Title 40 CFR Part 191
Subparts B and C
Compliance Recertification
Application
for the
Waste Isolation Pilot Plant

Appendix TRU WASTE

United States Department of Energy
Waste Isolation Pilot Plant

Carlsbad Field Office
Carlsbad, New Mexico

Appendix TRU WASTE

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ACRONYMS AND ABBREVIATIONS

AK	***acceptable knowledge***
BRAGFLO	***BRine And Gas FLOw code***
CBFO	***Carlsbad Field Office***
CCA	***Compliance Certification Application***
CCDF	***complementary cumulative distribution function***
CFR	***Code of Federal Regulations***
CH-TRU	***contact-handled transuranic (waste)***
CRA	***Compliance Recertification Application***
DOE, USDOE	***United States Department of Energy***
EDTA	***ethylene diamine tetra-acetate***
EPA, USEPA	***United States Environmental Protection Agency***
FEP	***feature, event, and process***
FR	***Federal Register***
K_d	***equilibrium constant for distribution between solution and solid***
LANL	***Los Alamos National Laboratory***
LWA	***Land Withdrawal Act***
NDA	***nondestructive assay***
NUTS	***NUclide Transport System code***
PA	***performance assessment***
PAPDB	***Performance Assessment Parameter DataBase***
PAVT	***Performance Assessment Verification Test***
RH-TRU	***remote-handled transuranic (waste)***
SNL	***Sandia National Laboratories***
TRU	***transuranic***
TWBIR	***TRU Baseline Inventory Report***
TWBID	***TRU Waste Baseline Inventory Data Base***
WAC	***Waste Acceptance Criteria***
WAP	***Waste Analysis Plan***
WIPP	***Waste Isolation Pilot Plant***
WSPF	***Waste Stream Profile Form***
WUF	***waste unit factor***
WWIS	***WIPP Waste Information System***

TRU WASTE-1.0 INTRODUCTION

The transuranic (TRU) waste inventory is expected to be updated for each recertification application. The updated inventory will be evaluated to determine the effect of the waste and waste characteristics on the long-term performance of the repository. The proper implementation of the following five steps will ensure compliance with Title 40 Code of Federal Regulations (CFR) Section 194.24:

(1) Collect/scale inventory data. As shown in Figure TRU WASTE-1, the update cycle begins with the compilation of waste inventory data. This includes the waste that has been emplaced in the repository and the waste that is anticipated for emplacement over the operational life of the Waste Isolation Pilot Plant (WIPP). The anticipated waste inventory data consist of waste that has been stored at TRU waste sites and projected estimates of waste to be generated. For the purposes of performance assessment (PA), the projected waste is then scaled to the allowable capacity that remains in the repository after accounting for the stored and emplaced waste. The combined data (emplaced plus stored plus scaled projected) account for the total WIPP waste inventory. The results of conducting Step 1 of this process for CRA-2004 are reported in Appendix DATA, Attachment F.

(2) Perform waste characterization analysis. The inventory is analyzed for new waste components and/or changes to existing waste components that might affect the repository system. This is a screening step using sensitivity analyses. If a component is determined to impact repository performance it is placed on the list of "significant" waste components. Some waste components indirectly influence repository performance and are placed on the list of "negligible" waste components. All other components are screened out and are not included in the PA calculations. The results of conducting Step 2 of this process for the CRA-2004 are reported in Section TRU WASTE-2.0.

(3) Establish repository waste component limits. Waste components identified as "significant" are examined to determine if changes in the previously established limits are needed. If the inventory update shows substantial changes to the "significant" waste components, the change may necessitate a new or different limit. A new or different waste component limit will be established based upon the impact to the repository. The results of conducting Step 3 of this process for the CRA-2004 are reported in Section TRU WASTE-3.0.

(4) Characterize Waste. Waste characterization methods are developed or refined to quantify the significant waste components. Waste characterization programs implement other regulatory requirements, but for purposes of CRA-2004, this appendix will only address those elements relevant to long-term compliance. The results of conducting Step 4 of this process for the CRA-2004 are reported in Section TRU WASTE-4.0.

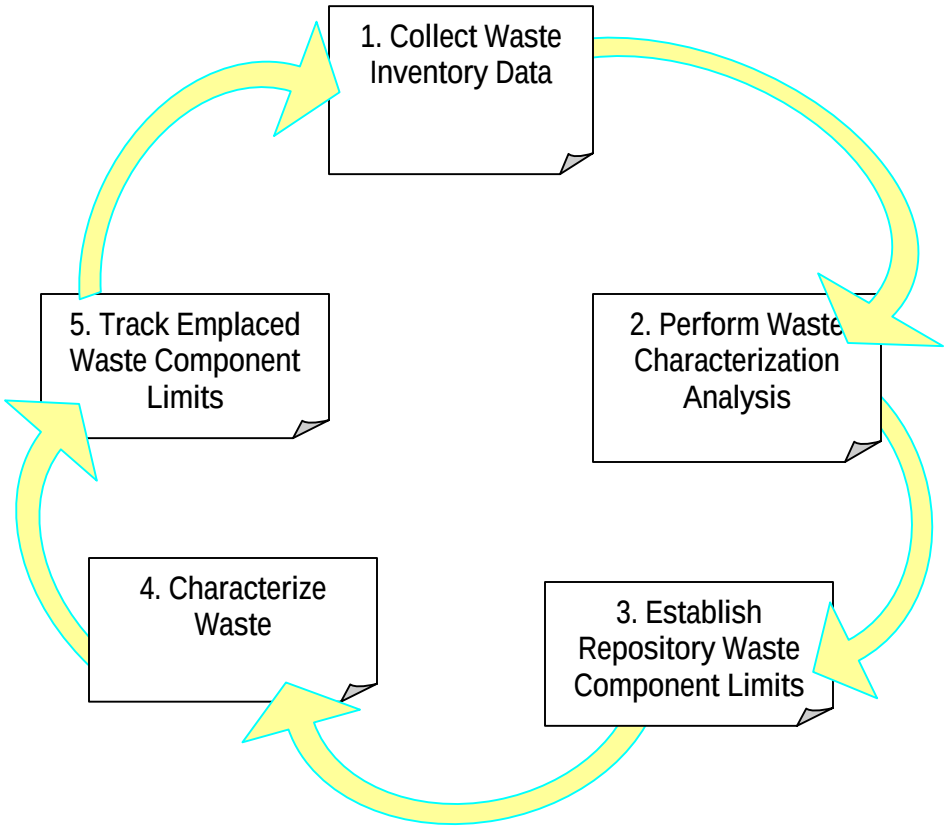

Figure TRU WASTE-1. Waste Characterization Cycle

***(5) Track emplaced waste component limits.** Waste component data are tracked and reported. The WIPP Waste Information System (WWIS) is used to capture the waste component data for waste emplaced in the repository. The WWIS is a tool used by the personnel at the TRU waste sites and at WIPP to control and track the waste emplaced in the repository. Once a year, the Department of Energy (DOE) provides the Environmental Protection Agency (EPA) with a report containing the values for each of the significant waste components. The emplaced waste data is compiled every five years (or as necessary) for updating the waste inventory, and the cycle repeats itself. The description of Step 5 of this process is reported in Section TRU WASTE-5.0.*

TRU WASTE-1.1 Purpose

This appendix provides information in accordance with 40 CFR § 194.24 for the waste characteristics and components important to the containment of waste in the disposal system over the regulatory performance period of 10,000 years. The characteristics and components of the waste are based on the current TRU waste descriptions and inventory presented in Appendix DATA, Attachment F. This appendix describes the assessment of the waste characteristics associated with the chemical, radiological, and physical composition of existing and projected TRU waste destined for disposal at the WIPP. It also identifies those waste

components that significantly influence waste characteristics, and establishes reasonable upper and lower waste component disposal limits. Based on the component limits and their associated uncertainties, a set of characterization techniques are established. Waste components are controlled, tracked, and inventoried upon emplacement in the repository. The cycle represented in Figure TRU WASTE-1 repeats as this characterization information provides key input data for future PAs to determine the impacts on the long-term containment of the disposal system.

Section TRU WASTE-2.0 addresses the requirements specified in 40 CFR § 194.24(b) to identify those waste components and their characteristics that can influence the containment of waste and that are included as inputs to the computer models used in PAs. This section identifies and assesses these parameters based on the DOE's current understanding of the disposal system behavior and the updated waste descriptions and inventory totals since submittal of the Compliance Certification Application (CCA). Section TRU WASTE2.3 also discusses the rationale for exclusion of specific waste characteristics or components expected not to influence releases from the disposal system.

Section TRU WASTE-3.0 shows the total limits for each identified significant component. This section addresses the requirement of 40 CFR § 194.24(c)(1) to establish limiting values for each component identified in Section TRU WASTE-2.0 as important to the performance of the repository system. The rationale for these limits is also discussed.

Section TRU WASTE-4.0 identifies and describes the methods used to quantify the limits for the waste components identified as potentially significant to the long-term performance of the disposal system. This section addresses the requirements of 40 CFR § 194.24(c)(2) and (3).

Section TRU WASTE-5.0 describes a system of controls (WWIS) that address the requirements of 40 CFR § 194.24(c)(4) and (5).

TRU WASTE-1.2 Scope

This appendix supercedes the information previously presented in the following appendices of the CCA:

- *Appendix WCA, Waste Characterization Analysis. The modeled long-term performance of the disposal system is evaluated based on current inventory information contained in Appendix DATA, Attachment F and on current disposal system behavior assumptions.*

- *Appendix WCL, Waste Component Limits. The limits for waste components determined important to the disposal system are established based on results of the CRA-2004 PA and the outcome of the current waste characterization analysis.*

- *Appendix WAP, Waste Analysis Plan. The characterization methods used to quantify the waste components determined important to the performance of the disposal system are established. Existing documentation that details the current characterization methods is referenced.*

TRU WASTE-2.0 WASTE CHARACTERIZATION ANALYSIS

Section TRU WASTE-2 summarizes relevant information on the emplaced and anticipated TRU waste inventories (detailed in Appendix DATA, Attachment F), identifies changes to PA and compliance assessment, and provides conclusions pertaining to whether the waste characteristics and waste components previously identified as significant to performance remain significant.

