-Canister Ceramic

5. Document Identifier (including Rev. No. and Change No., if applicable):
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Performance Assessment and Sensitivity Analyses of Disposal of Plutonium as Can-in-Canister Ceramic

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4. Revision/Change No.	5. Description of Revision/Change
REV 00	Initial Issue
REV 00 ICN 01	Interim Change Notice 01 In ICN 01 the error in the specific surface area for the Plutonium can-in-canister ceramic in Table 4.1-3 (Section 4.1, page 12) was corrected. The specific surface area was reported in units of m2/g instead of cm2/g. The TSPA model runs that included the specific surface area for Plutonium can-in-canister ceramic were repeated with the corrected values and the dose release figures presented in Sections 6.4 and 6.5 (pages 34 - 37, 41 -45) were corrected. Also, the output DTNs in Sections 6 and 7 were updated as a result of the corrections. However, this correction did not change noticeably the dose results and had no impact on the conclustions in Section 7.0. Only minor editorial changes were made in section 6.5.1 (page 38) and in the conclusions (page 46) unrelated to the correction of the specific surface area.

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1. PURPOSE

The purpose of this analysis is to examine whether there is a justification for using high-level waste (HLW) as a surrogate for plutonium disposal in can-in-canister ceramic in the total-system performance assessment (TSPA) model for the Site Recommendation (SR). In the TSPA-SR model, the immobilized plutonium waste form is not explicitly represented, but is implicitly represented as an equal number of canisters of HLW.

There are about 50 metric tons of plutonium in the U. S. Department of Energy inventory of surplus fissile material that could be disposed. Approximately 17 tons of this material contain significant quantities of impurities and are considered unsuitable for mixed-oxide (MOX) reactor fuel. This material has been designated for direct disposal by immobilization in a ceramic waste form and encapsulating this waste form in high-level waste (HLW). The remaining plutonium is suitable for incorporation into MOX fuel assemblies for commercial reactors (Shaw 1999, Section 2). In this analysis, two cases of immobilized plutonium disposal are analyzed, the 17-ton case and the 13-ton case (Shaw et al. 2001, Section 2.2). The MOX spent-fuel disposal is not analyzed in this report.

In the TSPA-VA (CRWMS M&O 1998a, Appendix B, Section B-4), the calculated dose release from immobilized plutonium waste form (can-in-canister ceramic) did not exceed that from an equivalent amount of HLW glass. This indicates that the HLW could be used as a surrogate for the plutonium can-in-canister ceramic. Representation of can-in-canister ceramic as a surrogate is necessary to reduce the number of waste forms in the TSPA model. This reduction reduces the complexity and running time of the TSPA model and makes the analyses tractable.

This document was developed under a Technical Work Plan (CRWMS M&O 2000a), and is compliant with that plan. The application of the Quality Assurance (QA) program to the development of that plan (CRWMS M&O 2000a) and of this Analysis is described in Section 2. The document is intended to be a source of information for subsequent revisions of the TSPA-SR (CRWMS M&O 2000b).

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this analysis report. In accordance with AP-3.10Q, *Analyses and Models,* and AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities,* a Technical Work Plan (CRWMS M&O 2000a) was developed, issued, and used in the preparation of this document. The Technical Work Plan (CRWMS M&O 2000a) and the associated activity were evaluated in accordance with AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities.* The AP-2.21Q activity evaluation determined that the preparation and review of this document is subject to the *Quality Assurance Requirements and Description*, DOE/RW-0333P, (QARD) (DOE 2000) requirements. The methods used to control the electronic management of data as requested by AP-SV.IQ, *Control of Electronic Management of Information*, were as specified in the Technical Work Plan (CRWMS M&O 2000a).

3. COMPUTER SOFTWARE AND MODEL USAGE

The analyses in this document were performed using the qualified numerical code GoldSim (GoldSim V.6.04.007, 10344-6.04.007-00) (Golder Associates 2000). The GoldSim software (Golder Associates 2000) was developed by Golder Associates as an update to the baseline software, RIP v.5.19.01 (Miller and Kossik, 1998). GoldSim is a Windows based program that is computationally similar to RIP, Version 5.19.01 that was used for TSPA calculations for the Viability Assessment (DOE 1998). GoldSim is designed so that probabilistic simulations can be conducted and represented graphically. GoldSim fulfills the specific functional requirements for the TSPA-SR.

Per Civilian Radioactive Waste Management (OCRWM) Procedure AP-SI.1Q, *Software Management*, a Software Activity Numbers (LV-2000-190) and Software Tracking Numbers (10344-6.04.007-00) were obtained for GoldSim from Configuration Management (CM). The GoldSim V. 6.04.007 was qualified according to AP-SI.1Q, *Software Management*. The GoldSim software is considered appropriate for this application and is being used within the range of validation/qualification.

The nominal multi-realization TSPA simulations was performed at the Performance Assessment Department, 1180 Town Center Drive, Building 15, Las Vegas, Nevada) on Dell PowerEdge Workstations 620 and 420 with Dual Pentium III Xeon and Dual Pentium III Processors, Dell PowerEdge Workstation 2200 with Dual Pentium Processors, and Dell PowerEdge Servers 6350 and 6300 Pentium III and Pentium II Xeon Processors. The hardware was operated under Windows NT 4.0 Operating System, Workstation and Server, Service Pack 5. The median-value, single-realization TSPA simulations were performed at Duke Engineering and Services, 9111 Research Boulevard, Austin, Texas. The simulations were conducted on a Dell Workstation 400 with a Pentium II Processor, and on a Dell PowerEdge Workstation 2200 with Dual Pentium Processors. The hardware was operated under Windows NT 4.0 Operating System, Workstation and Server, Service Pack 4.

4. INPUTS

Inputs for this analysis were obtained from the Fissile Materials Disposition Program Plutonium Immobilization Project (Shaw 1999; Shaw et al. 2001) and from the source term compiled by the Yucca Mountain Project (CRWMS M&O 1999b). The input from the Fissile Materials Disposition Program falls under the QARD definition of design input (DOE 2000, Section 3.2). Information from these sources is contained in tables in Section 4.1. The specific activity values used to obtain the data in 4.1-1 are presented in Attachment II, Table II-1. The radionuclide inventory for HLW is from the *Inventory Abstraction* (CRWMS M&O 2000c, Section 7, Table 34). Input information for radionuclide inventory for both the immobilized plutonium and HLW are considered to be appropriate for performance assessment of can-in-canister ceramic and no further confirmation of this design input is required. The physical parameters that are used in dissolution models for the waste forms analyzed and the dissolution models themselves are considered appropriate, because the range of sensitivity analyses conducted is larger than the range of uncertainty in these parameters and models.

4.1 DATA AND PARAMETERS

Data used in this analysis are similar to those used in past analyses of plutonium waste forms (CRWMS M&O 1998a, Appendix B). These data include the radionuclide for the plutonium ceramic and HLW. The radionuclide inventory for the plutonium ceramic is presented in Table 4.1-1 (Shaw et al. 2001, Table 4.3). The inventory was reported in Ci/canister (Shaw et al. 2001, Table 4.3) and is converted into grams/canister as input in the TSPA model based on the activity coefficients in Table II-1 (Attachment II). The radionuclide inventory for HLW is presented in Table 4.1-2 (CRWMS M&O 2000c, Section 7, Table 34) together with the 12.1 percent reduced inventory which is used as input in the TSPA model. The physical properties of the waste forms are presented in Table 4.1-3 (CRWMS M&O 1999b, Table 4; Shaw 1999, Table 6.2). The input files for the TSPA model include the nominal, median-value TSPA-SR base case (DTN: MO0009MWDMED01.020) and the nominal, multi-realization TSPA-SR model (DTN: MO0009MWDNM601.018). The nominal, median-value TSPA-SR model (DTN: MO0009MWDMED01.020) was superceded by DTN: MO0012MWDMED01.032 and the nominal, multi-realization TSPA-SR model (DTN: MO0009MWDNM601.018) was superceded by DTN: MO0012MWDNM601.033, MO00012MWDMIL01, which were not available at the onset of this analysis. The superceded models produce the same results, except for the ^{242}Pu dose rate, for which the biosphere dose conversion factor (BDCF) was corrected in DTN: MO0012MWDMED01.032 and DTN: MO0012MWDNM601.033, MO00012MWDMIL01.034. In this analysis, the BDCF of ^{242}Pu was corrected in the TSPA-SR models (DTN: MO0009MWDMED01.020, MO0009MWDNM601.018), such that it produces identical results when compared with results using the corrected data set, DTN: MO0012MWDMED01.032 and MO0012MWDNM601.033, MO00012MWDMIL01.034 (see assumption 5.6). Note that the description in DTN: MO0009MWDNM601.018 refers to model case runs that supercede the model runs associated with the TSPA-SR Rev. 00B report version, and describes additional internal tracking clarification.

Table 4.1-1. Radionuclide Inventory for Surplus Plutonium Used in Can-In-Canister Ceramic[a]

Isotope	Bounding Case	
	(Ci/canister)[b]	(g/canister)[c]
^{238}Pu	577	33.66
^{239}Pu	1,615	25,995
^{240}Pu	564	2,480
^{241}Pu	7,159	69.157
^{242}Pu	0.39	99.125
^{241}Am	1,334	387.95
^{234}U	< 0.13	20.82
^{235}U	2.03 E -3	938.11
^{236}U	5.8 E -4	8.955
^{238}U	1.88 E -2	55,843
^{237}Np	1.28 E -2	18.13

[a] (Shaw et al. 2001, Table 4.3)
[b] Includes only the radionuclides in the ceramic in the year 2010. Does not include radionuclides in the HLW.
[c] calculated using radionuclide activity coefficient in Table II-1 in Attachment II

Table 4.1-2. Radionuclide Inventories for High-Level Waste

Isotope	High-Level Waste Inventory[a] (g/waste package)	12.1 Percent Reduced High-Level Waste Inventory (g/waste package)
^{227}Ac	4.36E-04	3.832E-04
^{241}Am	6.03E+01	5.30E+01
^{243}Am	1.55E+00	1.36E+00
^{14}C	7.11E-03	6.25E-03
^{137}Cs	4.04E+02	3.55E+02
^{129}I	4.41E+01	3.88E+01
^{237}Np	1.78E+02	1.56E+02
^{231}Pa	7.44E-01	6.54E-01
^{210}Pb	1.31E-07	1.15E-07
^{238}Pu	5.69E+01	5.00E+01
^{239}Pu	3.52E+03	3.09E+03
^{240}Pu	3.39E+02	2.98E+02
^{242}Pu	6.25E+00	5.49E+00
^{226}Ra	1.52E-05	1.34E-05
^{228}Ra	6.51E-06	5.72E-06
^{90}Sr	2.67E+02	2.35E+02
^{99}Tc	7.01E+02	6.16E+02
^{229}Th	3.79E-03	3.33E-03
^{230}Th	7.00E-03	6.15E-03
^{232}Th	1.59E+04	1.40E+04
^{232}U	7.64E-04	6.72E-04
^{233}U	1.02E+01	8.97E+00
^{234}U	3.39E+01	2.98E+01
^{235}U	1.56E+03	1.37E+03
^{236}U	3.65E+01	3.21E+01
^{238}U	7.86E+05	6.91E+05

[a] (CRWMS M&O 2000c, Section 7, Table 34)

Table 4.1-3. Physical Characteristics of High-Level Waste, and Plutonium Ceramic

Waste Type	Matrix Dissolution	Matrix Surface Area (cm^2/g)	Fuel Volume (m^3)
High-Level Waste[a]	Glass model	5.705E-01[a]	0.636[d]
Plutonium Ceramic[b]	Ceramic model	347 to 3461[c]	0.0787[d]

[a] (CRWMS M&O 1999b, Table 4)
[b] (Shaw 1999, Table 6.2)
[c] Range shown to indicate need for sensitivity analyses of surface area
[d] (Shaw et al. 2001, Section 2.1)

4.2 CRITERIA

There are no criteria applicable to this analysis. Doses analyzed using the TSPA-SR model are compared to doses from waste forms that are included in the nominal case (i.e., HLW). This comparison is made to examine if the representation of the immobilized plutonium waste form by HLW in the TSPA-SR model is conservative. These analyses are not intended to address compliance to regulations or specific acceptance criteria in Issue Resolution Status Reports for Key Technical Issues. Those criteria will be addressed in the TSPA-SR itself (CRWMS M&O 2000b, Section 1.3).

4.3 CODES AND STANDARDS

There are no codes and standards associated with this analysis. Analyses of dose from disposal of immobilized plutonium waste in the potential repository at Yucca Mountain is compared to the dose from the TSPA-SR nominal case model at 20 kilometers. The dose is also compared to HLW that is one of the three waste forms included in the nominal case (e.g., DOE spent fuel, commercial spent fuel, and HLW).

5. ASSUMPTIONS

This section identifies assumptions that are essential for this calculation. The discussion of each assumption includes four elements: (1) a statement of the assumption; (2) the rationale for the assumption; (3) a statement of the need for further confirmation of the assumption (i.e., the "to be verified" (TBV) status); and (4) a statement of where the assumption is used in the analysis.

5.1 MODEL SOFTWARE

Assumption: The nominal-case model for TSPA-SR is assumed for the analyses in Section 6 below, including all assumptions incorporated into the nominal case (CRWMS M&O 2000d, Section 5) and the GoldSim software (Golder Associates 2000, STN: 10344-6.04.007-00).

Rationale: The nominal case model was developed to conduct calculations for the TSPA-SR and is appropriate for the calculations in Section 6 that are similar. The use of this model is consistent with the Technical Work Plan for this work (CRWMS M&O 2000a), and the calculations associated with *Total System Performance Assessment (TSPA) Model for Site Recommendation* (CRWMS M&O 2000d).

Confirmation Status: The TSPA-SR model was reviewed and approved under AP-3.10Q, *Analyses and Models.* No further confirmation was required for this analysis.

Use within the Analysis: The model was used to perform the simulations used to develop the results presented in Section 6.

5.2 RADIONUCLIDE INVENTORY

Assumption: The radionuclide inventory for the plutonium ceramic was taken from (Shaw et al. 2001, Table 4.3). It is assumed that the inventory for the 17-ton case (Shaw et al. 2001, Table 4.3) also applies to the 13-ton case. The radionuclide inventory for high-level

waste was developed in *Inventory Abstraction* (CRWMS M&O 2000c, Section 7, Table 34).

Rationale: The radionuclide inventories used in this analysis are appropriate because they were developed specifically for the TSPA-SR (high-level waste) or this analysis (plutonium ceramic). There is uncertainty in assuming that the inventory for the 17-ton case also applies to the 13-ton case. However, the sensitivity analyses for radionuclide inventory (Section 6.5.5) show that there is relatively little effect on the total dose due to a factor-of-five change in radionuclide inventory. A factor-of-five increase and decrease in radionuclide concentration was chosen to cover one-order of magnitude range of uncertainty in the input.

Confirmation Status: The inventory information for plutonium ceramic is considered as design input information and is appropriate for use in performance assessment. The range in isotope inventory used in sensitivity analyses in Section 6.5.5 is adequate to show that no further confirmation of the radionuclide inventory is required due to the small impact of a change in inventory. The radionuclide inventory for high-level waste is from an approved technical product (CRWMS M&O 2000c, Section 7, Table 34). No further confirmation of the radionuclide inventories from the referenced sources is required for this analysis.

Use within the Analysis: The radionuclide inventories were used in performing the simulations used to develop the results presented in Section 6.

5.3 WASTE PACKAGES

Assumption: Disposal is assumed to be one canister of can-in-canister ceramic in a HLW canister position in a standard co-disposal package along with four canisters of HLW. The central slot that is normally for DOE spent fuel is assumed to be left empty.