TRU WASTE-2.1 Introduction

TRU WASTE-2.1.1 Scope

Waste components are the elements that make up the waste (e.g., radionuclides, paper and other cellulosic materials, steel drums that contain the waste, solidified organic and inorganic sludges, etc.). These components have characteristics with the potential to impact disposal system performance. For example, paper is a component of the waste and a substrate for microbes in the repository. The ability of the paper to act as a substrate for microbial gas production is a characteristic of the paper. Microbes metabolizing paper can produce carbon dioxide, methane, and other gaseous metabolic products, which can increase the pressure in a waste panel and potentially impact the performance of the repository.

Sensitivity analysis is used to determine limiting values and associated uncertainties in the waste characteristics and components as required in 40 CFR § 194.24 (c). Sensitivity analyses and calculations related to features, events, and processes (FEPs) associated with the CCA, Performance Assessment Verification Test (PAVT) (DOE 1997), and Appendix PA have identified those waste characteristics and components that are included or excluded in the PA. Sections TRU WASTE-2.2 through 2.5 identify those waste components and waste characteristics and components that influence the containment of waste and thus are included as inputs to the computer codes used in PA.

TRU WASTE-2.1.2 Updated Estimate of TRU Waste Inventory

In the certification of WIPP, the EPA concluded that the estimates provided in Appendix BIR of the CCA represented the best information available at that time (Federal Register [FR] 63 27354, May 18, 1998). The EPA recognized that the WIPP waste inventory may change as the DOE characterizes the contents of containers of TRU waste prior to shipment to WIPP and as new wastes are generated in the future. The EPA also concluded that the WIPP waste inventory estimates provided in Appendix BIR of the CCA were sufficient for purposes of PA.

The inventory volume defined for WIPP emplacement to be used for PA calculations is the "disposal inventory." The WIPP Land Withdrawal Act (LWA), Pub. L. No. 104-201, 110 Stat. 2422 defines the total amount of TRU waste allowed in the WIPP as 175,564 m^3 (6,200,000 ft^3). The "Agreement for Consultation and Cooperation" limits the remote-handled (RH)-TRU waste inventory to 7,079 m^3 (250,000 ft^3) (State of New Mexico vs DOE 1981). By difference, the contact-handled (CH)-TRU waste inventory is limited to 168,485 m^3 (5,950,000 ft^3).

Since submittal of the CCA, DOE has updated its estimates of the TRU waste inventory destined for disposal in the WIPP. A complete description of that process and its results are presented in Appendix DATA, Attachment F. The following tables summarize information from Appendix DATA, Attachment F that pertains to waste characterization analysis. Table TRU WASTE-1 summarizes the current densities for the waste materials in the disposal inventory. Table TRU WASTE-2 summarizes the current activities for the radionuclides in the disposal inventory. Table TRU WASTE-3 summarizes the current mass of other important components in the disposal inventory.

Table TRU WASTE-1. Summary of Densities of Waste Materials

Waste Material	*Average Mass Density in CH-TRU Waste (kg/m^3)*	*Average Mass Density in RH-TRU Waste (kg/m^3)*
Fe-base Metal/Alloys	1.1×10^{2}	1.1×10^{2}
Al-base Metal/Alloys	1.4×10^{1}	2.5×10^{0}
Other Metal/Alloys	3.0×10^{1}	3.2×10^{1}
Other Inorganic Materials	4.2×10^{1}	3.5×10^{1}
Cellulosic Materials	5.8×10^{1}	4.5×10^{0}
Rubber Materials	1.4×10^{1}	3.1×10^{0}
Plastic Materials	4.2×10^{1}	4.9×10^{0}
Solidified Inorganic Material	7.7×10^{1}	3.9×10^{1}
Cement (Solidified)	2.9×10^{1}	8.7×10^{-1}
Vitrified Material	6.2×10^{0}	5.7×10^{-2}
Solidified Organic Material	1.6×10^{1}	4.0×10^{0}
Soils	1.9×10^{1}	2.6×10^{1}
Packaging Material, Steel	1.7×10^{2}	4.8×10^{2}
Packaging Material, Plastic	1.6×10^{1}	1.4×10^{0}
Packaging Material, Lead	1.4×10^{-2}	4.4×10^{2}

Source: Appendix DATA, Attachment F. Data reported in Appendix DATA, Attachment F includes information known by the TRU waste sites as of September 30, 2002.

Table TRU WASTE-2. Summary of Activities for Radionuclides in the Disposal Inventory (Decayed through 12/31/01)

Radionuclide	*CH-TRU Waste Concentration (Ci/m^3)*	*RH-TRU Waste Concentration (Ci/m^3)*	*CH-TRU Waste (Ci)*	*RH-TRU Waste (Ci)*
^{225}Ac	9.21×10^{-6}	5.20×10^{-6}	1.55×10^{0}	3.68×10^{-2}
^{227}Ac	3.00×10^{-6}	5.65×10^{-10}	5.06×10^{-1}	4.00×10^{-6}
^{228}Ac	2.84×10^{-5}	2.02×10^{-5}	4.79×10^{0}	1.43×10^{-1}
^{109m}Ag	7.49×10^{-10}	NR	1.26×10^{-4}	NR
^{110}Ag	2.61×10^{-16}	2.71×10^{-15}	4.40×10^{-11}	1.92×10^{-11}
^{110m}Ag	1.98×10^{-14}	2.06×10^{-13}	3.34×10^{-9}	1.46×10^{-9}

Table TRU WASTE-2. Summary of Activities for Radionuclides in the Disposal Inventory (Decayed through 12/31/01) — Continued

Radionuclide	CH-TRU Waste Concentration (Ci/m^3)	RH-TRU Waste Concentration (Ci/m^3)	CH-TRU Waste (Ci)	RH-TRU Waste (Ci)
^{241}Am	2.38×10^{0}	1.93×10^{0}	4.01×10^{5}	1.36×10^{4}
^{242}Am	2.79×10^{-7}	1.20×10^{-7}	4.70×10^{-2}	8.52×10^{-4}
^{242m}Am	2.83×10^{-7}	2.77×10^{-5}	4.78×10^{-2}	1.96×10^{-1}
^{243}Am	1.25×10^{-4}	1.01×10^{-4}	2.10×10^{1}	7.15×10^{-1}
^{245}Am	7.79×10^{-16}	NR	1.31×10^{-10}	NR
^{217}At	9.22×10^{-6}	5.21×10^{-6}	1.55×10^{0}	3.69×10^{-2}
^{137m}Ba	5.38×10^{-2}	4.74×10^{1}	9.06×10^{3}	3.36×10^{5}
^{210}Bi	1.53×10^{-5}	2.98×10^{-11}	2.58×10^{0}	2.11×10^{-7}
^{211}Bi	2.97×10^{-6}	5.58×10^{-10}	5.00×10^{-1}	3.95×10^{-6}
^{212}Bi	3.47×10^{-5}	3.82×10^{-4}	5.84×10^{0}	2.70×10^{0}
^{213}Bi	9.20×10^{-6}	5.20×10^{-6}	1.55×10^{0}	3.68×10^{-2}
^{214}Bi	3.73×10^{-5}	1.92×10^{-10}	6.29×10^{0}	1.36×10^{-6}
^{249}Bk	5.39×10^{-11}	NR	9.07×10^{-6}	NR
^{250}Bk	2.17×10^{-17}	NR	3.65×10^{-12}	NR
^{14}C	7.19×10^{-6}	2.90×10^{-4}	1.21×10^{0}	2.05×10^{0}
^{109}Cd	7.58×10^{-10}	NR	1.28×10^{-4}	NR
^{113m}Cd	NR	2.31×10^{-5}	NR	1.64×10^{-1}
^{141}Ce	NR	5.33×10^{-23}	NR	3.77×10^{-19}
^{144}Ce	2.11×10^{-9}	2.56×10^{-4}	3.56×10^{-4}	1.82×10^{0}
^{249}Cf	4.53×10^{-7}	1.18×10^{-7}	7.64×10^{-2}	8.37×10^{-4}
^{250}Cf	1.09×10^{-6}	2.11×10^{-6}	1.83×10^{-1}	1.50×10^{-2}
^{251}Cf	2.16×10^{-9}	2.25×10^{-8}	3.64×10^{-4}	1.59×10^{-4}
^{252}Cf	1.23×10^{-6}	2.50×10^{-6}	2.08×10^{-1}	1.77×10^{-2}
^{242}Cm	2.34×10^{-7}	1.01×10^{-7}	3.94×10^{-2}	7.15×10^{-4}
^{243}Cm	2.36×10^{-6}	6.92×10^{-5}	3.97×10^{-1}	4.90×10^{-1}
^{244}Cm	6.86×10^{-2}	3.82×10^{-2}	1.16×10^{4}	2.70×10^{2}
^{245}Cm	5.00×10^{-8}	1.50×10^{-6}	8.42×10^{-3}	1.06×10^{-2}
^{246}Cm	9.21×10^{-6}	9.53×10^{-5}	1.55×10^{0}	6.74×10^{-1}
^{247}Cm	1.65×10^{-15}	1.33×10^{-3}	2.77×10^{-10}	9.44×10^{0}
^{248}Cm	5.43×10^{-7}	2.58×10^{-7}	9.14×10^{-2}	1.83×10^{-3}
^{250}Cm	3.94×10^{-16}	NR	6.64×10^{-11}	NR
^{60}Co	5.85×10^{-6}	2.38×10^{-1}	9.85×10^{-1}	1.68×10^{3}
^{134}Cs	1.22×10^{-7}	4.75×10^{-3}	2.05×10^{-2}	3.36×10^{1}
^{135}Cs	NR	9.75×10^{-9}	NR	6.90×10^{-5}
^{137}Cs	5.73×10^{-2}	5.15×10^{1}	9.65×10^{3}	3.65×10^{5}
^{152}Eu	1.16×10^{-5}	9.82×10^{-2}	1.95×10^{0}	6.95×10^{2}
^{154}Eu	9.82×10^{-6}	5.98×10^{-2}	1.65×10^{0}	4.23×10^{2}
^{155}Eu	3.99×10^{-7}	2.61×10^{-3}	6.73×10^{-2}	1.85×10^{1}
^{55}Fe	NR	5.93×10^{-6}	NR	4.20×10^{-2}

Table TRU WASTE-2. Summary of Activities for Radionuclides in the Disposal Inventory (Decayed through 12/31/01) — Continued

Radionuclide	CH-TRU Waste Concentration (Ci/m^3)	RH-TRU Waste Concentration (Ci/m^3)	CH-TRU Waste (Ci)	RH-TRU Waste (Ci)
^{221}Fr	9.20×10^{-6}	5.20×10^{-6}	1.55×10^{0}	3.68×10^{-2}
^{223}Fr	4.10×10^{-8}	7.71×10^{-12}	6.91×10^{-3}	5.45×10^{-8}
^{152}Gd	2.61×10^{-19}	2.76×10^{-15}	4.40×10^{-14}	1.95×10^{-11}
^{3}H	1.29×10^{-3}	1.62×10^{-4}	2.17×10^{2}	1.15×10^{0}
^{129}I	3.04×10^{-9}	1.16×10^{-5}	5.12×10^{-4}	8.20×10^{-2}
^{85}Kr	2.74×10^{-6}	1.59×10^{-5}	4.62×10^{-1}	1.13×10^{-1}
^{54}Mn	NR	2.58×10^{-4}	NR	1.82×10^{0}
^{22}Na	2.32×10^{-12}	4.17×10^{-5}	3.91×10^{-7}	2.95×10^{-1}
^{93m}Nb	NR	3.88×10^{-8}	NR	2.75×10^{-4}
^{95}Nb	NR	1.06×10^{-17}	NR	7.53×10^{-14}
^{95m}Nb	NR	3.56×10^{-20}	NR	2.52×10^{-16}
^{59}Ni	4.54×10^{-7}	3.25×10^{-3}	7.64×10^{-2}	2.30×10^{1}
^{63}Ni	2.21×10^{-5}	1.58×10^{-1}	3.72×10^{0}	1.12×10^{3}
^{237}Np	2.85×10^{-5}	9.41×10^{-5}	4.80×10^{0}	6.66×10^{-1}
^{238}Np	1.40×10^{-9}	6.05×10^{-10}	2.36×10^{-4}	4.28×10^{-6}
^{239}Np	1.23×10^{-4}	8.87×10^{-6}	2.08×10^{1}	6.28×10^{-2}
^{240m}Np	7.75×10^{-12}	1.57×10^{-7}	1.31×10^{-6}	1.11×10^{-3}
^{231}Pa	7.19×10^{-6}	2.53×10^{-9}	1.21×10^{0}	1.79×10^{-5}
^{233}Pa	2.82×10^{-5}	3.26×10^{-7}	4.75×10^{0}	2.31×10^{-3}
^{234}Pa	5.49×10^{-8}	3.99×10^{-7}	9.25×10^{-3}	2.82×10^{-3}
$^{234}Pa^{m}$	4.22×10^{-5}	3.07×10^{-4}	7.11×10^{0}	2.17×10^{0}
^{209}Pb	9.21×10^{-6}	5.20×10^{-6}	1.55×10^{0}	3.68×10^{-2}
^{210}Pb	1.55×10^{-5}	3.02×10^{-11}	2.61×10^{0}	2.13×10^{-7}
^{211}Pb	2.97×10^{-6}	5.59×10^{-10}	5.01×10^{-1}	3.95×10^{-6}
^{212}Pb	3.46×10^{-5}	3.80×10^{-4}	5.82×10^{0}	2.69×10^{0}
^{214}Pb	3.74×10^{-5}	1.92×10^{-10}	6.30×10^{0}	1.36×10^{-6}
^{107}Pd	NR	4.07×10^{-10}	NR	2.88×10^{-6}
^{147}Pm	1.08×10^{-5}	4.96×10^{-2}	1.82×10^{0}	3.51×10^{2}
^{210}Po	1.55×10^{-5}	3.01×10^{-11}	2.60×10^{0}	2.13×10^{-7}
^{211}Po	9.05×10^{-9}	1.70×10^{-12}	1.53×10^{-3}	1.20×10^{-8}
^{212}Po	2.21×10^{-5}	2.43×10^{-4}	3.72×10^{0}	1.72×10^{0}
^{213}Po	9.01×10^{-6}	5.09×10^{-6}	1.52×10^{0}	3.60×10^{-2}
^{214}Po	3.74×10^{-5}	1.92×10^{-10}	6.30×10^{0}	1.36×10^{-6}
^{215}Po	2.97×10^{-6}	5.59×10^{-10}	5.00×10^{-1}	3.95×10^{-6}
^{216}Po	3.45×10^{-5}	3.80×10^{-4}	5.82×10^{0}	2.69×10^{0}
^{218}Po	3.68×10^{-5}	1.89×10^{-10}	6.19×10^{0}	1.34×10^{-6}
^{144}Pr	2.07×10^{-9}	2.51×10^{-4}	3.49×10^{-4}	1.78×10^{0}
^{236}Pu	2.60×10^{-9}	NR	4.38×10^{-4}	NR
^{238}Pu	9.55×10^{0}	5.10×10^{-1}	1.61×10^{6}	3.61×10^{3}

Table TRU WASTE-2. Summary of Activities for Radionuclides in the Disposal Inventory (Decayed through 12/31/01) — Continued

Radionuclide	CH-TRU Waste Concentration (Ci/m^3)	RH-TRU Waste Concentration (Ci/m^3)	CH-TRU Waste (Ci)	RH-TRU Waste (Ci)
^{239}Pu	3.92×10^{0}	7.59×10^{-1}	6.60×10^{5}	5.38×10^{3}
^{240}Pu	6.35×10^{-1}	2.37×10^{-1}	1.07×10^{5}	1.68×10^{3}
^{241}Pu	1.43×10^{1}	1.58×10^{1}	2.40×10^{6}	1.12×10^{5}
^{242}Pu	1.58×10^{-4}	6.69×10^{-5}	2.67×10^{1}	4.74×10^{-1}
^{243}Pu	1.63×10^{-15}	1.32×10^{-3}	2.74×10^{-10}	9.33×10^{0}
^{244}Pu	7.68×10^{-12}	1.56×10^{-7}	1.29×10^{-6}	1.10×10^{-3}
^{223}Ra	3.00×10^{-6}	5.64×10^{-10}	5.06×10^{-1}	3.99×10^{-6}
^{224}Ra	3.45×10^{-5}	3.80×10^{-4}	5.81×10^{0}	2.69×10^{0}
^{225}Ra	9.22×10^{-6}	5.21×10^{-6}	1.55×10^{0}	3.69×10^{-2}
^{226}Ra	3.78×10^{-5}	1.95×10^{-10}	6.37×10^{0}	1.38×10^{-6}
^{228}Ra	3.36×10^{-5}	2.38×10^{-5}	5.66×10^{0}	1.69×10^{-1}
^{106}Rh	9.36×10^{-10}	9.59×10^{-6}	1.58×10^{-4}	6.79×10^{-2}
^{219}Rn	2.97×10^{-6}	5.58×10^{-10}	5.00×10^{-1}	3.95×10^{-6}
^{220}Rn	3.45×10^{-5}	3.80×10^{-4}	5.82×10^{0}	2.69×10^{0}
^{222}Rn	3.74×10^{-5}	1.93×10^{-10}	6.31×10^{0}	1.36×10^{-6}
^{106}Ru	9.46×10^{-10}	9.60×10^{-6}	1.59×10^{-4}	6.79×10^{-2}
^{125}Sb	2.99×10^{-8}	6.18×10^{-4}	5.04×10^{-3}	4.38×10^{0}
^{126}Sb	NR	5.89×10^{-9}	NR	4.17×10^{-5}
^{126m}Sb	NR	4.21×10^{-8}	NR	2.98×10^{-4}
^{79}Se	7.84×10^{-10}	6.29×10^{-6}	1.32×10^{-4}	4.46×10^{-2}
^{147}Sm	2.83×10^{-15}	9.69×10^{-13}	4.78×10^{-10}	6.86×10^{-9}
^{151}Sm	3.37×10^{-4}	8.20×10^{-2}	5.68×10^{1}	5.80×10^{2}
^{121m}Sn	NR	7.28×10^{-8}	NR	5.15×10^{-4}
^{126}Sn	NR	4.21×10^{-8}	NR	2.98×10^{-4}
^{90}Sr	3.41×10^{-1}	3.48×10^{1}	5.75×10^{4}	2.46×10^{5}
^{99}Tc	9.93×10^{-4}	2.25×10^{-2}	1.67×10^{2}	1.59×10^{2}
^{123}Te	4.02×10^{-10}	NR	6.78×10^{-5}	NR
^{123m}Te	2.96×10^{-24}	NR	4.98×10^{-19}	NR
^{125m}Te	7.24×10^{-9}	1.50×10^{-4}	1.22×10^{-3}	1.06×10^{0}
^{227}Th	2.92×10^{-6}	5.50×10^{-10}	4.93×10^{-1}	3.89×10^{-6}
^{228}Th	3.49×10^{-5}	3.85×10^{-4}	5.89×10^{0}	2.72×10^{0}
^{229}Th	9.23×10^{-6}	5.21×10^{-6}	1.55×10^{0}	3.69×10^{-2}
^{230}Th	6.02×10^{-7}	5.31×10^{-8}	1.01×10^{-1}	3.76×10^{-4}
^{231}Th	2.10×10^{-6}	7.38×10^{-6}	3.53×10^{-1}	5.23×10^{-2}
^{232}Th	3.92×10^{-5}	3.08×10^{-5}	6.61×10^{0}	2.18×10^{-1}
^{234}Th	4.23×10^{-5}	3.07×10^{-4}	7.12×10^{0}	2.17×10^{0}
^{207}Tl	2.95×10^{-6}	5.55×10^{-10}	4.98×10^{-1}	3.93×10^{-6}
^{208}Tl	1.24×10^{-5}	1.37×10^{-4}	2.09×10^{0}	9.71×10^{-1}
^{209}Tl	2.03×10^{-7}	1.14×10^{-7}	3.41×10^{-2}	8.10×10^{-4}

Table TRU WASTE-2. Summary of Activities for Radionuclides in the Disposal Inventory (Decayed through 12/31/01) — Continued