Rationale: This assumption is consistent with the current waste-package design for disposal of immobilized plutonium ceramic (CRWMS M&O 2000e, Figure 6). The assumption is conservative, because it produces the largest number of waste packages that will yield the largest dose. The number of canisters of immobilized plutonium contained in a waste package will be determined by criticality analyses that are beyond the scope of this analysis.

Confirmation Status: Differences in the configuration and numbers of canisters of can-in-canister ceramic per co-disposal package are investigated through sensitivity analyses of the number of packages required (in Section 6) and show some effect on dose results. Because the effects of this assumption are investigated for both the extremes of the possible waste-package configurations (one and five canisters per waste package), it does not require confirmation. In addition, the configuration of one canister of can-in-canister ceramic per waste package yields the largest dose, and is thus is conservative configuration.

Use within the Analysis: The waste-package assumption was used in performing the simulations used to develop the results presented in Section 6.

5.4 STAINLESS STEEL DEGRADATION AND CLADDING

Assumption: No credit is assumed for the stainless-steel canister that contains either HLW or can-in-canister ceramic for the analyses in Section 6. The stainless-steel canisters are assumed to fail at the time of waste-package failure.

Rationale: This assumption is considered reasonably conservative, because it yields more rapid release of radionuclides from the waste form than would actually occur. For example, the waste form would not begin to dissolve until after the stainless-steel canister fails. Therefore, taking no credit for the stainless-steel canister is conservative because more radionuclides are available for release from the failed waste package than would be, if credit had been taken for stainless steel.

Confirmation Status: Due to the conservatism that more radionuclides are available for release from the failed waste package because of the assumption of no credit for stainless steel, the assumption does not require confirmation.

Use within the Analysis: The assumption of no credit for delay of radionuclide release due to the stainless-steel canister is used to perform the simulations used to develop the results presented in Section 6.

5.5 DISSOLUTION MODEL

Assumption: The physical parameters that are used in dissolution models for the waste forms analyzed and the dissolution models themselves are considered appropriate for this analysis.

Rationale: The parameters and associated dissolution models are consistent with those used in the current TSPA-SR model (CRWMS M&O 2000d) and previous TSPA analyses (CRWMS M&O 1998a, Appendix B). The specific parameters and dissolution models for the ceramic waste form are based on accepted data (Shaw et al. 2001). Sensitivity analyses of the physical parameters used in the dissolution models (Section 6.5) show relatively little effect on the total dose rate. The range in sensitivity analyses conducted is larger than the range of uncertainty in these parameters and models.

Confirmation Status: Due to the lack of sensitivity of dose to surface area and the choice of dissolution model, this assumption does not require confirmation.

Use within the Analysis: The dissolution models and associated physical parameters were used to develop the results presented in section 6.

5.6 TSPA-SR MODEL

Assumption: It is assumed that the input data sets for the median-value TSPA-SR model (DTN: MO0009MWDMED01.020) and for the nominal, multi-realization TSPA-SR model (DTN: MO0009MWDNM601.018) were appropriate for use in this analysis.

Rationale: For the evaluation of the different median-value cases of immobilized plutonium can-in-canister ceramic, the nominal case of the median-value TSPA-SR model was used (DTN: MO0009MWDMED01.020), which was superceded by DTN MO0012MWDMED01.032. For the evaluation of the multi-realization case of immobilized plutonium can-in-canister ceramic, the nominal, multi-realization TSPA-SR model was used (DTN: MO0009MWDNM601.018), which was superceded by DTN: MO0012MWDNM601.033, MO00012MWDMIL01.034). In all preceding models, the

BDCF for ^{242}Pu was given in Rem/yr per pCi/l instead of mRem/yr per pCi/l, resulting in calculated dose rates for ^{242}Pu that were underestimated by a factor of 1000. This was corrected in the superceded TSPA-SR models (DTN: MO0012 MWDMED01.032 , MO0012MWDNM601.033, MO00012MWDMIL01.034) which were not available at the onset of this analysis.

Confirmation Status: Test cases were run using both input data sets; (DTN: MO0009MWDMED01.020, MO0009MWDNM601.018) with the correction factor of 1000 for the ^{242}Pu dose rate, and the corrected data set, DTN: MO0012MWDMED01.032 and DTN: MO0012MWDNM601.033, MO00012MWD MIL01.034, respectively. For these two test cases, the two models produced identical results with the correction factor for ^{242}Pu applied. Except for this ^{242}Pu dose rate, the two models produced the same results. In this analysis, the BDCF for ^{242}Pu was corrected in the nominal, median-value TSPA-SR model (DTN: MO0009MWDMED01.020) and in the nominal, multi-realization TSPA-SR model (DTN: MO0009MWD NM601.018). Consequently, no further confirmation is required.

Use within the analysis: The nominal, median value TSPA-SR model was used to develop the specific TSPA models for the immobilized plutonium can-in-canister ceramic, which are presented in section 6.

6. ANALYSIS

6.1 BACKGROUND

Of the about 50 metric tons of plutonium in the DOE inventory of surplus fissile, approximately 17 tons of this material has been designated for direct disposal by immobilization in a ceramic waste form and encapsulation of this waste form in HLW. However, the total quantity of plutonium that will be immobilized has not yet been finalized and only about 13 tons of plutonium are currently considered for immobilization (Shaw et al. 2001, Section 2.2). As recommended by Shaw et al. (2001, Section 2.2) two cases of immobilized plutonium disposal are analyzed, the 17-ton case and the 13-ton case.

The encapsulated plutonium waste form is can-in-canister ceramic. Can-in-canister ceramic is a waste form in which plutonium ceramic disks are placed in 28 cans that each contain 9.2 kilograms of ceramic (Shaw 1999, Table 2.1). These cans are then encapsulated in HLW glass in a HLW canister (Shaw 1999, Page 3). For the baseline design, the 28 cans displace 12.1 percent (Shaw et al. 2001, Section 2.1) of the volume of a standard HLW canister (see Section 6.3).

In the previous TSPA-VA (CRWMS M&O 1998a, Appendix B, Section B-4), the analysis of the immobilized plutonium indicated that the HLW could be used a surrogate for the plutonium can-in-canister ceramic waste form. The calculated dose release from immobilized plutonium waste form (can-in-canister ceramic) did not exceed that from an equivalent amount of HLW glass. A surrogate of HLW is implicitly used to represent immobilized plutonium in the TSPA-SR model, and the justification of the use of this surrogate in the TSPA-SR model is the objective of this analysis.

6.2 TOTAL SYSTEM PERFORMANCE ASSESSMENT SUMMARY

This section is included to give the reader a brief summary of the TSPA-SR model as an aid in the interpretation of the results contained in Section 6.4 and 6.5. A more detailed discussion of the model is contained in the TSPA-SR report (CRWMS M&O 2000b, Sections 1 and 2). In general, the process for constructing a TSPA may be described as a pyramid with the most detailed supporting information and models near the base and the most abstracted model at the apex of the pyramid (Figure 6.2-1). The Performance Assessment Pyramid (Figure 6.2-1) shows how more detailed underlying information builds the technical basis for the total system model. The breadth of the lowest level of the pyramid represents the complete suite of process and design data and information (i.e., field and laboratory studies that are the first step in understanding the system). The next (higher) level indicates how data feed into conceptual models that describe the behavior of the individual system components.

The next (higher) level represents the synthesis of information from the lower levels of the pyramid into computer models. At this level, the subsystem behavior may be described by linking models together into subsystem representations. This is also the level where performance assessment modeling usually begins.

The TSPA models are usually referred to as abstracted models. The term “abstraction” is used to connote the development of a simplified mathematical and/or numerical model that reproduces and bounds the results of an underlying, more detailed process model, if necessary, because of computational constraints or lack of information. The term abstraction is used here to indicate the extraction of essential information. Abstraction is not synonymous with simplification. If a particular component model can not be simplified without losing essential aspects of the model, it ceases to move up the pyramid and becomes part of a TSPA calculation tool at that level of detail.

The upper level of the pyramid shows the final level of distillation of information into the most critical aspects necessary to represent the total system. At this level, all of the models are linked together. These are the models used to forecast system behavior and estimate the likelihood that the behavior will ensure long-term safety and comply with regulations.

Figure 6.2-2 is a more detailed, but still simplified, view of information flow among the component models: Unsaturated-zone flow (and seepage), thermal hydrology, engineered barrier system geochemistry, waste package and drip shield degradation, waste form degradation, engineered barrier system (EBS) transport, unsaturated-zone transport, saturated zone (SZ) flow and transport, biosphere, and volcanism. The figure does not show all of the couplings among TSPA-SR component models but does illustrate major model connections, abstractions, and information feeds.

Figures 6.2-3a and 6.2-3b give a more detailed description of information flow in the TSPA-SR, showing the principal pieces of information passed between the various component models. Figure 6.2-3a shows the overall system, while Figure 6.2-3b shows the details of EBS.

The overall information flow forms the basis for the architecture of the TSPA-SR computer code. The integrating program that links all the various component codes is GoldSim (Golder

Associates 2000). It is a probabilistic sampling program that ties all the component models, codes, and response surfaces together in a coherent structure that allows for consistent parameter sampling among the component models. The GoldSim program is used to conduct either single-realization or multi-realizations simulations of the entire system.

Figure 6.2-4, in conjunction with Figure 6.2-2, provides an understanding of the TSPA-SR code architecture (i.e., the actual computer codes used and the connections and information transfer between codes). The figure includes both the codes run before the GoldSim program and those run in real time and coupled to, or within, the GoldSim program. In general terms, the major components modeled within GoldSim are as follows:

- Mountain-scale unsaturated-zone flow
- Seepage of water into emplacement drifts
- Drift-scale unsaturated-zone thermal hydrology
- EBS environment
- Drip-shield and waste-package degradation
- Cladding degradation
- Waste-form degradation
- EBS transport
- Unsaturated-zone transport
- Saturated-zone transport
- Biosphere transport
- Disruptive events

A more detailed discussion of these components may be found in the TSPA-SR (CRWMS M&O 2000b, Section 2.2).

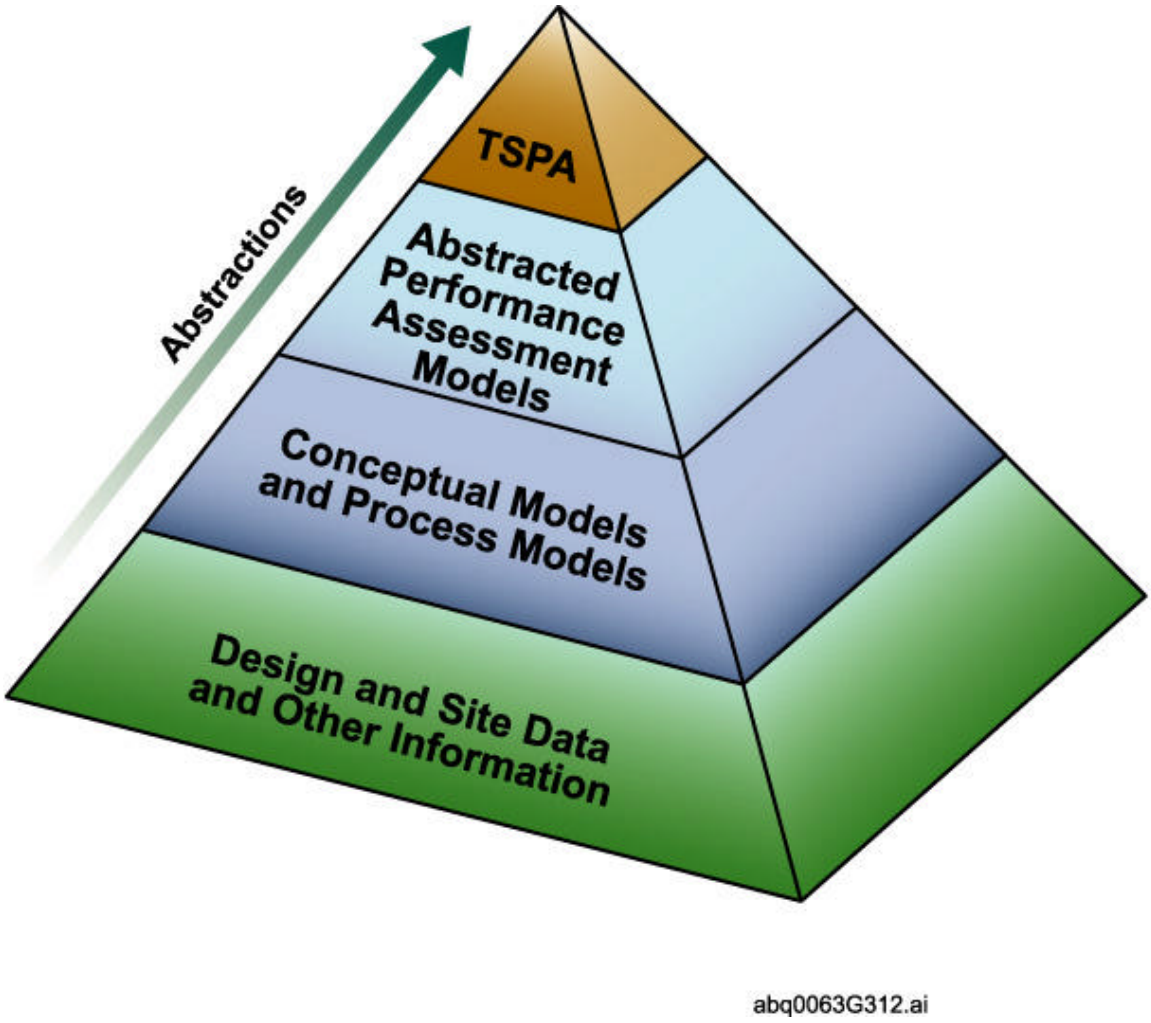


Figure 6.2-1. Performance Assessment Information Flow Pyramid (CRWMS M&O 2000b, Figure 1.1-1)

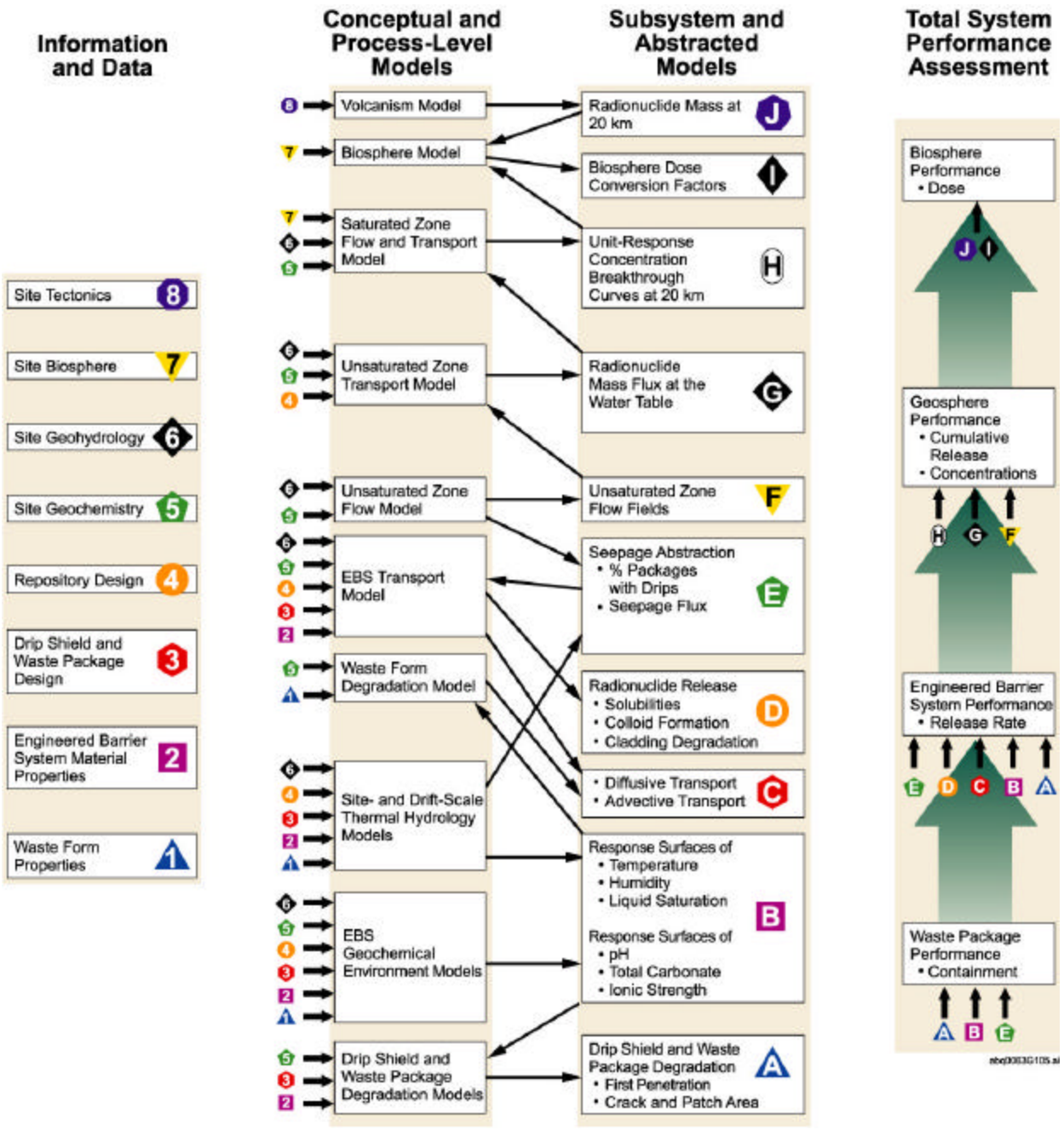


Figure 6.2-2. Simplified Representation of Information Flow in the Total System Performance Assessment among Data, Process Models, and Abstracted Models (CRWMS M&O 2000b, Figure 2.2-1)