Radionuclide	CH-TRU Waste Concentration (Ci/m^3)	RH-TRU Waste Concentration (Ci/m^3)	CH-TRU Waste (Ci)	RH-TRU Waste (Ci)
^{232}U	9.76×10^{-6}	3.57×10^{-4}	1.64×10^{0}	2.53×10^{0}
^{233}U	7.34×10^{-3}	4.82×10^{-3}	1.24×10^{3}	3.41×10^{1}
^{234}U	9.95×10^{-4}	3.07×10^{-3}	1.68×10^{2}	2.17×10^{1}
^{235}U	7.84×10^{-6}	1.33×10^{-4}	1.32×10^{0}	9.42×10^{-1}
^{236}U	7.70×10^{-7}	2.01×10^{-4}	1.30×10^{-1}	1.42×10^{0}
^{237}U	1.28×10^{-4}	2.48×10^{-6}	2.15×10^{1}	1.75×10^{-2}
^{238}U	1.45×10^{-4}	1.83×10^{-2}	2.44×10^{1}	1.30×10^{2}
^{240}U	7.60×10^{-12}	1.54×10^{-7}	1.28×10^{-6}	1.09×10^{-3}
^{90}Y	3.41×10^{-1}	3.43×10^{1}	5.74×10^{4}	2.43×10^{5}
^{91}Y	NR	1.15×10^{-16}	NR	8.11×10^{-13}
^{65}Zn	1.38×10^{-15}	NR	2.32×10^{-10}	NR
^{93}Zr	6.68×10^{-9}	4.79×10^{-5}	1.13×10^{-3}	3.39×10^{-1}
^{95}Zr	NR	4.84×10^{-18}	NR	3.43×10^{-14}
Total:	3.16×10^{1}	1.88×10^{2}	5.33×10^{6}	1.33×10^{6}

Note: NR = Not Reportable
Source: Appendix DATA, Attachment F. Data reported in Appendix DATA, Attachment F includes information known by the TRU waste sites as of September 30, 2002.

1

Table TRU WASTE-3. Summary of Masses for Other Important Components

Component	Mass Contained in the Disposal Inventory (kg)
Acetic Acid	1.42×10^{2}
Sodium Acetate	8.51×10^{3}
Citric Acid	1.19×10^{3}
Sodium Citrate	4.00×10^{2}
Oxalic Acid	1.38×10^{4}
Sodium Oxalate	3.39×10^{4}
Sodium EDTA	2.56×10^{1}
Nitrate	2.51×10^{6}
Sulfate	4.21×10^{5}
Phosphate	1.05×10^{5}
Cement	1.2×10^{7}

Source: Appendix DATA, Attachment F. Data reported in Appendix DATA, Attachment F includes information known by the TRU waste sites as of September 30, 2002. Masses reported here are based on the disposal volume as defined in Appendix TRU WASTE, Section 2.1.2.

2

TRU WASTE-2.2 Summary of Waste Components and Characteristics

TRU WASTE-2.2.1 Waste Characterization Analysis

Tables TRU WASTE-4, TRU WASTE-5, and TRU WASTE-6 summarize the waste characteristics and waste components considered in this section. These tables provide:

- *a list of the waste characteristics and components expected to have significant effect on disposal system performance (included in PA),*
- *a list of the waste characteristics and components expected to have negligible effect on disposal system performance, and*
- *a list of waste characteristics and components that were considered and excluded.*

Table TRU WASTE-4 lists the waste characteristics and components that are included in PA because they would be expected to have a significant impact on repository performance. The waste characteristics and components listed in Table TRU WASTE-4 are identical to those listed in Table WCA-2 of the CCA. None of the inventory changes described in Appendix DATA, Attachment F led to an alternate conclusion regarding the relative importance of individual waste characteristics and components for PA.

Table TRU WASTE-4. Waste Characteristics and Components Used in Performance Assessment: Characteristics Expected to Have a Significant Effect on Disposal System Performance

Characteristic	*Component*	*Effect on Performance*	*Section of Appendix TRU WASTE*
Radioactivity of Each Isotope	*Radionuclides*	*Used in Calculating Normalized Releases*	*2.3.1, 2.3.2*
TRU Radioactivity at Closure	*α-Emitting TRU Radionuclides, half-life > 20 Years*	*Determines Waste Unit Factor (WUF)*	*2.3.1*
Solubility	*Radionuclides*	*Actinide Mobility*	*2.4.1*
Colloid Formation	*Radionuclides, Soils, Cellulosic, Plastic, and Rubber (CPR) Materials*	*Actinide Mobility*	*2.4.2*
Redox State	*Radionuclides*	*Actinide Mobility*	*2.4.1*
Redox Potential	*Ferrous Metals*	*Actinide Oxidation State; Actinide Mobility*	*2.4.1.1*
Gas (H_2) Generation	*Ferrous Metals*	*Increase in H_2 Pressure*	*2.4.1.2, 2.5.1*
Microbial Substrate: CH_4 Generation	*Cellulosic Materials*	*Increase in Gas Pressure*	*2.4.1.2, 2.5.1*
Microbial Substrate: CH_4 Generation	*Plastic, Rubber Materials*	*Increase in Gas Pressure*	*2.4.1.2, 2.5.1*
Particle Diameter	*Solid Waste Components*	*Spalling Release*	*2.5.2*

Table TRU WASTE-4. Waste Characteristics and Components Used in Performance Assessment: Characteristics Expected to Have a Significant Effect on Disposal System Performance — Continued

Characteristic	Component	Effect on Performance	Section of Appendix TRU WASTE
Microbial Nutrients: CH_4 Generation	Sulfates	Increase in Gas Pressure	2.5.1
Microbial Nutrients: CH_4 Generation	Nitrates	Increase in Gas Pressure	2.5.1
Compressibility and Shear Strength	Solid Waste Components	Effect on Creep Closure, Cuttings, Caving, Spallings	2.5.2

Table TRU WASTE-5 lists the waste characteristics and components that are included in PA, but would be expected to have a negligible impact on performance. For example, the impact of microbially generated CO_2 on performance is insignificant because the CO_2 will react with the MgO, forming Mg carbonate minerals that greatly reduce the impact of CO_2 on pH. The waste characteristics and components listed in Table TRU WASTE-5 are identical to those listed in Table WCA-3 of the CCA. None of the inventory changes described in Appendix DATA, Attachment F led to an alternate conclusion regarding the relative importance of individual waste characteristics and components for PA. Actual sensitivities of the analysis to waste characteristics and components are described in Appendix PA. The relationships between components, characteristics, and PA codes is illustrated in Figure TRU WASTE-2.

Table TRU WASTE-5. Waste Characteristics and Components Used in Performance Assessment: Characteristics Expected to Have a Negligible Effect on Disposal System Performance

Characteristic	Component	Effect on Performance	Section of Appendix TRU WASTE
Permeability	Solid Waste Components	Negligible Effect on Brine Movement, Gas Storage	2.5.2
Porosity	Solid Waste Components	Negligible Effect on Brine Movement	2.5.2
Microbial Nutrients, CO_2 Generation	Sulfates[1]	Negligible: MgO Reacts with CO_2	2.4.1.2
Microbial Nutrients, CO_2 Generation	Nitrates[1]	Negligible: MgO Reacts with CO_2,	2.4.1.2, 2.5.1
Microbial Substrate: CO_2 Generation	Cellulosic Materials	Negligible: MgO Reacts with CO_2	2.4.1.2, 2.5.1
Microbial Substrate: CO_2 Generation	Plastic Materials, Rubber Materials	Negligible: MgO Reacts with CO_2	2.4.1.2, 2.5.1
Gas Generation	Water in the Waste	Enhances Initial Gas Generation	2.5.1

[1] *These components are significant to gas generation and are therefore also listed in Table TRU WASTE-4.*