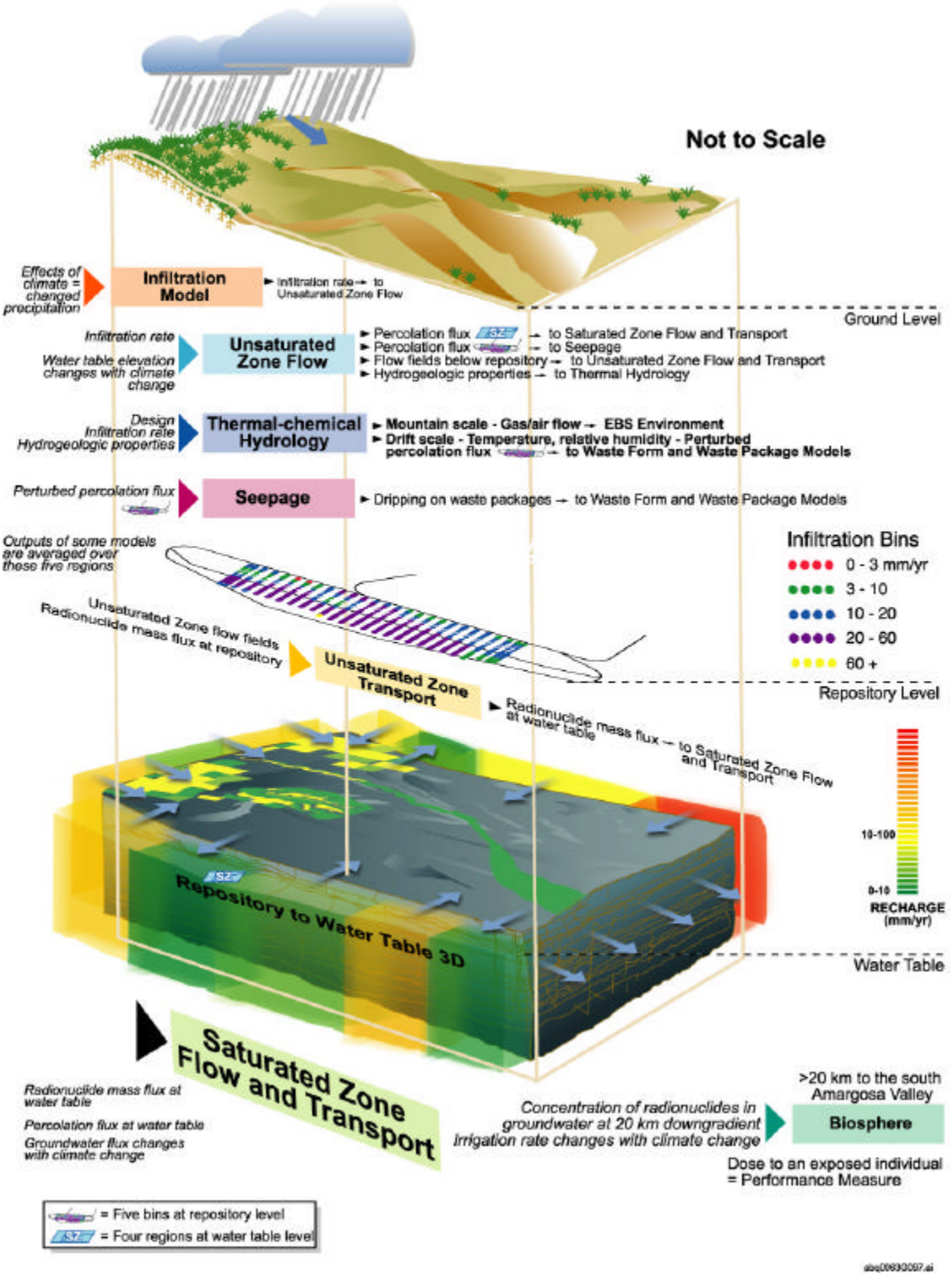


Figure 6.2-3a. Detailed Representation of Information Flow in the Total System Performance Assessment Model for the Site Recommendation (CRWMS M&O 2000b, Figure 2.2-2a)

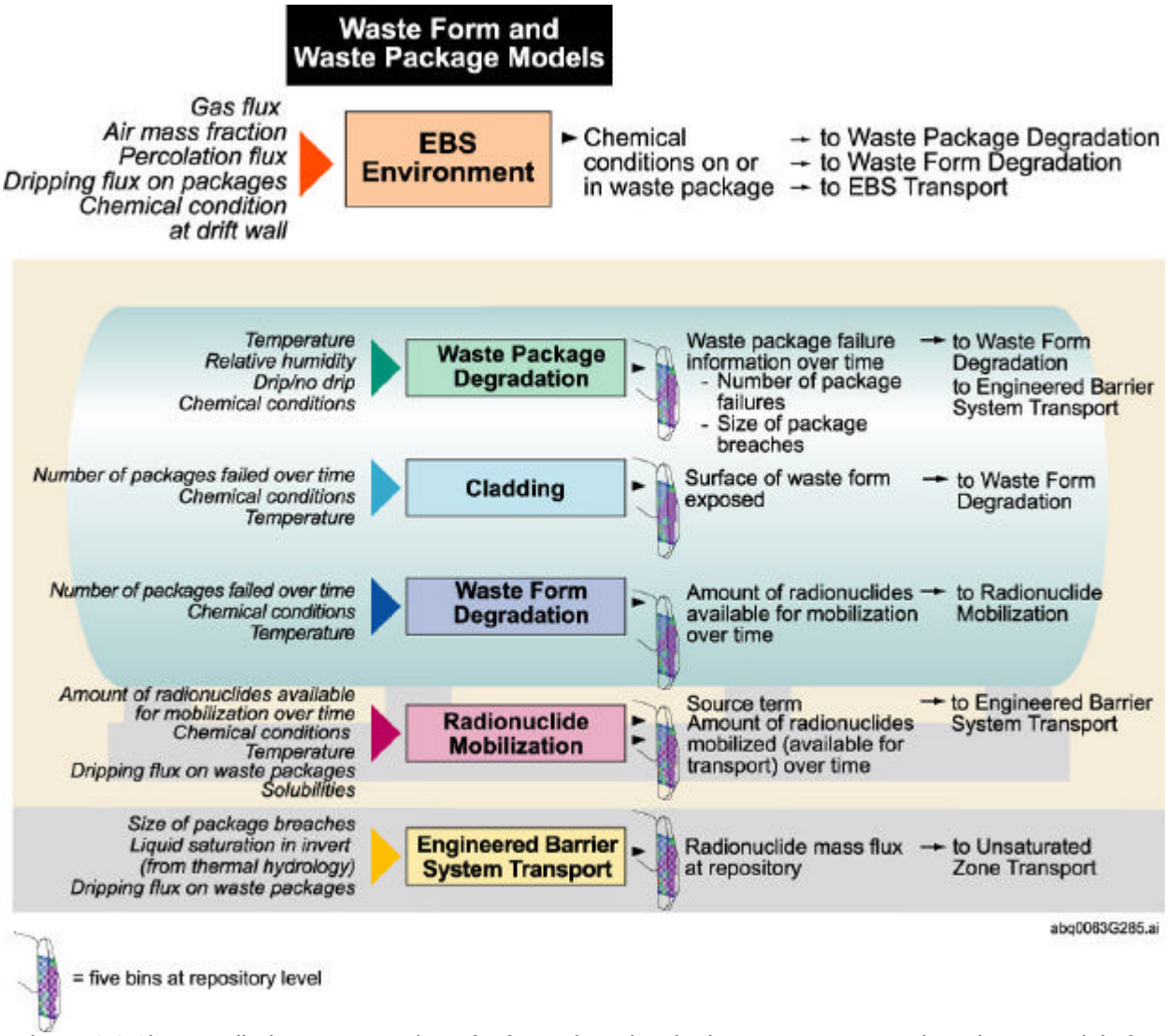


Figure 6.2-3b. Detailed Representation of Information Flow in the Waste Form and Package Models for the Site Recommendation (CRWMS M&O 2000b, Figure 2.2-2b)

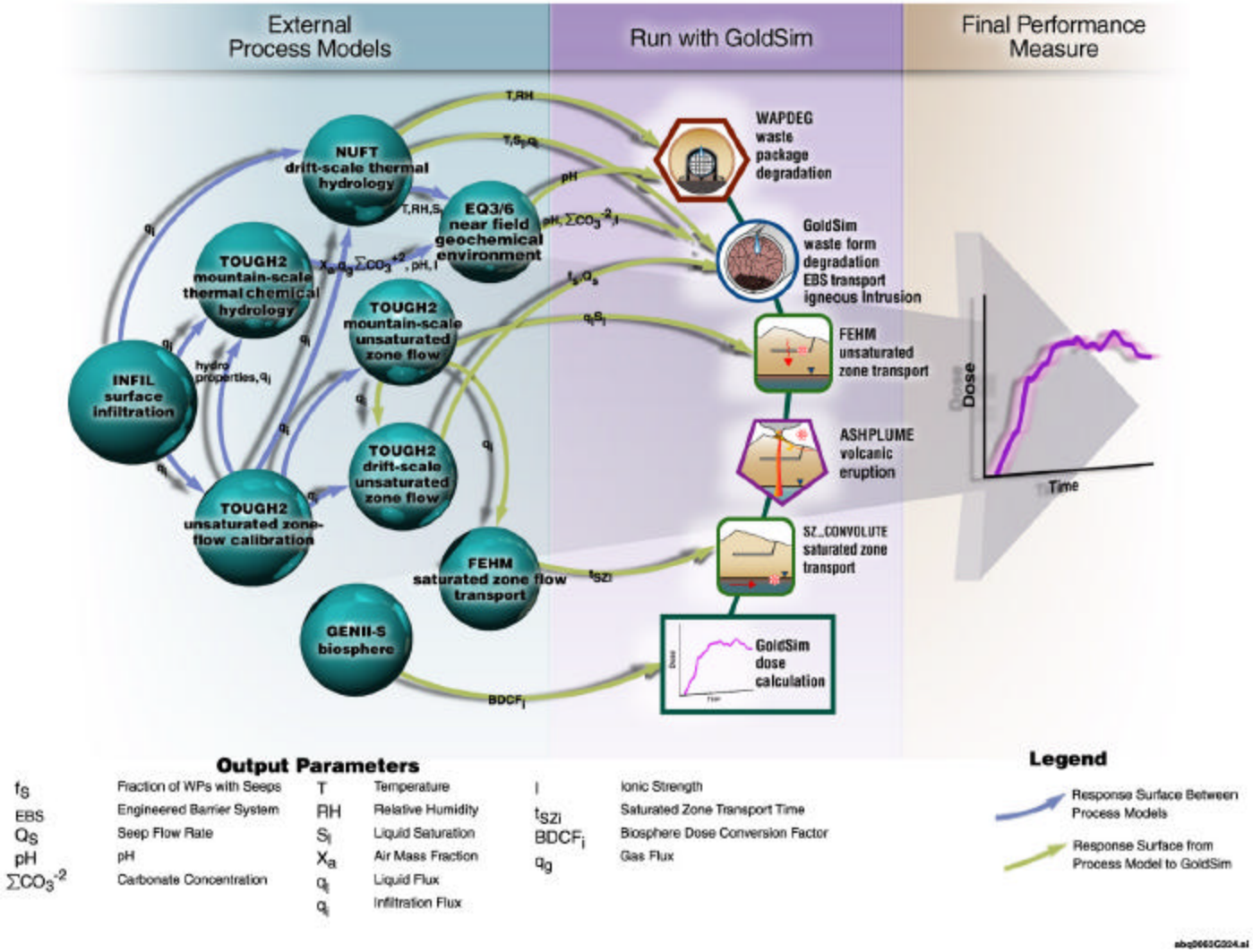


Figure 6.2-4. Code Architecture and Transfer of Information among Models used for the Total System Performance Assessment for the Site Recommendation (CRWMS M&O 2000b, Figure 2.2-3)

6.3 SOURCE TERM

The source term is comprised of the waste packages, the waste forms they contain, and the radionuclide inventory in the waste forms. The dissolution of the waste forms depends on their chemical and physical properties. The waste forms included in the TSPA-SR model and their waste packaging are shown in Figure 6.3-1 and the loading of the waste package types into the repository is shown in Figure 6.3-2. The source term for the immobilized plutonium waste form, can-in-canister ceramic is described below.

6.3.1 Waste Packaging

Figure 6.3-3 shows the waste package for disposal of immobilized plutonium. The waste package has an outer barrier of Alloy 22 (a nickel alloy) and an inner barrier of stainless steel (316NG) (CRWMS M&O 1999a, Section 5.3.2). The spent fuel canister, the HLW canisters, and the can-in-canister ceramic canisters are also composed of stainless steel (304L) (Figure 6.3-4) (Shaw 1999, Section 2, Table 2.2). The plutonium ceramic disks are placed in 28 cylindrical cans, 20 inches long and 3 inches in diameter, and each can contains 9.2 kilograms of plutonium can-in-canister ceramic waste (Shaw 1999, Table 2.1). For disposal of 17 tons of plutonium approximately 700 canisters of can-in-canister ceramic are required and for 13 tons of plutonium approximately 535 canisters are required (Shaw et al. 2001, Table 2.3).

6.3.2 Radionuclide Inventories

The radionuclide inventory for the can-in-canister ceramic is provided in Table 4.1-1 for the 17-ton case (Shaw et al. 2001, Table 4.3) and it is assumed that this inventory also applies to the 13-ton case (Assumption 5.2). For the analyses that follow, the ^{241}Pu shown in Table 4.1-1 was decayed to ^{241}Am and added to the amount of ^{241}Am shown in Table 4.1-1. Table 4.1-2 shows the radionuclide inventory for the HLW (CRWMS M&O 2000c, Section 7, Table 34).

6.3.3 Waste Form Dissolution Models

Dissolution models for ceramic and for HLW glass are presented below. The models are for the waste form itself (i.e., no affect of packaging or cladding is considered).

6.3.3.1 Ceramic

Information from leach testing of plutonium ceramic (Shaw 1999, Section 6, Figure 6.2) suggests that the dissolution follows the Arrhenius relationship:

$$k = k_o \exp [-Q/RT] \qquad \text{(Eq. 6-1)}$$

where

- k = leaching rate ($g/m^2/day$)
- Q = activation energy (kJ/mol)
- R = the gas constant (8.3145 J/mol/^oK)
- T = temperature (^oK)

k_o = a constant for the specific reaction ($g/m^2/day$)

Data from leaching tests for the range of 25 to 90 °C provides a best-fit value for Q of 66.85 kJ/mol (16.0 kcal/mol where 1.0 kcal = 4.18597 kJ) and k_o of 1.16×10^6 $g/m^2/day$ (Shaw 1999, Section 6, Figure 6.2).

In previous performance assessments (CRWMS M&O 1996, Section 3.2.3; CRWMS M&O 1998b, Section 3.5; CRWMS M&O 2000f, Section 6.3.5.3) the composition of the ceramic was assumed to be similar to that of Synroc-C, a titanate ceramic (Reeve et al. 1989, Table 1). Reeve (Reeve et al. 1989, Eq. 1) proposed that the cumulative release from Synroc-C to be:

$$Q = Q_0 + \theta + S\ F\ t/A \qquad \text{(Eq. 6-2)}$$

where

Q = release rate per unit surface area (g/m^2)

Q_0 = instantaneous release from grain boundaries and metastable phases (g/m^2)

θ = complex kinetic function that accounts for ionic diffusion, selective matrix attack, etc (g/m^2)

S = solubility of the matrix (g/m^3)

F = groundwater flow rate (m^3/day)

A = surface area (m^2)

t = time (days).

Lappa (Lappa 1995, p. 3) states that it is likely that the long-term release from the Synroc-C is controlled by the third term (S F t /A) of the Equation 6-2. Lappa indicated that in using deionized water at 70°C, the available data support a matrix solubility of less than or equal to 0.007 g/m^3 based on a long-term leaching rate of less than or equal to 10^{-4} $g/m^2/day$, and proposed that the temperature effect on the leaching rate of Synroc-C be described by:

$$R = \alpha\ 10^{-\beta(1000/T)} \qquad \text{(Eq. 6-3)}$$

where

R = leaching rate ($g/m^2/day$)

T = temperature (°K)

α, β = constants

Based on the Synroc-C data of Ringwood et al. (1988), Lappa (Lappa 1995, p. 3) proposed $\beta \approx 1.0$°K and $\alpha \approx 0.082$ $g/m^2/day$ using the long-term leaching rate of 10^{-4} $g/m^2/day$ at 70°C. The release rate can be calculated by multiplying R by the surface area (S) and the elapsed time (t). The radionuclides are released from the waste form based on its alteration rate, and are then transported at a rate dependent on whether they are alteration-controlled or solubility-limited

radionuclides. This dissolution model has been used in past performance assessments (CRWMS M&O 2000f, Section 6.3.5.3; CRWMS M&O 1997, Section 3.5.3).

6.3.2.2 High-Level Waste

The HLW glass-degradation model is implemented in the form of an analytical expression containing parameters that account for the pH, temperature, surface area, and the combined effects of glass composition and the composition of the leaching solution on the rate of glass corrosion. Conservative estimates of the parameter values were derived from laboratory data. Implementation of the model for the TSPA-SR analysis requires the input of temperature and pH data. The model for glass dissolution under immersion is based on the rate expression for aqueous dissolution of borosilicate glass. The rate expression to calculate the dissolution rate of HLW glass in an aqueous solution is given by (CRWMS M&O 2000c, Section 7):

$$DR = S_{im}\, k_{eff}\, 10^{\eta\, pH} \exp(-E_a/RT) \qquad \text{(Eq. 6-4)}$$

where,

$$k_{eff} = k_o\,(1 - Q/K) \qquad \text{(Eq. 6-5)}$$

with the coefficients in the above equations defined as follows:

- DR = dissolution rate of the glass (mass/time)
- S_{im} = surface area of glass immersed in water (area)
- k_{eff} = effective dissolution rate constant (mass/(area-time))
- k_o = intrinsic dissolution rate (mass/(area-time))
- Q = concentration of dissolved silica (mass/volume)
- K = fitting parameter equal to apparent silica saturation concentration (mass/volume)
- η = pH dependence coefficient (dimensionless)
- E_a = effective activation energy (kJ/mol)
- R = gas constant (8.31451 kJ/(mol-^oK))
- T = absolute temperature (^oK)

By selecting a conservative bounding value for k_{eff}, the model simplifies to an equation in three parameters (η, E_a, S_{im}) and two independent variables (pH and T). Values for S_{im}, pH, and T depend on the exposure conditions (CRWMS M&O 2000c, Section 7). Equations 6-4 and 6-5 are incorporated into the TSPA-SR model for the calculation of the HLW glass-dissolution rate. The model parameters k_{eff}, η, and E_a are represented using statistical distributions to account for uncertainty (CRWMS M&O 2000d, Section 6.3.4.4, Table 6-51). Distributions for both high and low pH are used. The surface area of the glass, S_{im}, is a constant equal to 0.0000563 m^2/g (CRWMS M&O 2000d, Section 6.3.4.4, Table 6-51) and R, the universal gas constant, is as previously defined. The pH and T in Equation 6-4 vary with time and are computed in the TSPA model.

At the initiation of a simulation, the TSPA model samples a value from each of the parameter distributions. The TSPA model then calculates the glass-dissolution rates for both high- and low-pH cases. Once both dissolution rates have been calculated, the model compares the high-pH and low-pH dissolution rates and selects the larger of the two rates. Finally, the rate per surface area is multiplied by the geometric surface times a factor of 20 (CRWMS M&O 2000d, Section 6.3.4.4).

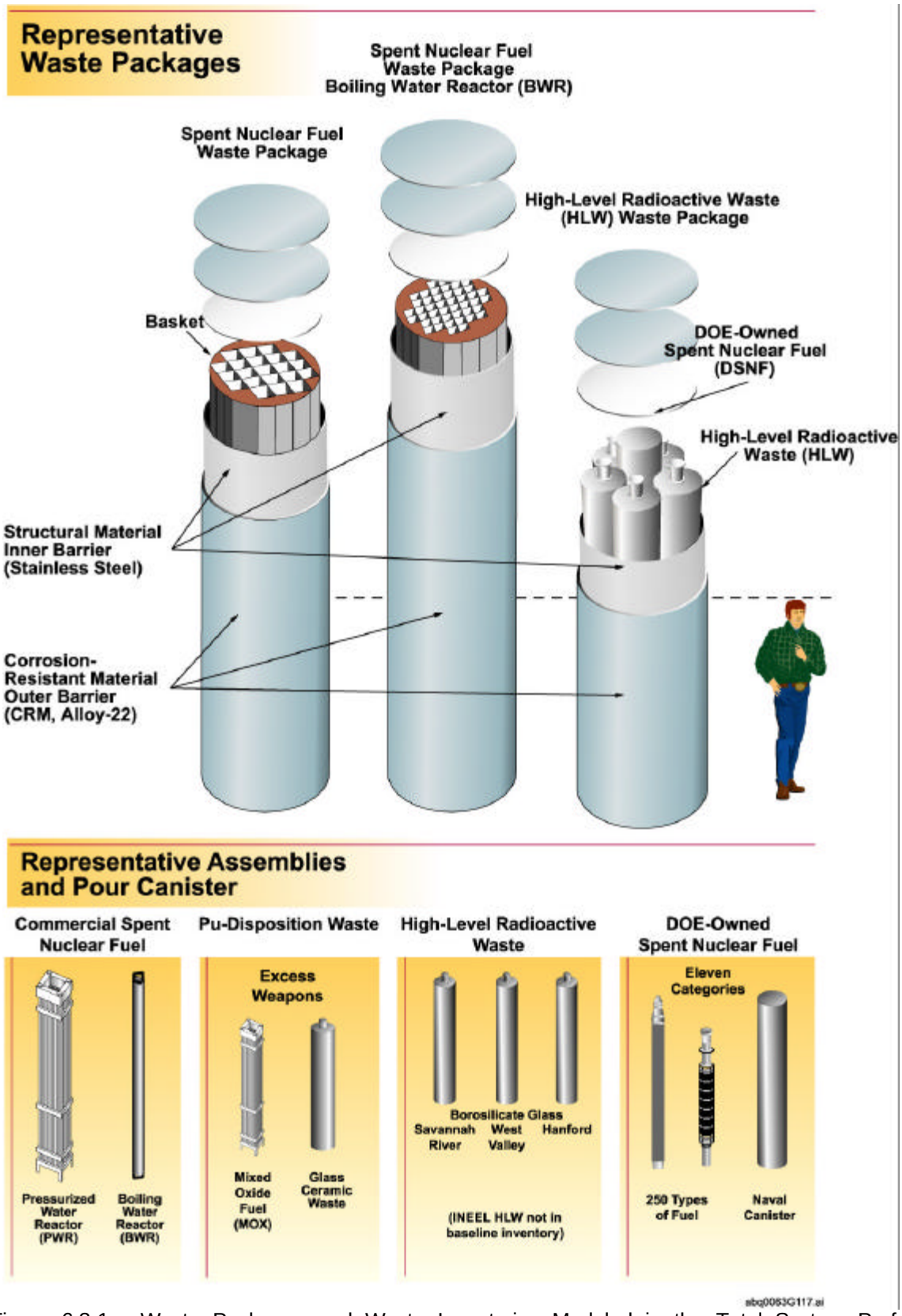


Figure 6.3-1. Waste Packages and Waste Inventories Modeled in the Total System Performance Assessment Nominal Case (CRWMS M&O 2000b, Figure 2.1-9)

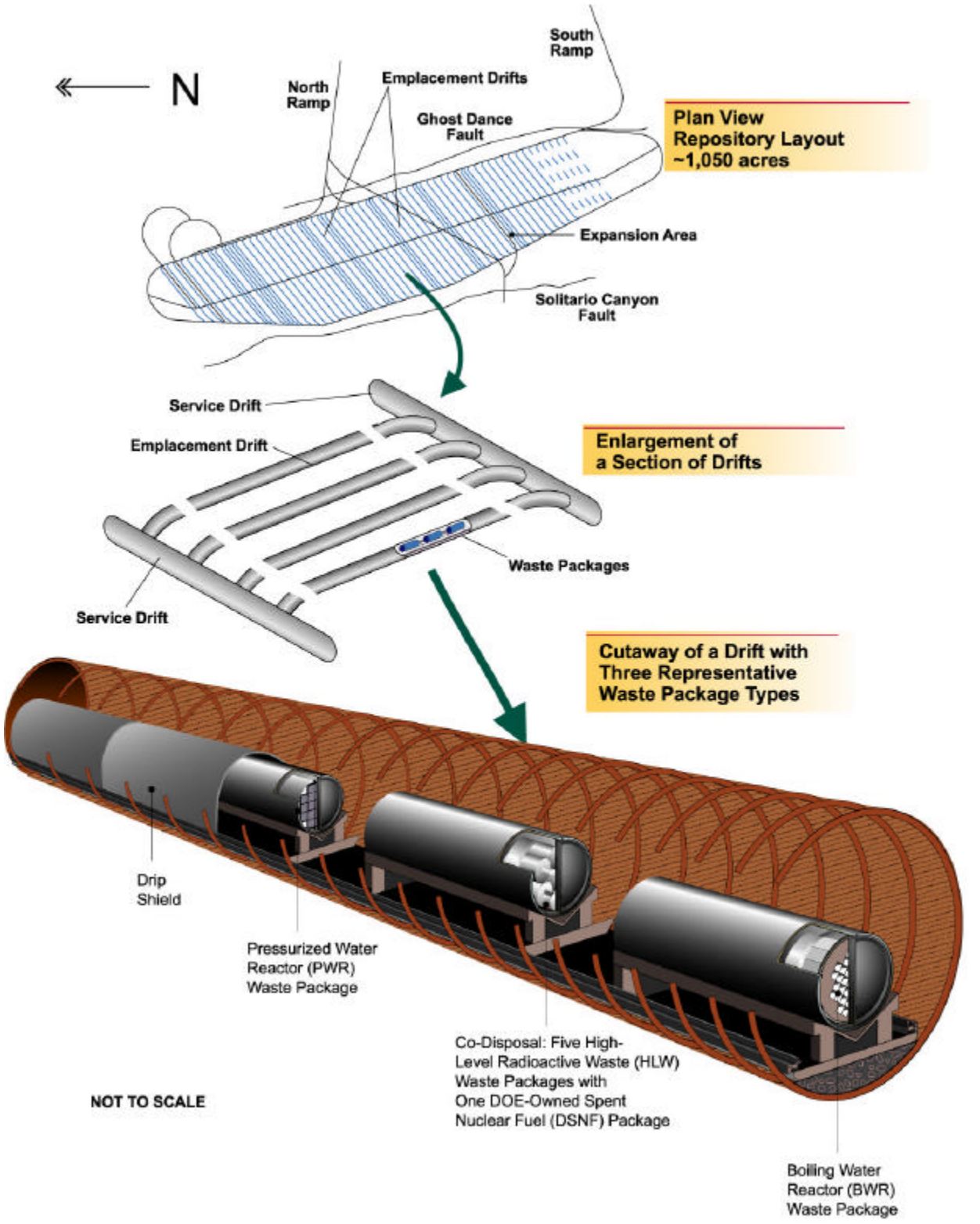


Figure 6.3-2. Repository Layout and Drift Loading with Representative Waste Packages (CRWMS M&O 2000b, Figure 1.7-1)

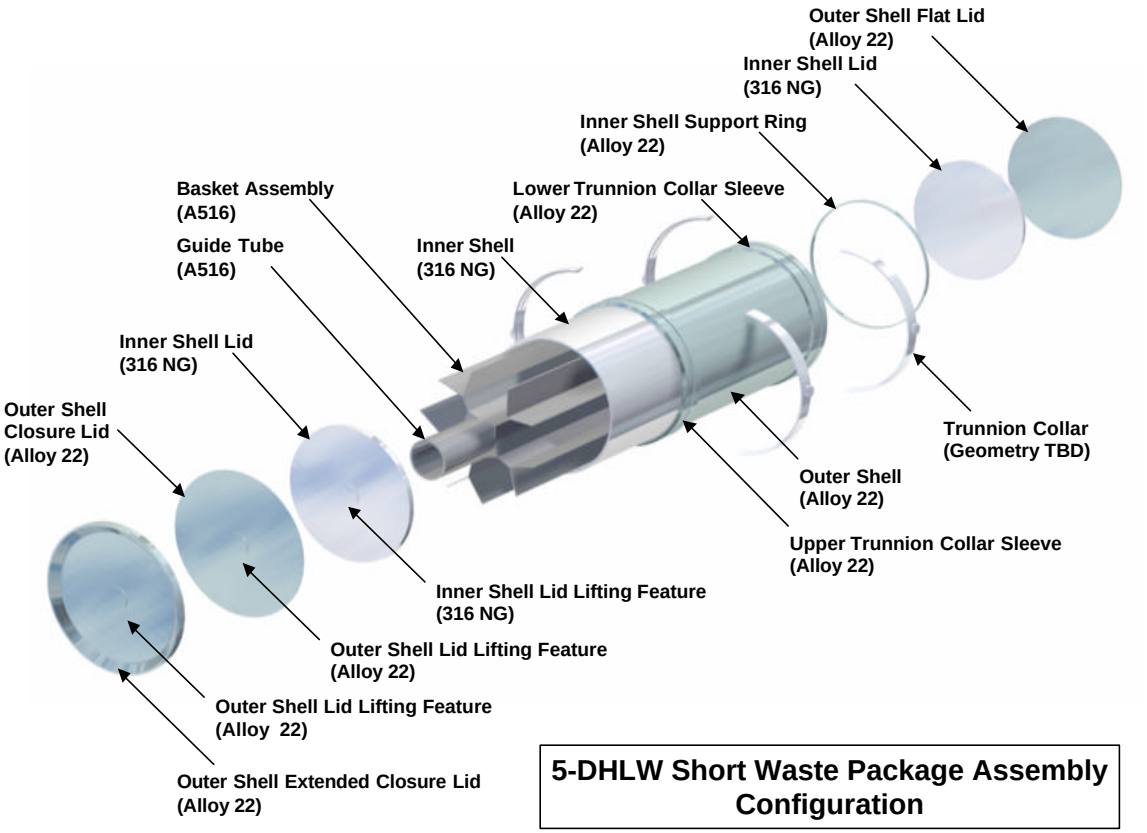


Figure 6.3-3. Waste Package for Disposal of High-Level Waste and Immobilized Plutonium Can-in-Canister Ceramic (CRWMS M&O 2000e, Figure 6)