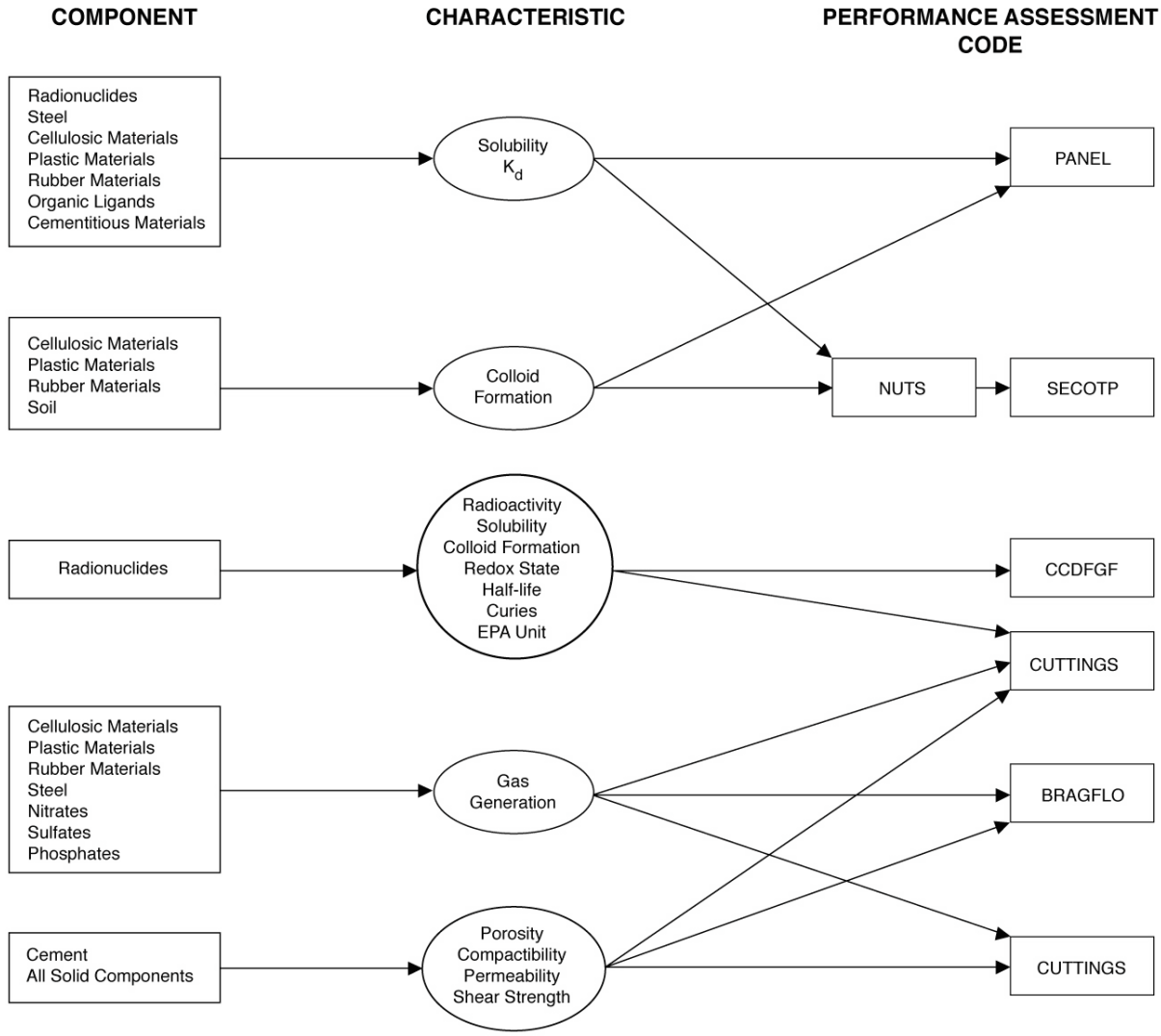

Figure TRU WASTE-2. Waste Components, the Associated Waste Characteristics, and a Performance Assessment Code Related to Each Characteristic

Table TRU WASTE-6 lists the waste characteristics and components that are excluded from PA. Some of these excluded characteristics, however, can indirectly influence performance. For example, the ability of nonferrous metals to bind organic ligands prevents those ligands from increasing actinide solubility, which is considered in PA analyses. The waste characteristics and components listed in Table TRU WASTE-6 are identical to those listed in Appendix WCA, Table WCA-4, in the CCA. None of the inventory changes described in Appendix DATA, Attachment F led to an alternate conclusion regarding the relative importance of individual waste characteristics and components for PA.

Table TRU WASTE-6. Waste Characteristics and Components Not Used in Performance Assessment

Characteristic	Component	Effect on Performance
Cellulosic Materials Radiolysis	Radionuclides	Negligible Effect On Total CO_2
Explosivity	Other Organic Compounds	None
Brine Radiolysis	Radionuclides	Negligible Effect On Actinide Valence
Galvanic Action	Nonferrous Metals	Negligible
Complexation With Actinides[1]	Soil And Humic Material[1]	Actinide Mobility
Buffering Action[1]	Cement[1]	Negligible: Reacts With CO_2 And $MgCl_2$
Heat Of Solution	Cement	Negligible
Ca^{2+} Binding To Organic Ligands	Cement	Negligible Compared To Other Metals
Binding To Organic Ligands[1]	Ferrous Metals[1]	Can Reduce Actinide Mobility
Buffering Action[1]	Ferrous Metals[1]	Actinide Mobility
Galvanic Action	Ferrous Metals	Negligible
Binding To Organic Ligands[1]	Ferrous Alloy Components[1]	Can Reduce Actinide Mobility
Redox Reactions	Nonferrous Metals	Negligible Compared To Iron
Binding To Organic Ligands[1]	Nonferrous Metals[1]	Can Reduce Actinide Mobility
Complexation With Actinides	Organic Ligands	Negligible
Gas Generation	Al And Other Nonferrous Metals	Negligible Relative To Steels
Microbial Nutrients, CO_2 Generation	Phosphates	Negligible Because MgO Reacts With CO_2
Microbial Nutrients: CH_4 Generation	Phosphates[1]	Negligible
Heat Generation	RH-TRU	Negligible
Electrochemical Processes	Sulfate, Nitrate, Phosphate	Negligible

[1] *Waste characteristics and components that influence performance indirectly by influencing components and characteristics listed in Table TRU WASTE-5.*

Each waste characteristic shown in Tables TRU WASTE-4 and TRU WASTE-5 is reflected in one or more parameters that are used in PA. The PA parameters are compiled in the Performance Assessment Parameter Database (PAPDB) (presented in Appendix PA, Attachment PAR).

TRU WASTE-2.2.2 Relationship Between Inventory Data and Performance Assessment

Appendix DATA, Attachment F provides both WIPP-level data and waste stream-level data on the radionuclide inventory for the WIPP. Performance assessment models generally use the WIPP-level data, normalized to a base year (2001) and scaled up to the full WIPP capacity. The one exception to this approach is the cuttings/caving model, which uses scaled waste stream level data to capture potential variations in the CH-TRU waste.

The relationship between Appendix DATA, Attachment F data and PA is shown in Figure TRU WASTE-3. As Figure TRU WASTE-3 shows, the waste stream level data are used only in modeling direct release by cuttings and cavings (see Appendix PA for additional information). This direct release scenario includes the probability of penetrating each of the 693 CH-TRU waste streams or a single RH-TRU waste stream that represents all of the 86 RH-TRU waste streams, as discussed in Section 6.4.12.4 and in Appendix PA.

This approach for cuttings and cavings releases represents the potential variations in the CH-TRU waste. This approach is necessary because the size scale for cuttings and cavings is on the order of the drill bit diameter, which is less than the diameter of a 55-gallon drum (8- to 12 in versus 24 in). A cuttings and cavings intrusion would, therefore, extract waste from three specific drums (assuming that drums are stacked three high in the disposal rooms), rather than sampling from a larger volume of waste.

In contrast, scenarios in which radionuclides would be released in brine, either directly to the surface or through the Culebra reservoir, assume that the mobility of radionuclides in brine results in an essentially homogeneous mixture of radionuclides. Brine flow would contact a much larger portion of the waste than the direct release of cuttings and cavings. For brine-related release pathways, the total radionuclide inventory is more applicable than the inventory of a particular waste stream. Performance assessment, therefore, uses the average (WIPP-level) inventory from all TRU waste sites, as shown in Figure TRU WASTE-3. In a similar fashion, spall releases use WIPP-level data because this mechanism is assumed to release waste from a volume larger than several drums, averaging out variations in waste streams.

Decay of radionuclides in the TRU waste will produce some radioactive daughter products that must be accounted for in the waste inventory. Therefore, to provide a current inventory estimate for the CRA-2004, all radionuclide values reported in Appendix DATA, Attachment F are decayed to the end of 2001. The PA calculations begin at the time of closure of the WIPP facility. Therefore, PA calculations further decay the inventory to the end of year 2033.

TRU WASTE-2.3 Components That Affect Performance: Curie Content

The radioactivity of a particular radionuclide, often called the activity, is significant to two different aspects of compliance: (1) inclusion in the waste unit factor, which is the normalization factor for the release limits given in Table TRU WASTE-7, and (2) inclusion in the source term for the compliance demonstration. The waste unit factor is based only on TRU wastes that are alpha (α)-emitters with a half-life greater than 20 years, while the complementary cumulative distribution function (CCDF) is based on the full inventory of all radionuclides in the repository. This section, therefore, includes two subsections: TRU WASTE-2.3.1, components relevant to inclusion in the waste unit factor; and TRU WASTE-2.3.2, components relevant to inclusion in CCDFs for each applicable scenario.

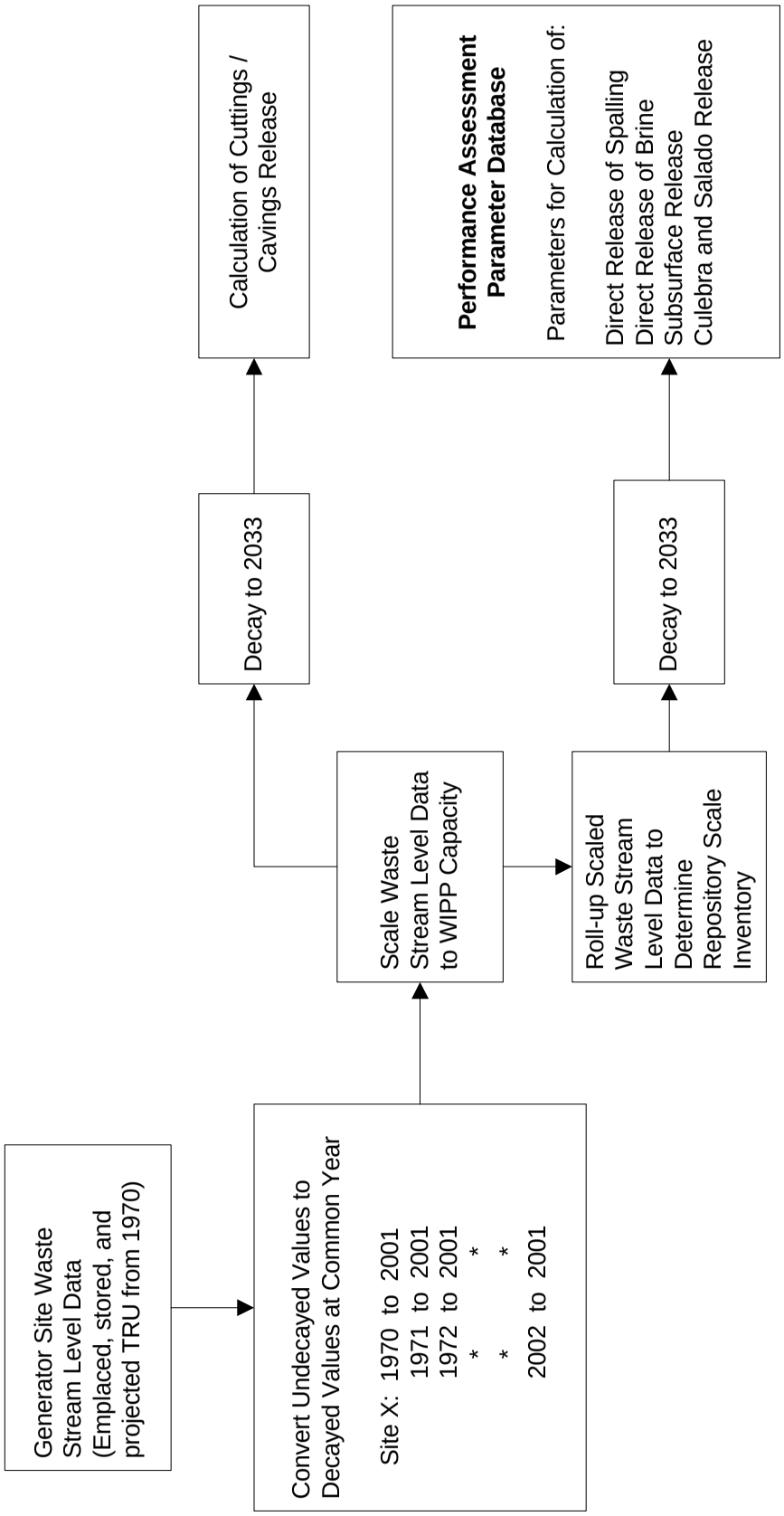

Figure TRU WASTE-3. Flow Chart for Inventory Input into Performance Assessment Waste Components, the Associated Waste Characteristics, and a Performance Assessment Code Related to Each Characteristic