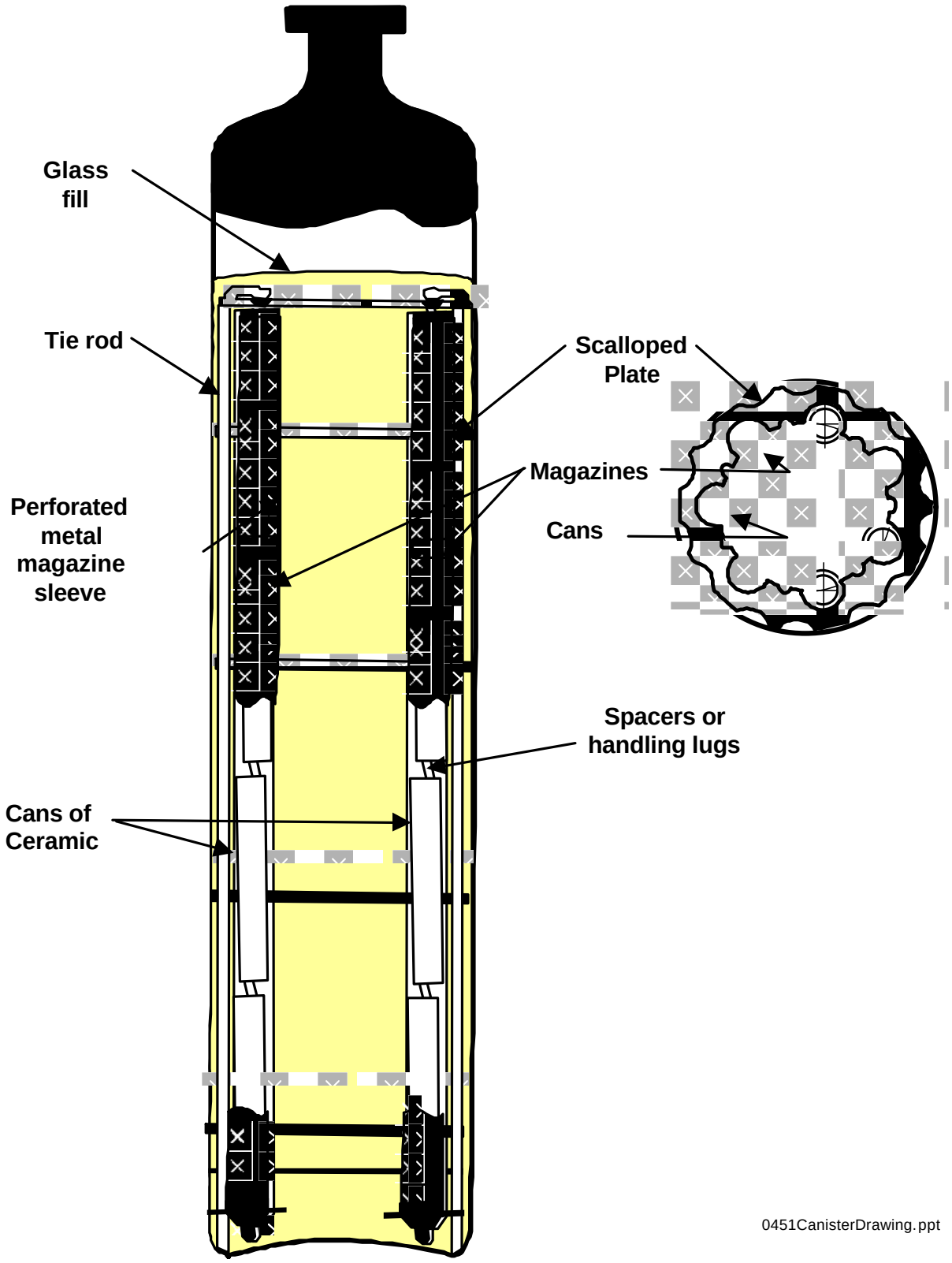


Figure 6.3-4. Schematic Diagram of Immobilized Plutonium Can-in-Canister Ceramic (CRWMS M&O 1999b, Figure 3)

6.4 DOSE RESULTS

The performance-assessment analyses of the plutonium immobilized in a ceramic waste form examine the contribution from the disposal of 17 tons and 13 tons of plutonium as can-in-canister ceramic to the dose rate 20 kilometers from the repository. For this analysis, the specific inventory and physical properties of the ceramic waste form (Tables 4.1-1 and 4.1-3) were implemented in the nominal case of the median-value TSPA-SR model (DTN: MO0009MWDMED01.020). In addition to the ceramic waste form, the contribution of the HLW (Table 4.1-2) used to encapsulate the ceramic waste form was considered in the model. For the ceramic waste form the ceramic volume is 0.0787 m^3 (Table 4.1-3), which corresponds to a volume displacement in the HLW canister of 12.1 percent of the base design (Shaw et al. 2001, Section 2.1). Shaw et al. (2001, Section 2.1) gave a range in total HLW glass volume. For this analysis, the HLW glass volume encapsulating the ceramic waste form was assumed to be 0.636 m^3 and the HLW radionuclide inventory per waste package was reduced by 12.1 percent from that given in Table 4.1-2.

The 17-ton and the 13-ton cases require 700 and 535 waste packages (Shaw et al. 2001, Table 2.3), respectively, assuming the same radionuclide inventory (Table 4.1-1). The TSPA-SR model does not include ^{241}Pu in its list of radionuclides, only its daughter product ^{241}Am. Because of the same atomic weight and the relatively short half live of ^{241}Pu compared to ^{241}Am, the inventory of ^{241}Pu, given in Table 4.1-1, was added to the inventory of ^{241}Am in the TSPA model. In the simulations in this report, the LLNL ceramic dissolution model (Equation 6-1, Section 6.3.3.1) is used to describe the dissolution of ceramic. As mentioned in Section 5.6, the BDCF for ^{242}Pu was corrected in the TSPA-SR model (DTN: MO0009MWDMED01.020) that was used as the basis for the implementation of the immobilized plutonium can-in-canister ceramic.

For the 17-ton case, considering only the immobilized plutonium can-in-canister ceramic waste form, the potential range in the total dose release due to uncertainty in various input parameters was investigated in a multi-realization simulation. For this simulation, the nominal case of the 100 realization TSPA-SR model was used (DTN: MO0009MWDNM601.018, see Section 4.1) to implement the specific inventory and physical properties of the ceramic waste form (Tables 4.1-1 and 4.1-3). The input and output data from the 100-realization simulation for 17 tons of the immobilized plutonium can-in-canister waste form are recorded in DTN: MO0107MWDMUL03.008.

The total dose results from the 100 realizations are described by the 5^{th} and 95^{th} percentile and by the mean and median of the probability distribution (Figure 6.4-1). In addition, the calculated total-dose history from the corresponding single-realization, median-value simulation is included in Figure 6.4-1 for comparison with the median curve from the probabilistic run. The input and output data from the median-value simulation are given in DTN: MO0107MWDMED03.007.

The calculated total-dose rates from the median-value simulation compare well with the early time of the median curve from the multi-realization simulation (Figure 6.4-1). However, the median-value simulation displays a relatively sharp peak of 14.4 mRem/yr at 150,000 years exceeding the mean curve of the multi-realization simulation that peaks at 11.4 mRem/yr, whereas the median curve peaks at about 4.5 mRem/yr after 200,000 years. Following the peak,

the total dose rate from the median-value simulation declines sharply and levels off at about 3 mRem/yr until 300,000 years, after which the calculated dose-history curve shows a linear decline. In comparison, the multi-realization simulations yield relatively smooth curves for the mean and median. For comparison, the peak dose rates from the 5^{th} and 95^{th} percentile curves are as high as 0.5 and 67.6 mRem/yr, respectively.

The dose histories for the eight major radionuclides for the 17-tons of plutonium can-in-canister ceramic from the median-value simulation are shown in Figure 6.4-2. The dominant radionuclide contributing most to the total dose is ^{239}Pu, irreversibly attached to waste-form colloids (^{239}IC), followed by ^{237}Np that has a peak dose rate of 3.2 mRem/yr after about 300,000 years. The peak dose for ^{239}IC (13,0 mRem/yr) occurs at 155,000 years, followed by a rapid decline below that of ^{239}Pu after about 200,000 years. The dose-rate increase for ^{237}Np is somewhat delayed compared to ^{239}IC. In addition to ^{239}IC and ^{237}Np, the other major radionuclides include ^{239}Pu, ^{242}Pu, ^{227}Ac, ^{242}IC, ^{230}Th, and ^{229}Th (^{242}IC is ^{242}Pu irreversibly attached to waste-form colloids).

The results of the median-value simulation for the 13-ton case are shown in Figure 6.4-3. The peak total-dose rate decreased from 14.4 mRem/yr in the 17-ton case to 11.5 mRem/yr in the 13-ton case. The relative contributions of the eight major radionuclides remain the same, except that the peak dose for ^{231}Pa exceeds that for ^{230}Th and replaced ^{229}Th as one of the eight major radionuclides. This is probably caused by differences in solubility-limited dissolution of the parent radionuclides for ^{229}Th and ^{231}Pa, causing a slightly lower release of the ^{241}Am relative to ^{239}Pu for the 13-ton case (535 WP) than for the 17-ton case (700 WP).

The dose contribution from the HLW glass that is used to encapsulate the ceramic waste form was calculated by considering the HLW inventory reduced by 12.1 percent (Table 4.1-2) to account for the volume reduction due to the displacement of the ceramic waste form. The dose contributions for the 17-ton (700 waste packages) and 13-ton (535 waste packages) cases are shown in Figures 6.4-4 and 6.4-5, respectively. The results indicate peak dose rates of 2.25 and 1.72 mRem/yr for the 17-ton and 13-ton cases, respectively, contributed mainly by ^{237}Np, followed closely by ^{239}IC that peaks earlier at about 130,000 years (Figures 6.4-4 and 6.4-5). Similar to the ceramic waste form, the dose rate increase for ^{237}Np lags behind and peaks at about 240,000 years.

The dose release rates from the simulations with both the plutonium ceramic waste form and the associated HLW glass combined in a single waste package for the 17-ton and 13-ton cases are shown in Figures 6.4-6 and 6.4-7, respectively. For the 17-ton case, the peak dose rate decreased slightly from 14.4 mRem/yr to 14.0 mRem/yr (Figure 6.4-6). For the 13-ton case, the peak dose rate decreased slightly from 11.5 mRem/yr to about 10.7 mRem/yr (Figure 6.4-7). In both cases, ^{239}IC is the dominant radionuclide contributing to the early peak at about 150,000 years, followed by a second, lower peak that is dominated by ^{237}Np. The slight decrease in the dose rates for the cases with the combined inventory compared to the peak dose from the corresponding ceramic waste form (Figures 6.4-2 and 6.4-3) is due to solute-limited dissolution of the some radionuclides.

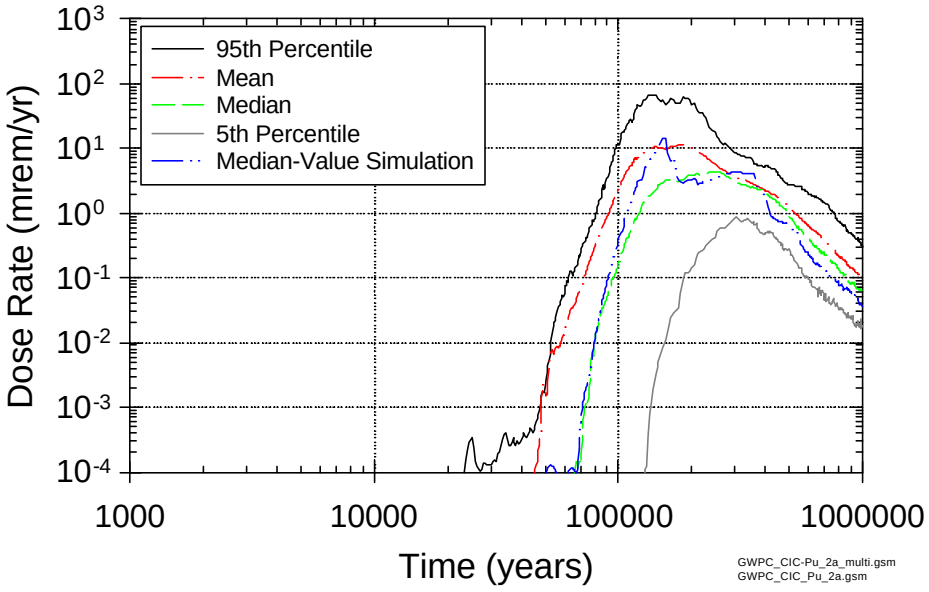


Figure 6.4-1. Simulated Total Dose-Rate Histories for the Nominal, 100 Realization Case of 17 Tons of Plutonium in Ceramic at 20 Kilometers over 1,000,000 Years (DTN: MO0107MWDMUL03.008); also shown is the nominal, median-value simulation for comparison (DTN: MO0107MWDMED03.007).

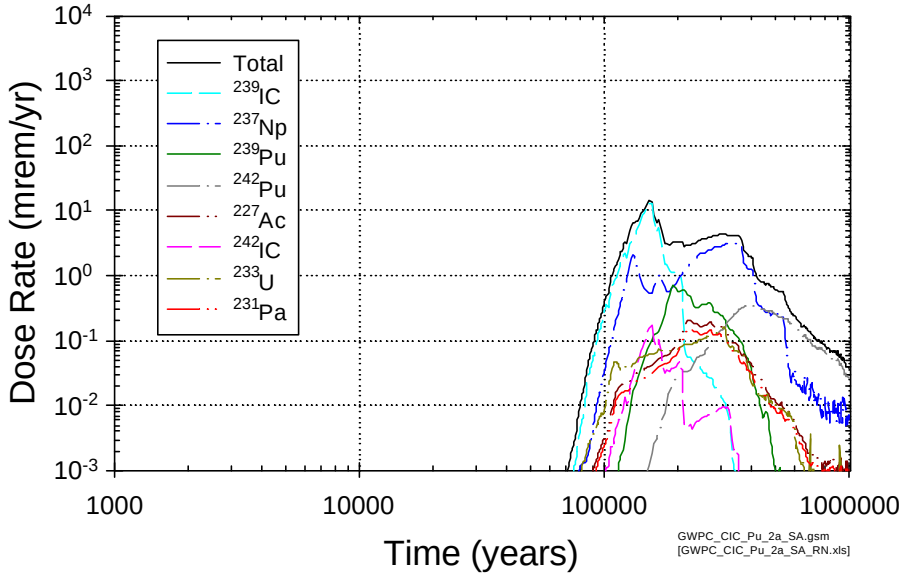


Figure 6.4-2. Median-Value Dose History of Selected Radionuclides from Ceramic in Can-in-Canister Ceramic at 20 Kilometers over 1,000,000 Years for the 17-Ton Case (DTN: MO0107MWDMED03.007)

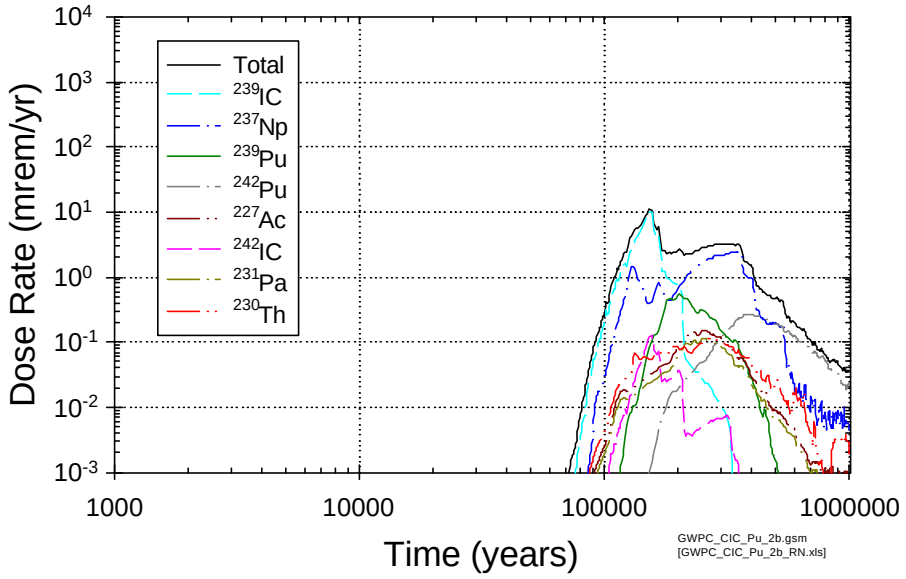


Figure 6.4-3. Median-Value Dose History of Selected Radionuclides from Ceramic in Can-in-Canister Ceramic at 20 Kilometers over 1,000,000 Years for the 13-Ton Case (DTN: MO0107MWDMED03.007)

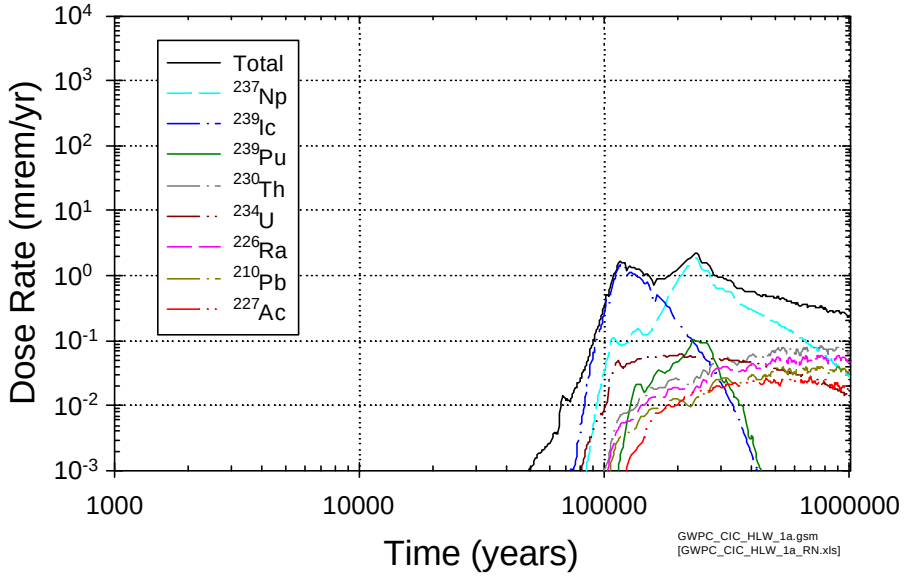


Figure 6.4-4. Median-Value Dose History of Selected Radionuclides from High-Level Waste used to Encapsulate the Ceramic in Can-in-Canister Ceramic at 20 Kilometers over 1,000,000 Years for the 17-Ton Case (DTN: MO0107MWDMED03.007).

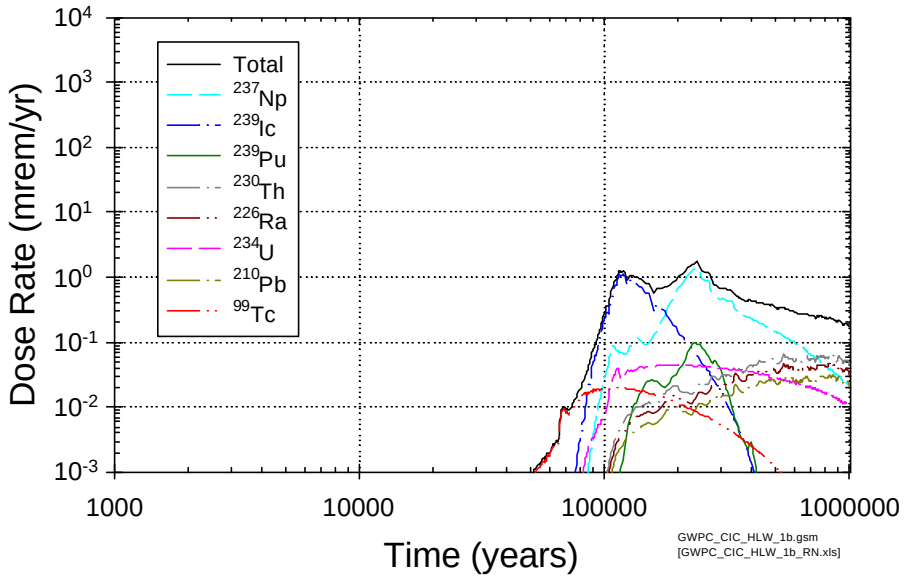


Figure 6.4-5. Median-Value Dose History of Selected Radionuclides from High-Level Waste used to Encapsulate the Ceramic in Can-in-Canister Ceramic at 20 Kilometers over 1,000,000 Years for the 13-Ton Case (DTN: MO0107MWDMED03.007).

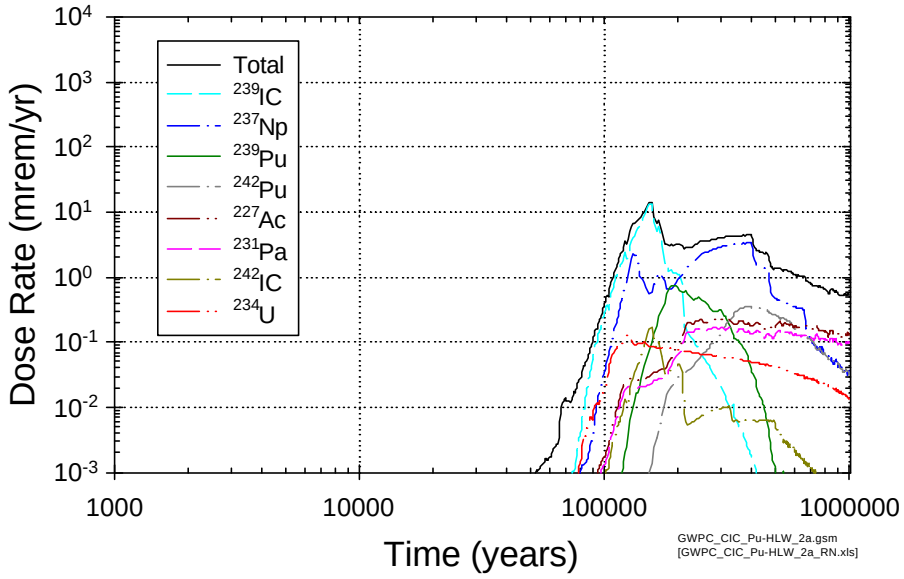


Figure 6.4-6. Median-Value Dose History of Selected Radionuclides from Ceramic and High-Level Waste in Can-in-Canister Ceramic at 20 Kilometers over 1,000,000 Years for the 17-Ton Case (DTN: MO0107MWDMED03.007).

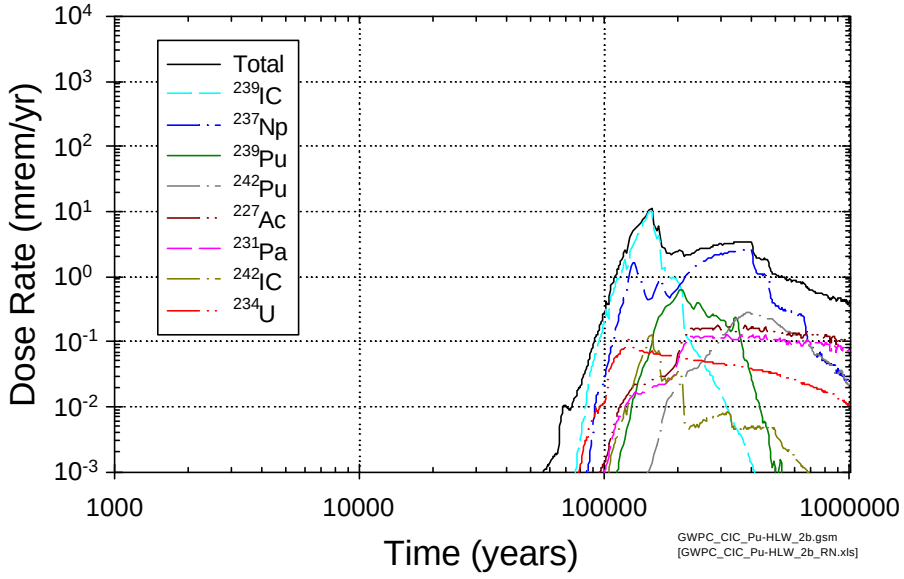


Figure 6.4-7. Median-Value Dose History of Selected Radionuclides from Ceramic and High-Level Waste in Can-in-Canister Ceramic at 20 Kilometers over 1,000,000 Years for the 13-Ton Case (DTN: MO0107MWDMED03.007).

6.5 SENSITIVITY ANALYSES

For the sensitivity analysis of the plutonium can-in-canister ceramic waste form, the uncertainty in the physical characteristics of the ceramic waste form, the radionuclide inventory, and the number of waste packages on the total dose release are investigated. In addition, the uncertainty associated with waste-form colloid formation is examined. Furthermore, the total dose contribution from the ceramic waste form is compared to the nominal case of the TSPA-SR model and to an equivalent number of canisters of HLW using the TSPA-SR model.

6.5.1 High-Level Waste Equivalent and Nominal-Case Repository

A comparison between the total dose from the combined plutonium ceramic and HLW glass (using 12.1 percent reduced HLW inventory) and an equivalent number of canisters of HLW (the complete HLW inventory is found in Table 6.4-2), for the 17-ton and the 13-ton cases, is shown in Figures 6.5-1 and 6.5-2, respectively. Both cases show that the total dose for the equivalent HLW is noticeably lower than the total dose from the can-in-canister ceramic. However, for the total amount of HLW contained in the repository the radionuclide inventory for the surplus plutonium was included in the radionuclide inventory for the HLW (CRWMS M&O 2000c, Attachment I).

The total-dose history from the ceramic waste form for the 17-ton case and the total dose release from the nominal, median-value TSPA-SR model (DTN: MO0009MWDMED01.020) are compared in Figure 6.5-3. The calculated dose rates indicate that the peak dose from the 17-ton case is more than one order of magnitude lower than the peak dose from the nominal, median-value TSPA-SR case.

6.5.2 Dissolution Rate of Ceramic

As mentioned above, the dissolution of the ceramic waste form is represented by the LLNL ceramic dissolution model (Equation 6-1, Section 6.3.3.1). In previous performance assessments, a dissolution model based on Synroc ceramic (Equations 6-2 and 6-3, Section 6.3.3.1) was used. A comparison of the dissolution rates between the two ceramic models and that for HLW glass is shown in Figure 6.5-4. Both ceramic models depend on the waste-package temperature. The dissolution model for HLW glass also depends, in addition to waste-package temperature, on the pH of the dissolving solution (Equation 6-4). Waste-package temperature varies through time and between the different model regions. The repository consists of five regions at the repository level, called Bins (Figure 6.2-3a), accounting for different infiltration ranges and associated variations in temperatures. In addition, pH varies for the different drip conditions (e.g., for always dripping, intermediate dripping, and no-dripping conditions), that are differentiated in the model.

For comparison, the dissolution rates for the different ceramic models and for the HLW glass are given for Bin-1, and for the HLW glass always dripping (AD) conditions were used (Figure 6.5-4). Figure 6.5-4 shows that the dissolution rate of HLW glass is more than one order of magnitude greater than that for the ceramic models at early times. At late time, when the waste-package temperature decreases, the dissolution rates decrease. The two ceramic models start out

at the same rate, but the dissolution rate from the LLNL ceramic model decreases more than the dissolution rate from the Synroc ceramic model (Figure 6.5-4).

The potential effect of the different ceramic dissolution models on the total dose release is investigated for the 17-ton case using, in addition to the LLNL ceramic dissolution model, the Synroc ceramic model and comparing them to a case assuming instantaneous dissolution of the ceramic waste form. The results are shown in Figure 6.5-5, indicating no noticeable differences in the total dose rates for the three cases, except at late times when the LLNL ceramic dissolution model yields somewhat higher dose rates than the Synroc ceramic model. However, there is no noticeable increase in total dose release using instantaneous dissolution of the ceramic waste form (Figure 6.5-5), indicating that the release from the failed waste packages is controlled by the solubility of the actinides and the release of colloids.

In a separate simulation, the glass dissolution model that has higher dissolution rates compared to the ceramic dissolution models (Figure 6.5-4) was used for the 17-ton case. The resulting total dose rate did not differ from the case with the LLNL ceramic dissolution model (Figure 6.5-6).

6.5.3 Surface Area of Ceramic

The physical properties of the ceramic waste (Table 4.1-3) indicate a wide range in specific surface area. The TSPA simulations, shown above, used the greater value of 3,461 m^2/g for the specific surface area. The potential range in specific surface area was examined in a simulation with the 17-ton case ceramic waste form, incorporating the smaller value of 347 m^2/g for comparison. The resulting total dose history for these two cases is shown in Figure 6.5-7, indicating that the potential uncertainty in specific surface area for the ceramic waste form has negligible impact on the total dose release.

6.5.4 Amount of Colloids

The results in Section 6.4 indicate that there is significant contribution to total dose from ^{239}Pu irreversibly attached to colloids (^{239}IC). The dose from these colloids exceeds the peak dose from ^{237}Np for the ceramic waste form (Figures 6.4-2 and 6.4-3) and is close to the peak dose from ^{237}Np for HLW (Figures 6.4-4 and 6.4-5). In the TSPA-SR model the ^{239}IC concentration, representing ^{239}Pu that is irreversibly attached to the waste-form colloids, is calculated as a function of the ionic strength of the solution, and is bounded by a minimum and maximum value (CRWMS M&O 2000d, Section 6.3.4.6). To evaluate the uncertainty in how much ^{239}Pu is transported in colloid form, the calculated ^{239}IC concentration is set to the maximum value in the TSPA model.

The resulting total dose history for the 17-ton case with maximum colloid concentrations for the waste-form colloids, compared to the base case (Figure 6.4-2), is shown in Figure 6.5-8. The calculation, using maximum waste form colloid concentrations, indicates a peak-dose increase from 14.4 mRem/yr to 26.8 mRem/yr that is associated with an increase in peak dose in ^{239}IC from 13.3 mRem/yr to 25.4 mRem/yr (Figure 6.5-8). Besides the significant increase in the dose rate for ^{239}IC, the other major radionuclides show only minor changes in the dose rate.

6.5.5 Radionuclide Inventory

The potential uncertainty in the radionuclide inventory for the plutonium can-in-canister ceramic waste form is examined by increasing and decreasing the radionuclide inventory given in Table 4.1-1 by a factor of five, respectively. The results of these simulations for the 17-ton case compared to the base case (Figure 6.4-2) is shown in Figure 6.5-9. An increase in the radionuclide inventory by a factor of five results in an increase in peak dose from 14.4 mRem/yr to 26.8 mRem/yr. Moreover, the second peak dominated by ^{237}Np is broader, resulting in dose rates of about 7 mRem/yr from about 200,000 through 800,000 years.