Table TRU WASTE-7. EPA Release Limits and Normalized Release Limits for Radionuclides

Radionuclide	Release Limit per Million Ci of TRU Radionuclides[1] (Ci)	Release Limit for the WIPP Normalized by Total from Table TRU WASTE-8 (Ci)
Americium: ^{241}Am or ^{243}Am	100	248
Carbon: ^{14}C	100	248
Cesium: ^{135}Cs, or ^{137}Cm	1,000	2,480
Iodine: ^{129}I	100	248
Neptunium: ^{237}Np	100	248
Plutonium: ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu	100	248
Radium: ^{226}Ra	100	248
Strontium: ^{90}Sr	1,000	2,480
Technetium: ^{99}Tc	10,000	24,800
Thorium: ^{230}Th or ^{232}Th	10	24.8
Tin: ^{126}Sn	1,000	2,480
Uranium: ^{233}U, ^{234}U, ^{235}U, ^{236}U, or ^{238}U	100	248
Any other α-emitting radionuclide with a half-life greater than 20 years	100	248
Any other radionuclide with a half-life greater than 20 years that does not emit α particles	1,000	2,480

[1] In Appendix A of 40 CFR Part 191, this column is in terms of metric tons heavy metal, and the equivalence to Ci of TRU is presented in Footnote e to the table.

TRU WASTE-2.3.1 Radioactivity Included in the Waste Unit Factor

The WUF is the number of millions of curies (Ci) of α-emitting TRU radionuclides with half-lives longer than 20 years (40 CFR Part 191, Appendix A), based on the TRU waste inventory to be disposed. In the WIPP, 2.48×10^6 Ci (see Table TRU WASTE-8) of TRU waste are estimated to be in the repository at closure, so the WUF is 2.48. In CCA Section 4.2.1, the DOE reported the activity of TRU isotopes that contribute to the WUF at closure to be[1] 3.44×10^6 Ci, with a WUF of 3.44. The current WUF (now 2.48 at closure) reflects the updated TRU waste inventory as described in Section TRU WASTE-2.1.2 (greater detail is available in Appendix DATA, Attachment F).

The number of EPA units of a radionuclide is the activity (in Ci) of the radionuclide divided by the release limit for that radionuclide. EPA units are important because the containment requirement for the repository is expressed in EPA units. Section TRU WASTE-2.3.1 discusses current EPA units in more detail.

[1] The value for the WUF in the CCA was inconsistently described; Chapter 4, Section 4.2.1 correctly listed the WUF that was used in the CCA PA as 3.44. CCA Appendix WCA Sections 1.4.2 and WCA Attachment WCA 8.1 incorrectly stated the 1995 decayed value of 4.07 was used in the CCA PA, however the preface to Attachment WCA.8.2 identified and corrected the error. During the EPA's review of the CCA, EPA required DOE to recalculate a new WUF of 3.59 that was ultimately included in the EPA's PAVT (EPA 1998). After the certification, the DOE incorporated the PAVT WUF value of 3.59 in the compliance baseline through an EPA approved change request (EPA 2002).

Table TRU WASTE-8. Radionuclides That Contribute to the Waste Unit Factor

Nuclide	Half-Life (years)	Inventory at Closure (Ci)	Percent of Waste Unit Factor
^{241}Am	4.33×10^{2}	4.58×10^{5}	1.82×10^{1}
^{242m}Am	1.41×10^{2}	2.11×10^{-1}	8.48×10^{-6}
^{243}Am	7.37×10^{3}	2.17×10^{1}	8.63×10^{-4}
^{249}Cf	3.51×10^{2}	7.24×10^{-2}	2.88×10^{-6}
^{251}Cf	9.00×10^{2}	5.10×10^{-4}	2.03×10^{-8}
^{243}Cm	2.91×10^{1}	4.07×10^{-1}	1.62×10^{-5}
^{245}Cm	8.50×10^{3}	1.92×10^{-2}	7.62×10^{-7}
^{246}Cm	4.76×10^{3}	2.22×10^{0}	8.80×10^{-5}
^{247}Cm	1.56×10^{7}	9.45×10^{0}	3.75×10^{-4}
^{248}Cm	3.48×10^{5}	9.32×10^{-2}	3.70×10^{-6}
^{237}Np	2.14×10^{6}	1.01×10^{1}	4.00×10^{-4}
^{238}Pu	8.77×10^{1}	1.25×10^{6}	4.98×10^{1}
^{239}Pu	2.41×10^{4}	6.65×10^{5}	2.64×10^{1}
^{240}Pu	6.56×10^{3}	1.08×10^{5}	4.30×10^{0}
^{242}Pu	3.75×10^{5}	2.71×10^{1}	1.08×10^{-3}
^{244}Pu	8.00×10^{7}	1.10×10^{-3}	4.38×10^{-8}
TOTAL		2.48×10^{6}	-

Source: Leigh 2003a

As an example, using EPA units, the ^{239}Pu inventory at closure would be 6.65×10^{5} Ci (Table TRU WASTE-8), and the release limit for ^{239}Pu would be 248 Ci, so the number of EPA units is calculated as:

$$\frac{6.65 \times 10^{5}\ \text{Ci}}{248\ \text{Ci}} = 2.68 \times 10^{3}\ \text{EPA units.} \qquad (1)$$

The release limit for ^{239}Pu is given by the waste unit factor (2.48) multiplied by the release limit per million Ci of TRU. The release limit per million Ci is given in Table TRU WASTE-7, which is a copy of Table 1 in Appendix A, 40 CFR Part 191. The value for ^{239}Pu is 100 Ci, giving a release limit of 248 Ci. The calculation of WUF, EPA units, and release limits uses the method established for the CCA (described above).

With a mix of radionuclides, each radionuclide is normalized with respect to its release limit, and the sum of all releases must have

- *less than one chance in 10 of exceeding the release limit, and*
- *less than one chance in 1,000 of exceeding ten times the release limit.*

The sum of releases in EPA units is expressed by

$$Rj = \frac{1}{fw}\left[\frac{Q1j}{L1} + \frac{Q2j}{L2} + \ldots\right] = \sum_{i=1}^{nR} \frac{Qij}{fwLi} \leq \left\{\begin{matrix}1 \text{ with a probability of } 0.1 \\ 10 \text{ with a probability of } 0.001\end{matrix}\right\} \qquad (2)$$

where

R_j is the total release in EPA units under scenario j,

f_w is the WUF,

Q_{ij} is the cumulative release for radionuclide i under scenario j,

L_i is the EPA release limit for radionuclide i, and

nR is the number of radionuclides contributing to the release.

The regulatory time period over which these releases are summed is 10,000 years. A brief explanation of these release limits is given in Sanchez (1996), and a comprehensive discussion of the background for these limits is provided in EPA (1985).

Figure TRU WASTE-4 is a flow diagram for the selection of those radionuclides in the inventory that contribute to the WUF. As noted above, not all radionuclides are included in this factor. For example, ^{90}Sr is excluded because it is not a TRU radionuclide, and is not an α-emitter. Even uranium is excluded because it is not a TRU radionuclide, defined as elements with atomic numbers greater than 92.

The radionuclides that are included in the WUF are listed in Table TRU WASTE-8. As noted in the table, the relevant inventory at closure is 2.48×10^6 Ci, resulting in a WUF of 2.48. This analysis was performed using data from Appendix DATA, Attachment F.

It is worthwhile to note that the inventory in Table TRU WASTE-8 is dominated by americium and plutonium, the same elements that dominated the inventory for the CCA. More specifically, the radionuclides ^{238}Pu, ^{239}Pu, ^{240}Pu, and ^{241}Am capture 99.9 percent of the WUF. The combined activity at emplacement of ^{241}Am, ^{238}Pu, ^{239}Pu, and ^{240}Pu is orders of magnitude greater than the combined activity of the remaining radionuclides.

TRU WASTE-2.3.2 Radioactivity Included in the Source Term for Performance Assessment

Unlike the WUF, all reported radionuclides are included in a demonstration of compliance and must therefore be considered for inclusion in the source term for PA. A comprehensive list of radionuclides in the waste is in Appendix DATA, Attachment F, which provides the inventory basis for the CRA-2004. Many of these radionuclides are present in such small quantities that their impact on long-term performance is negligible. That is, their total combined initial inventory in EPA units is much less than one percent so they will have negligible impact on compliance.