Decreasing the inventory by a factor of five results in a decrease in peak dose from 14.4 mRem/yr to 7.3 mRem/yr. The inventory reduction also causes the second peak dominated by ^{237}Np to narrow significantly, which is followed by a rapid decline after 200,000 years (Figure 6.5-9).

6.5.6 Number of Waste Packages

The uncertainty in the number of waste packages required for the disposal of the plutonium can-in-canister waste form is investigated by reducing the number of waste packages by a factor of five from 700 to 140 waste packages, using the same radionuclide inventory, given in Table 4.1-1. The impact of the reduced number of waste packages is shown in Figure 6.5-10, indicating a reduction in peak dose from 14.4 mRem/yr to 3.1 mRem/yr. The overall shape of the total-dose history curve is shifted to lower total dose rates, except at early times, where the simulation with 140 packages indicates a local peak. This is due to effects of the discrete failure of a limited number of waste packages at specific time intervals.

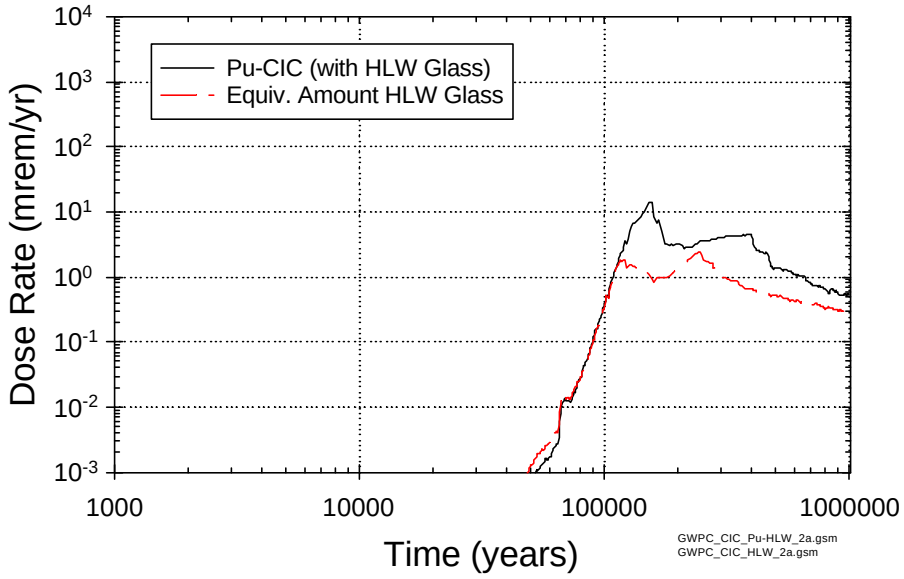


Figure 6.5-1. Comparison of the Total Dose Rate from the Combined Ceramic and High-Level Waste Glass for the 17-Ton Case and Total Dose Rate for the same Number of Canisters of High Level Waste (DTN: MO0107MWDMED03.007).

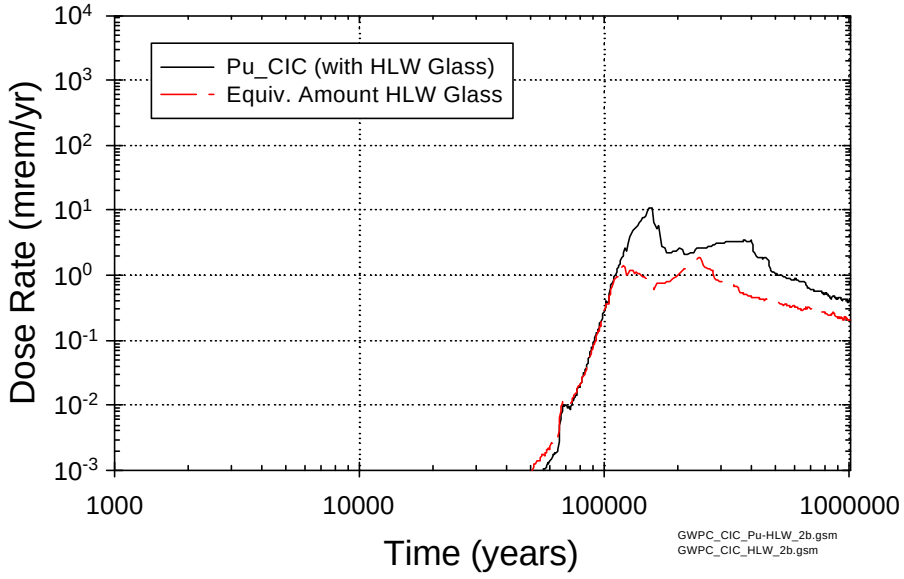


Figure 6.5-2. Comparison of the Total Dose Rate from the Combined Ceramic and High-Level Waste Glass for the 13-Ton Case and Total Dose Rate for the same Number of Canisters of High-Level Waste (DTN: MO0107MWDMED03.007)

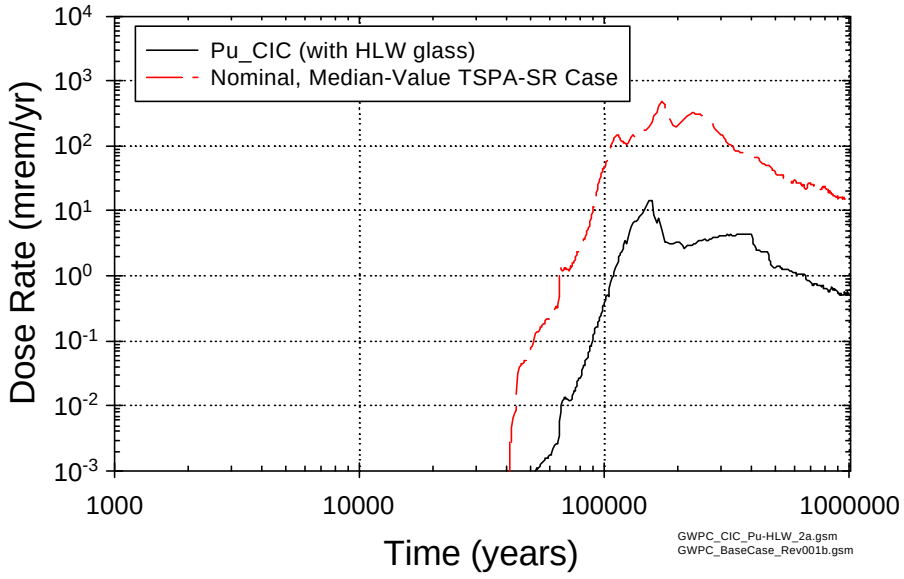


Figure 6.5-3. Comparison of the Total Dose Rate from Can-in-Canister Ceramic in the 17-Ton Case (DTN: MO0107MWDMED03.007) to the Total Dose Rate from the Nominal, Median-Value TSPA-SR Case (DTN: MO0009MWDMED01.020).

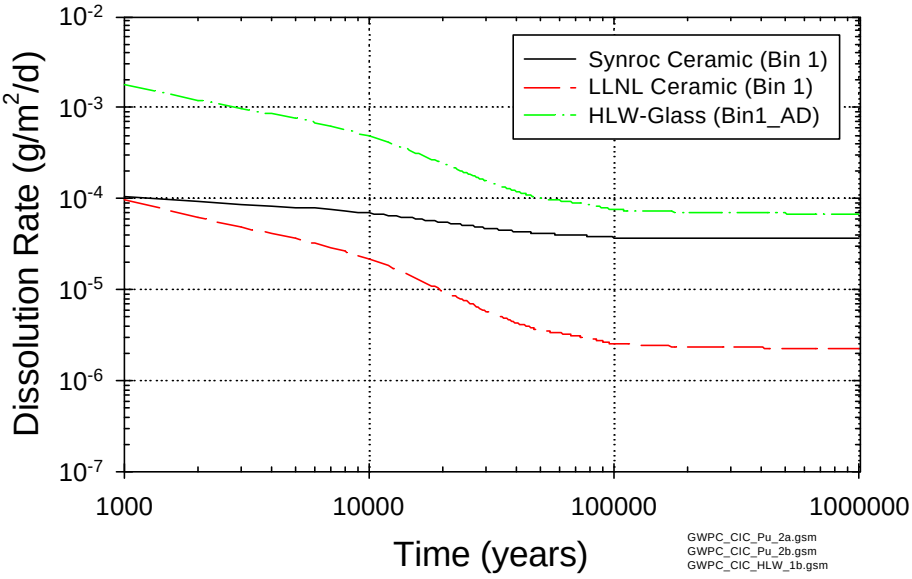


Figure 6.5-4. Comparison of Dissolution Rates for High-Level Waste, Synroc Ceramic, and LLNL Ceramic for the 17-Ton Case (DTN: MO0107MWDMED03.007).

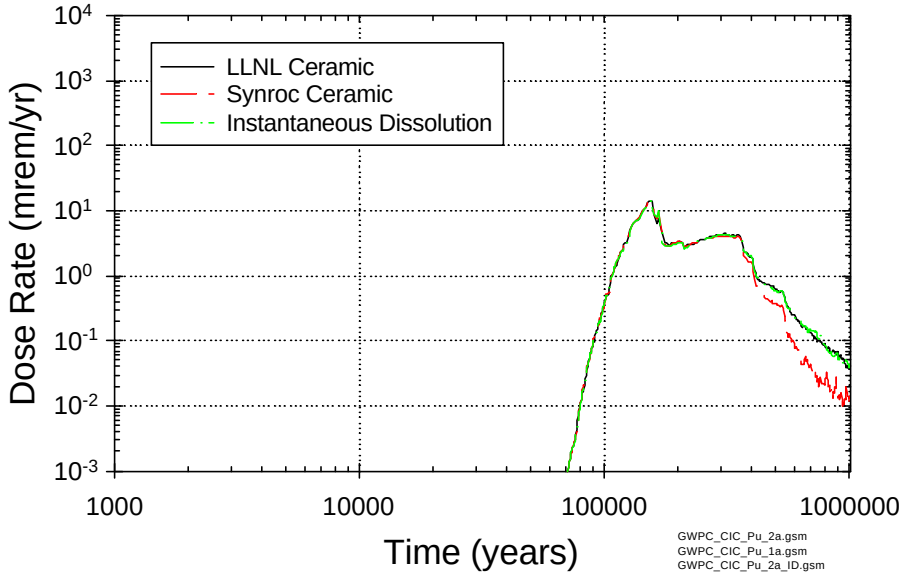


Figure 6.5-5. Comparison of Total Dose Rate from Ceramic, using the LLNL and Synroc Ceramic Model to the Total Dose Rate, using Instantaneous Dissolution of Ceramic (17-Ton Case) (DTN: MO0107MWDMED03.007).

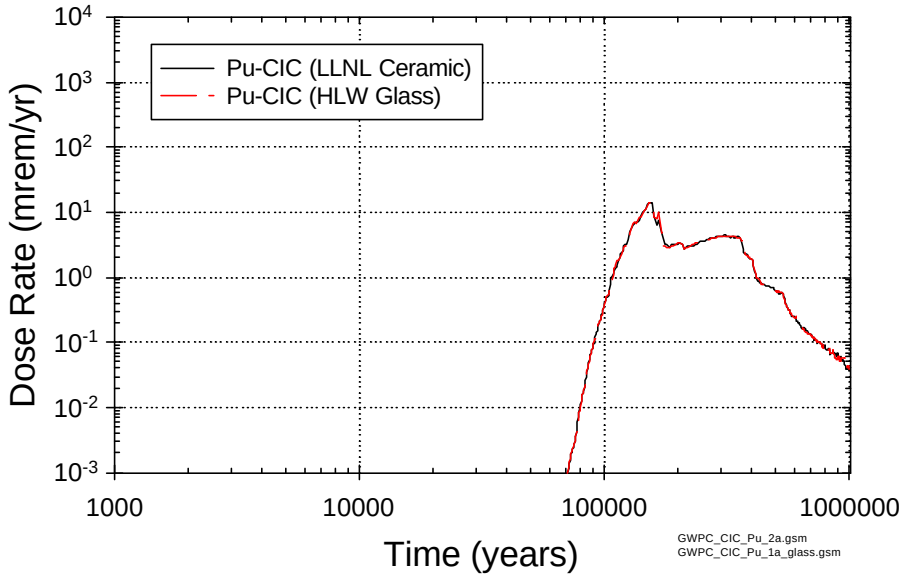
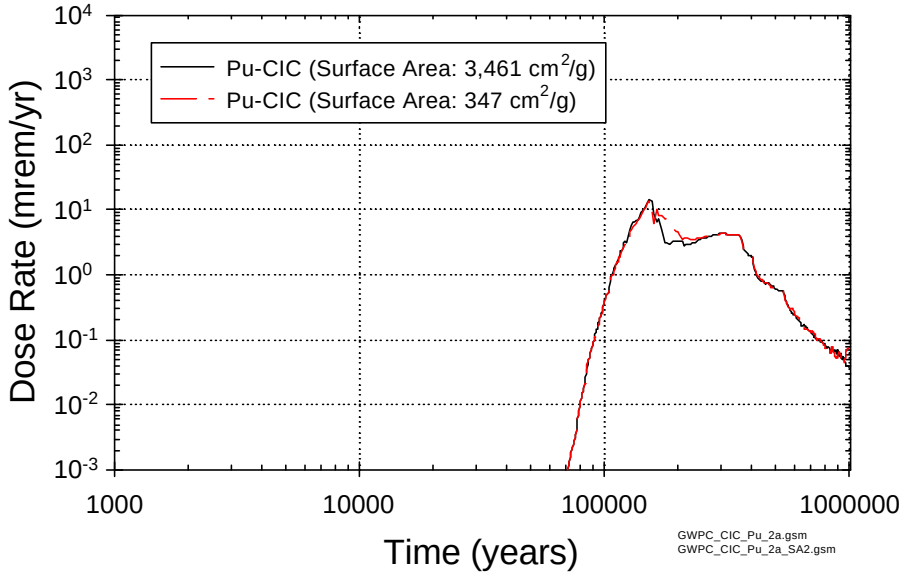


Figure 6.5-6. Comparison of Total Dose Rate from the 17-Ton Case using the LLNL Ceramic Compared to Using the High-Level Waste Glass Dissolution Model for the Ceramic (DTN: MO0107MWDMED03.007).



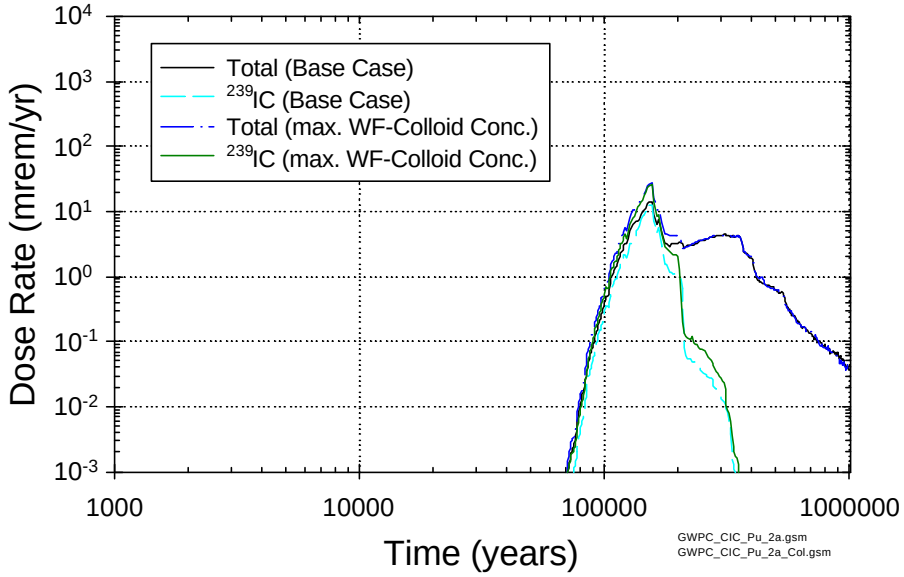


Figure 6.5-7. Sensitivity of Total Dose-Rate History at 20 Kilometers over 1,000,000 Years to Uncertainty in Surface Area of Ceramic for the 17-Ton Case (DTN: MO0107MWDMED03.007).Figure 6.5-8. Sensitivity of Dose-Rate History at 20 Kilometers over 1,000,000 Years to Uncertainty in Amount of Colloids Formed from Dissolution of the Ceramic in HLW for the 17-Ton Case (DTN: MO0107MWDMED03.007).