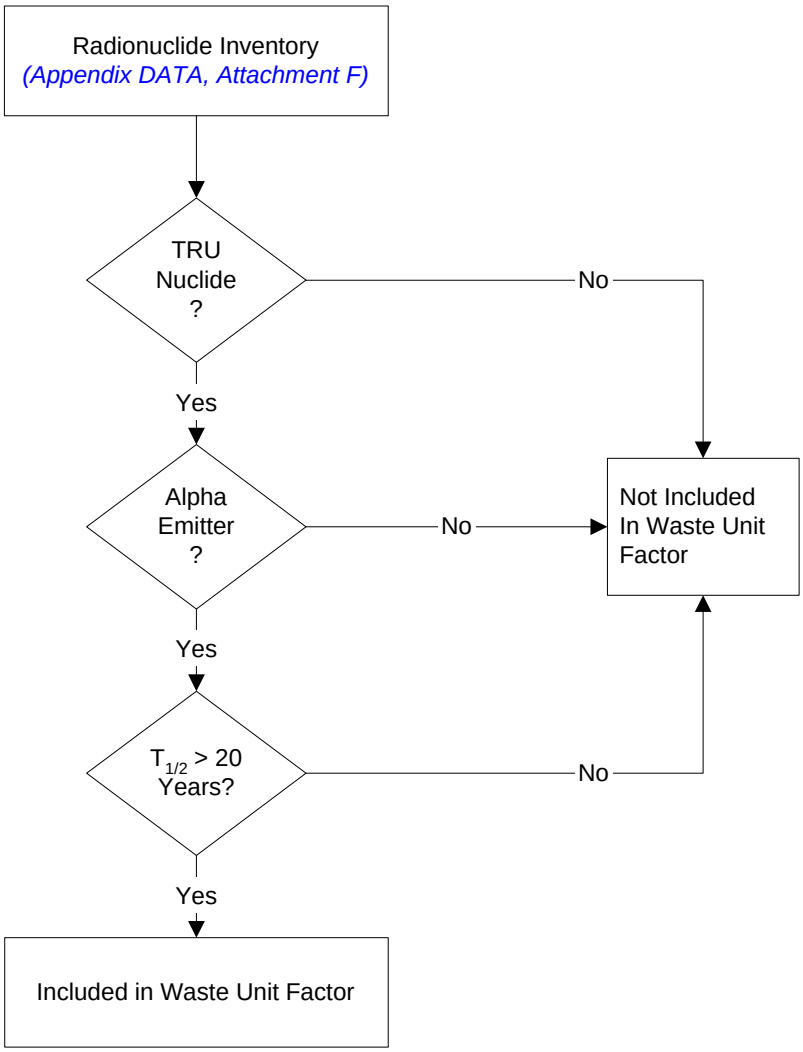

Figure TRU WASTE-4. Flow Diagram for Including Radionuclides in the Waste Unit Factor

Two different release pathways are used in PA: (1) direct releases comprised of (a) material brought to the surface by cuttings, cavings, spalling, and (b) brine under pressure that flows to the surface during a drilling intrusion through the repository; and (2) releases to the accessible environment in brine that moves through the subsurface, primarily the Culebra aquifer. Note that the time scales for these two releases are quite different. The direct release during drilling events (Item 1) occurs within a few days. The flow and transport of radionuclides through the Culebra (Item 2) will require hundreds to thousands of years.

Different radionuclides are used for these pathways because of the time-scale differences and different release media (solid particles containing radionuclides or brine containing radionuclides) as well as the computational efficiency of each computer code used in the PA calculations. Figure TRU WASTE-5 is a flow diagram for selecting radionuclides for different release mechanisms according to the criteria of Table TRU WASTE-7. The result of applying these criteria to the radionuclides in Appendix DATA, Attachment F is shown in

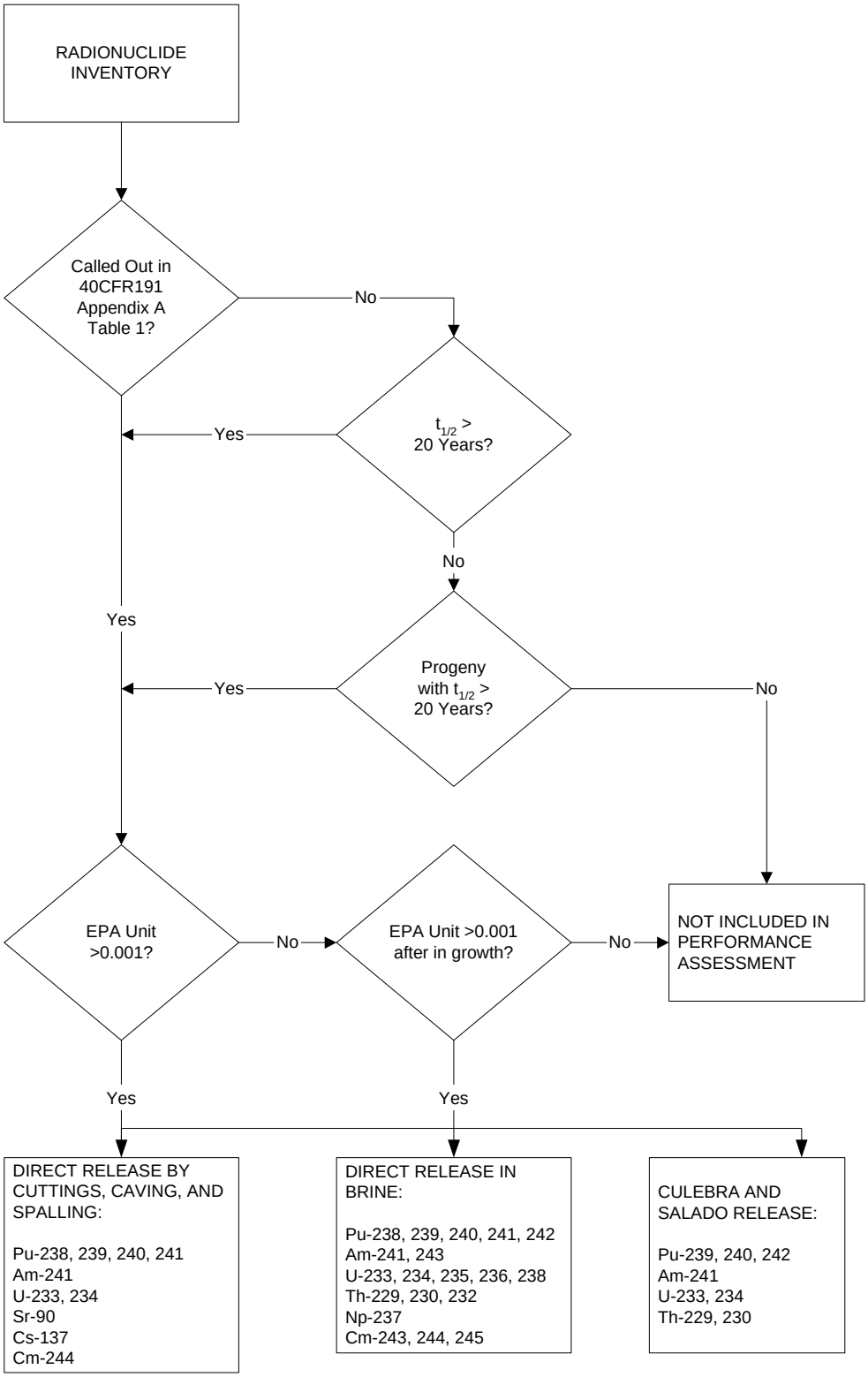

Figure TRU WASTE-5. Flow Diagram for Selecting Radionuclides for the Release Pathways Conceptualized by Performance Assessment (The top part of the diagram describes the criteria for selecting radionuclides in Table TRU WASTE-9)

Table TRU WASTE-9. Radionuclides Included in the Performance Assessment Source Term

Radionuclide	Current Inventory Values			Release Calculations (1)			
	Inventory at Closure (Ci)	EPA Units		Cuttings, Cavings, & Spall Release	Direct Brine Release	Salado Release	Culebra Release
		At Closure	At 10,000 years				
^{238}Pu	1.25×10^{6}	5.04×10^{3}	2.61×10^{-23}	×	×	(2)	(2)
^{239}Pu	6.65×10^{5}	2.68×10^{3}	2.01×10^{3}	×	×	×	×
^{241}Am	4.58×10^{5}	1.84×10^{3}	2.48×10^{-4}	×	×	×	×
^{240}Pu	1.08×10^{5}	4.36×10^{2}	1.51×10^{2}	×	×	c	c
^{137}Cs	1.79×10^{5}	7.19×10^{1}	0.00×10^{0}	×	--	--	--
^{90}Sr	1.42×10^{5}	5.71×10^{1}	0.00×10^{0}	×	--	--	--
^{233}U	1.27×10^{3}	5.12×10^{0}	4.91×10^{0}	×	×	c	c
^{229}Th	5.39×10^{0}	2.17×10^{-2}	3.04×10^{0}	--	×	c	c
^{234}U	3.19×10^{2}	1.28×10^{0}	3.03×10^{0}	×	×	×	×
^{230}Th	1.76×10^{-1}	7.07×10^{-3}	2.64×10^{0}	--	×	×	×
^{238}U	1.54×10^{2}	6.21×10^{-1}	6.21×10^{-1}	--	×	--	--
^{237}Np	1.01×10^{1}	4.06×10^{-2}	4.27×10^{-1}	--	×	--	--
^{232}Th	6.83×10^{0}	2.75×10^{-1}	2.75×10^{-1}	--	×	--	--
^{226}Ra	6.28×10^{0}	2.53×10^{-2}	2.07×10^{-1}	--	--	--	--
^{210}Pb	4.94×10^{0}	1.99×10^{-2}	2.07×10^{-1}	--	×	--	--
^{242}Pu	2.71×10^{1}	1.09×10^{-1}	1.07×10^{-1}	--	×	c	c
^{243}Am	2.17×10^{1}	8.75×10^{-2}	5.74×10^{-2}	--	×	--	--
^{236}U	1.65×10^{0}	6.66×10^{-3}	8.62×10^{-2}	--	×	--	--
^{235}U	2.28×10^{0}	9.18×10^{-3}	3.21×10^{-2}	--	×	--	--
^{14}C	3.25×10^{0}	1.31×10^{-2}	3.90×10^{-3}	--	--	--	--
^{232}U	3.07×10^{0}	1.23×10^{-2}	0.00×10^{0}	--	--	--	--
^{227}Ac	9.57×10^{-1}	3.85×10^{-3}	8.06×10^{-3}	--	--	--	--
^{231}Pa	1.21×10^{0}	4.88×10^{-3}	8.06×10^{-3}	--	--	--	--
^{243}Cm	4.07×10^{-1}	1.64×10^{-3}	0.00×10^{0}	--	×	--	--
^{248}Cm	9.32×10^{-2}	3.75×10^{-4}	3.68×10^{-4}	--	×	--	--
^{245}Cm	1.92×10^{-2}	7.72×10^{-5}	3.97×10^{-5}	--	×	--	--
^{244}Pu	1.10×10^{-3}	4.44×10^{-6}	4.47×10^{-6}	--	×	--	--
^{244}Cm	2.51×10^{3}	(3)	(3)	×	×	--	--
^{241}Pu	5.38×10^{5}	(3)	(3)	×	×	--	--
Percent of EPA Units at closure represented by nuclides in source term				99.98%	98.71%	48.95%	48.95%
Percent of EPA Units at 10,000 years represented by nuclides				99.65%	99.99%	99.92%	99.92%

Source: Leigh 2003b

(1) See Section 6.3 for a discussion of scenarios analyzed by PA and the release pathways.