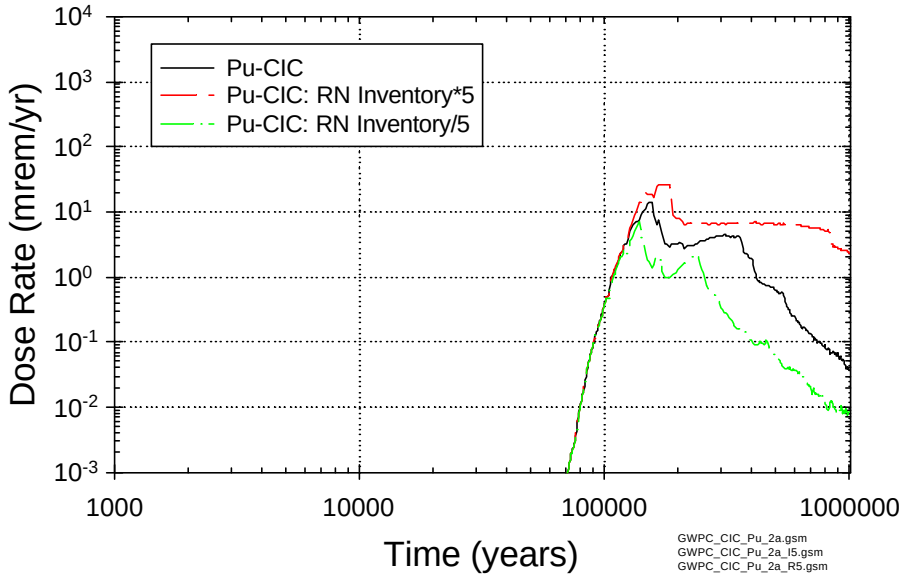


Figure 6.5-9. Sensitivity of Total Dose-Rate History at 20 Kilometers over 1,000,000 Years to Uncertainty in the Radionuclide Inventory of Plutonium Can-in-Canister Ceramic for the 17-Ton Case (DTN: MO0107MWDMED03.007).

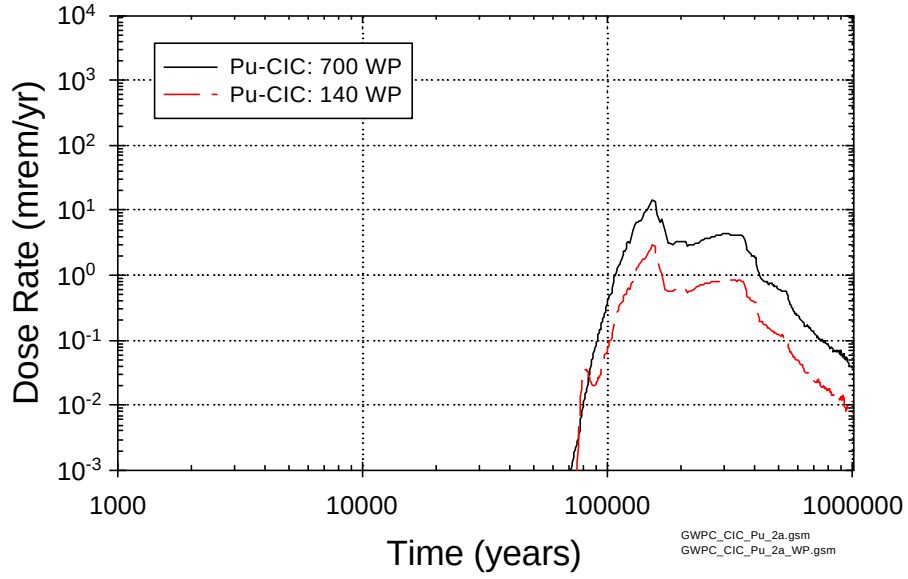


Figure 6.5-10. Sensitivity of Dose-Rate History at 20 Kilometers over 1,000,000 Years from Can-in-Canister Ceramic to a Factor of Five Decrease in the Number of Waste Packages for the 17-Ton Case (DTN: MO0107MWDMED03.007).

7. CONCLUSIONS

The TSPA-SR nominal-case model (CRWMS M&O 2000d) was used in this analysis, incorporating the radionuclide inventory and physical characteristics of the plutonium can-in-canister ceramic waste form into the nominal, 100-realization TSPA-SR model (DTN: MO0009MWDNM601.018) and into the nominal, median-value TSPA-SR model (DTN: MO0009MWDMED01.020). The nominal, median-value TSPA-SR model (DTN: MO0009MWDMED01.020) was superceded by DTN: MO0012MWDMED01.032 and the nominal, 100-realization TSPA-SR model (DTN: MO0009MWDNM601.018) was superceded by DTN: MO0012MWDNM601.033, MO0012MWDMIL01.034, which were not available at the onset of this analysis. The two models produce the same results, except for the ^{242}Pu dose rate, for which the BDCF was corrected in DTN: MO0012MWDMED01.032 and in DTN: MO0012MWDNM601.033. In this analysis, the BDCF of ^{242}Pu was corrected in the TSPA-SR model (MO0009MWDMED01.020, MO0009MWDNM601.018), such that it produces identical results when compared with the results using the corrected data set, DTN: MO0012MWDMED01.032 and DTN: MO0012MWDNM601.033 (see assumption 5.6).

Performance assessment and sensitivity analyses of the can-in-canister ceramic were conducted to evaluate the potential use of HLW as a surrogate for the immobilized plutonium waste form in the TSPA-SR model (DTN: MO0107MWDMED03.007, MO0107MWDMUL03.008). For the evaluation, the dose-rate histories for the can-in-canister ceramic were compared to the same number of HLW canisters and sensitivity analyses were conducted in areas where uncertainty exists to determine whether the inclusion of the plutonium can-in-canister ceramic waste form as HLW is appropriate. The following conclusions can be made:

- The dose from the immobilized plutonium waste form, can-in-canister ceramic is significantly higher (about a factor of five) than that from an equivalent number of canisters of high-level waste. This higher dose is primarily due to ^{239}Pu colloids from the ceramic and to a larger amount of ^{237}Np in the surplus plutonium than is contained in the high-level waste.

- The use of HLW as surrogate for immobilized plutonium in the TSPA-SR model is not strictly justified, because the current analysis indicated a noticeably higher dose rate than the equivalent number of HLW canisters. On the other hand, the total dose rate from the immobilized plutonium is more than one order of magnitude lower than the total dose rate from the TSPA-SR nominal case and does not significantly contribute to the total dose from the repository. The total inventory of immobilized surplus plutonium was incorporated into the radionuclide inventory for the HLW used in the TSPA-SR model and is accounted for in analyses of the entire repository (CRWMS M&O 2000c, Attachment I). Due to its relatively small contribution to total dose and the fact that the surplus plutonium is accounted for in its radionuclide inventory, HLW could be used as a surrogate for the immobilized plutonium for all practical purposes. On an individual canister basis, the peak dose rates from HLW are somewhat lower than from the equivalent amount of immobilized plutonium. The higher peak dose from immobilized plutonium is due to significantly higher dose rates from waste-

form colloids. The colloid model used in the TSPA-SR model will be subject to further refinement in the future.

- The peak dose from the 17-ton case of can-in-canister ceramic is approximately a factor of 15 below that of the nominal, median-value TSPA-SR case (DTN: MO0009MWDMED01.020).

- The dissolution rate using the LLNL ceramic model is more than one order of magnitude below that of high-level waste glass. The dissolution model used previously for ceramic (based on Synroc) has dose releases between that assuming the LLNL ceramic dissolution model and that assuming a high-level waste glass-dissolution model.

- Comparison of dose history using different dissolution models for the ceramic shows little difference. The models used in the comparison include LLNL ceramic, Synroc ceramic, high-level waste glass, and instantaneous dissolution. The reason that the dissolution model has little affect on dose history is that the dose is controlled by colloid release and by solubility controlled release from the waste packages.

- The uncertainty in the ceramic surface area has no significant affect on dose history.

- The uncertainty in the rate of formation of colloids has a significant effect on the dose rate history. This effect is due to colloids being a primary contributor to the total dose rate from can-in-canister ceramic.

- Uncertainty in radionuclide inventory in the surplus plutonium does not translate directly into uncertainty in total dose rate. For example, an increase of a factor of five in radionuclide inventory only doubles the peak dose rate while decreasing the radionuclide inventory by a factor of five decreases the peak total dose rate by a factor of seven. This result is because the peak dose from the can-in-canister ceramic is largely controlled by the amount of ^{239}Pu colloids that are released from the waste package.

- A change in the number of waste packages used for disposal of the can-in-canister ceramic translates directly into a change in dose rate history. For a factor of five decrease in the number of waste packages there is an approximate factor of five decrease in dose rate.

8. INPUTS AND REFERENCES

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8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

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8.3 SOURCE DATA, LISTED BY DATA-TRACKING NUMBER

8.3.1 Input Data

MO0009MWDMED01.020. Median Value Realization AMR Base Cases for the TSPA_SR Model. TSPA_SR, Rev. 00B, Cases SR00_037NE6, SR00_038NE6 and SR00_001IE5. Base Case; No Backfill; Median Value Realization. Submittal date: 09/26/2000. Submit to RPC URN-0727

MO0012MWDMED01.032. Median Value Realization AMR Base Cases contained in MDL-WIS-PA-000002 REV 00, TSPA_SR Model Cases SR00_073NE6, SR00_038NE6 and SR00_001IE5. Submittal date: 12/12/200. Submit to RPC URN-0792

MO0009MWDNM601.018. Million-Year Sensitivity Cases for the Nominal Scenario. TSPA_SR, Rev. 00B, Case SR00_023NM6 and Case SR00_024NM6. Submittal date: 09/20/2000. Submit to RPC URN-0667 (superceded by MO0012MWDNM601.033 and MO0012MWDMIL01.034)

MO0012MWDNM601.033. Nominal Million-Year Base Case contained in TDR-WIS-PA-000001 REV 00 ICN 01, Figure 4.1-19, Nominal Scenario, 1,000,000 Years, No Backfill, Constant Transition Climate after 2,000 Years. Submittal date: 12/12/2000. Submit to RPC URN-0830.

MO0012MWDMIL01.034. Million-year Sensitivity Cases for the Nominal Scenario, Secondary Phases and Log-term Climate Change, contained in TDR-WIS-PA-000001 REV 00 ICN 01, Nominal Scenario; No Backfill; 100 Realizations, 1,000,000 years. Submittal date: 12/12/00, Submit to RPC URN-0829.

8.3.2 Output Data

MO0107MWDMED03.007. Plutonium Can-in-Canister Ceramic Performance-Assessment Model: Million Year, Median-Value Simulations. Submittal date: 07/11/2001.

MO0107MWDMUL03.008. Plutonium Can-in-Canister Ceramic Performance-Assessment Model: Million Year, Multi-realization Simulations. Submittal date: 07/11/2001.

8.4 SOFTWARE

Golder Associates 2000. *Software Code: GoldSim.* 6.04.007. PC, Windows NT. 10344-6.04.007-00.

9. ATTACHMENTS

Attachments	Title
I	ACRONYMS AND ABBREVIATIONS
II	SPECIFIC ACTIVITIES FOR RADIONUCLIDES

ATTACHMENT I
ACRONYMS AND ABBREVIATIONS

ACRONYMS AND ABBREVIATIONS

ASHPLUME	Model used for volcanic ash plumes
BDCF	Biosphere Dose Conversion Factor
CIC	Can-in-Canister
CRWMS	Civilian Radioactive Waste Management System
CM	Configuration Management
DIRS	Document Input Reference System
DOE	U.S. Department of Energy
EBS	Engineered Barrier System
EQ3/6	Geochemical process model
GENII-S	Biosphere process model
GoldSim	Probabilistic model used for TSPA-SR
FEHM	Ground water flow and transport process model
HLW	High-Level Waste
ITOUGH2	Inverse process model for TOUGH2
LLNL	Lawrence Livermore National Laboratory
M&O	Management and Operating Contractor
MOX	Mixed Oxide
NUFT	Near field thermal hydrology process model
OCRWM	Office of Civilian Radioactive Waste Management
SR	Site Recommendation
SZ	Saturated Zone
SZ_CONVOLUTE	Convolution integral used for saturated zone transport
TBV	To Be Verified
TOUGH2	Unsaturated zone flow process model
UZ	Unsaturated Zone
TSPA-VA	Total Systems Performance Assessment Viability Assessment
WAPDEG	Waste Package Degradation “model”

ATTACHMENT II
SPECIFIC ACTIVITIES FOR RADIONUCLIDES

Table II-1. Specific Activity Values Used to Estimate the Radionuclide Inventory in Grams

Nuclide	Molecular Weight (g)	Half life (yr)[a]	Decay Rate (1/yr)[b]	Specific Activity (Ci/g)[c]
^{227}Ac	227	21.773	3.1835E-02	7.24E+01
^{241}Am	241	432	1.6045E-03	3.44E+00
^{243}Am	243	7.37E+03	9.4050E-05	2.00E-01
^{14}C	14	5715	1.2097E-04	4.47E+00
^{137}Cs	137	3.03E+01*	2.2877E-02	8.61E+01
^{129}I	129	1.60E+07	4.3322E-08	1.73E-04
^{237}Np	237	2.14E+06	3.2390E-07	7.06E-04
^{231}Pa	231	3.28E+04	2.1133E-05	4.72E-02
^{210}Pb	210	22.3	3.1083E-02	7.64E+01
^{238}Pu	238	87.74	7.9000E-03	1.71E+01
^{239}Pu	239	2.41E+04	2.8749E-05	6.21E-02
^{240}Pu	240	6.56E+03	1.0566E-04	2.27E-01
^{241}Pu	241	14.35 *	4.8303E-02	1.04E+02
^{242}Pu	242	3.76E+05	1.8435E-06	3.93E-03
^{226}Ra	226	1600	4.3322E-04	9.90E-01
^{228}Ra	228	5.76	1.2034E-01	2.73E+02
^{90}Sr	90	2.91E+01*	2.3819E-02	1.37E+02
^{99}Tc	99	2.13E+05	3.2542E-06	1.70E-02
^{229}Th	229	7.30E+03	9.4952E-05	2.14E-01
^{230}Th	230	7.54E+04	9.1929E-06	2.06E-02
^{232}Th	232	1.40E+10	4.9511E-11	1.10E-07
^{232}U	232	6.89E+01*	1.0060E-02	2.24E+01
^{233}U	233	1.59E+05	4.3539E-06	9.65E-03
^{234}U	234	2.45E+05	2.8292E-06	6.24E-03
^{235}U	235	7.04E+08	9.8458E-10	2.16E-06
^{236}U	236	2.34E+07	2.9596E-08	6.48E-05
^{238}U	238	4.47E+09	1.5514E-10	3.37E-07

[a] Lide 1995, pp. 11-28 to 11-132, except * from DOE 1987, Table 1B.1
[b] Decay Rate = ln(0.5)/-half life(yr)
[c] Specific Activity = -358000/(((ln(0.5)/Decay Rate))*Molecular Weight)