(2) ^{238}Pu was included in the Salado transport calculations but the release to the Culebra was too low to merit calculation of its transport within the Culebra. The EPA unit percent total at closure increases to 98.71% with ^{238}Pu added; the percent at 10,000 years is unaffected. ^{241}Pu and ^{244}Cu are not regulated by 40 CFR Part 191, but are included because their daughters, ^{241}Am and ^{240}Pu respectively, are significant to performance.

× indicates an isotope included in calculation

c indicates isotopes that are combined for transport with isotopes having similar characteristics

Table TRU WASTE-9. The inventory analysis that follows Figure TRU WASTE-5 is documented in Leigh (2003b). Table TRU WASTE-9 also lists the radionuclides used for specific release mechanisms. The EPA unit at 10,000 years (the end of the regulatory period) is also shown in Table TRU WASTE-9, because some nuclides experience considerable ingrowth, but not enough to affect the domination by the most prevalent radionuclides ^{239}Pu and ^{240}Pu. The ^{241}Am component is also important for the first 3,000 years after closure.

TRU WASTE-2.3.2.1 Radionuclides Included in Direct Releases by Cuttings, Cavings, and Spalling

The 10 isotopes listed in the column headed "Cuttings/Cavings/Spall Release" in Table TRU WASTE-9 are used to model direct release by cuttings, cavings, or spalling. Release is assumed to occur when containers of CH-TRU or RH-TRU waste are breached during a borehole intrusion. The amount of radionuclides in the source term is estimated from the inventory per drum of the waste stream penetrated, including decay and ingrowth. Details of the EPA unit distribution in the waste streams are provided in Fox (2003). The direct release scenario is discussed in greater detail in Section 6.4.12.4.

Eight of the listed isotopes comprise more than 99.9 percent of the EPA units for the entire regulatory period and are identified in Leigh (2003b) as important radionuclides for direct release. The other two are included because they are parent nuclides of significant daughters. Inclusion of 99 percent or more of the EPA unit provides an accurate representation of the source term, while maintaining efficiency in computation by limiting the total number of isotopes to 10. The addition of the many radionuclides that make up the final 0.1 percent does not provide additional benefit in understanding the long-term behavior of the repository (see Leigh 2003b).

TRU WASTE-2.3.2.2 Radionuclides Included in Direct Releases of Brine to the Surface

Direct release of brine to the surface can carry radionuclides that are dissolved in the brine or sorbed on colloidal particles.

The radionuclides released in direct release of brine to the surface include several isotopes that comprise negligible fractions of the total EPA unit, but must be included in the source term because of their influence on the total quantity of dissolved radionuclides. This influence occurs because the isotopes of a radionuclide will dissolve based on mass ratio, rather than the activity ratio, in which they are present in the waste. That is, if 90 percent of the mass of uranium in the waste is ^{238}U (for example), 90 percent of the dissolved uranium in moles/liter will be ^{238}U, even though 90 percent of the radioactivity will not be from ^{238}U.

The EPA units of ^{90}Sr and ^{137}Cs at closure are large enough that an explanation is needed for not including them in the source term for direct release of brine. Although the EPA units of ^{90}Sr and ^{137}Cs are initially large (57 for ^{90}Sr and 72 for ^{137}Cs), rapid decay from a short half-life (about 30 years) results in negligible impact on the PA for these two isotopes. The lack of impact on compliance is explained below.

The ^{90}Sr and ^{137}Cs components decay by about 90 percent during the first 100 years after closure, when borehole intrusions are excluded due to the active institutional controls that will

be implemented following WIPP closure. During this time period, the EPA unit of ^{137}Cs decays from 72 down to 7.1 for the whole repository, while ^{90}Sr decays from 57 to 5.3. At 200 years, the EPA unit for both ^{137}Cs and ^{90}Sr is below 1.0, again for the whole repository.

In addition to the rapid decay, the results of the PA show that were an individual borehole intrusion to occur at 100 years, it would release about six EPA units (5.5 units, see Appendix PA), which is much less than the total inventory. Even at 350 years, when either isotope decays down to 0.03 percent of the initial inventory, the maximum volume of brine release would be only 0.01 m^3. In summary, the rapid decay of ^{137}Cs and ^{90}Sr and the negligible volumes of brine release at early times provide the basis for excluding these isotopes from the inventory.

The ^{14}C component is not included in this (or any) source term. Any ^{14}C transported out of the repository will be diluted by the large excess of nonradioactive carbon. This was demonstrated in Wang (1996a) in which there were 0.2 moles of ^{14}C out of 3×10^8 moles of carbon in the cellulosic materials, or one part in 100 million. Although the ^{14}C inventory has been updated, the ratio of ^{14}C to nonradioactive carbon remains the same.

TRU WASTE-2.3.2.3 Radionuclides Included in Releases to the Culebra Aquifer

Release of brine from the repository to the Culebra also potentially carries dissolved and colloidal radionuclides. The nine radionuclides in the source term for Culebra release include those that dominate the EPA unit for all but the earliest part of the regulatory period. Other less prevalent radionuclides are excluded because they would comprise a negligible fraction of the EPA unit or because transport through the Culebra is sufficiently slow that shorter-lived radionuclides would decay to negligible amounts before reaching the accessible environment. The selection of the nine radionuclides is discussed in Leigh (2003b).

Of the nine radionuclides, only ^{239}Pu, ^{241}Am, ^{234}U, and ^{230}Th are transported separately in PA. Isotopes of the same element will be transported together, unless their half-lives differ greatly. The movement of most of the radionuclides can be calculated indirectly. This concept was presented in detail in Garner (1996):

- *The ^{233}U component can be combined with ^{234}U for transport because their half-lives are similar.*
- *Similarly, ^{229}Th can be combined with ^{230}Th, because they will be in a fixed ratio to each other. The ^{232}Th component can be dropped because it is a constant small fraction of the EPA unit throughout the regulatory period.*
- *The ^{240}Pu and ^{242}Pu components can be combined with ^{239}Pu; their long half-lives also indicate a fixed ratio between them.*
- *The ^{238}Pu component will have decayed to about 0.5 percent of its initial inventory after 700 years, and its contribution to the EPA unit will be negligible because travel time in the Culebra is much greater than 700 years.*

The ^{239}Pu and ^{240}Pu components dominate the EPA limit during the regulatory period, and ^{241}Am is also a factor for the first 3,000 years. Toward the end of the regulatory period, ^{230}Th has grown by about 2.5 orders of magnitude, ^{229}Th by about 1.5 orders of magnitude, and ^{234}U by a factor of three, but all are still small fractions of the EPA unit. The ^{226}Ra component grows during the regulatory period, but even at 10,000 years would comprise a very small fraction of the EPA limit.

Calculation of radionuclide inventories for this transport mechanism is presented in Leigh (2003c.)

TRU WASTE-2.3.2.4 Radionuclides Included in Releases Through the Salado

In the PA results (Appendix PA), there is one vector in which brine is released through the Salado to the accessible environment. As a result, the radionuclides that could potentially contribute to releases via this pathway are considered.

Release of brine from the repository through the Salado (either to the Culebra or to the accessible boundary) can also potentially carry dissolved and colloidal radionuclides. The nine radionuclides in the source term for Salado release include those that dominate the EPA unit for all but the earliest part of the regulatory period. Other less prevalent radionuclides are excluded, because they would comprise a negligible fraction of the EPA unit or because transport through the Salado is sufficiently slow that shorter-lived radionuclides would decay to negligible amounts before reaching the accessible environment. The selection of the nine radionuclides is discussed in Leigh (2003b.)

TRU WASTE-2.3.2.5 Radionuclides Excluded From Source Terms

A large number of radionuclides were not included in any source term because they did not survive the screening process outlined in Figure TRU WASTE-5. Table TRU WASTE-10 lists those excluded radionuclides that have not already been discussed, and indicates (marked with an "×" in Table TRU WASTE-10) the reason for their exclusion.

TRU WASTE-2.4 Radionuclide Characteristics: Solubility and Colloid Formation

The major characteristics of the radionuclides that are expected to affect disposal system performance are (1) solubility and (2) the tendency to form or sorb to colloidal particles. Except for direct release from drilling (cutting) and caving, in which particles containing radionuclides will be released with circulation of drilling mud, radionuclides are mobilized for transport from the repository either in brine or as colloidal particles transported by brine. Gas-phase transport is not expected to occur (see Appendix PA, Attachment SCR).

All isotopes of a particular radioactive element exhibit essentially identical characteristics of solubility, colloid formation, and sorption.

Table TRU WASTE-10. Radionuclides Excluded From All Source Terms

Radionuclide	*Reason for Exclusion*[3]		
	Short Half-life and Progeny with Short Half-life[1]	*Small EPA Unit*	*Negligible*[2] *Ingrowth*
^{225}Ac	×	*NA*	*NA*
^{227}Ac	×	*NA*	*NA*
^{228}Ac	×	*NA*	*NA*
^{109m}Ag	×	*NA*	*NA*
^{110}Ag	×	*NA*	*NA*
^{110m}Ag	×	*NA*	*NA*
^{242}Am	×	*NA*	*NA*
^{242m}Am	*NA*	×	×
^{245}Am	×	*NA*	*NA*
^{217}At	×	*NA*	*NA*
^{137m}Ba	×	*NA*	*NA*
^{210}Bi	×	*NA*	*NA*
^{211}Bi	×	*NA*	*NA*
^{212}Bi	×	*NA*	*NA*
^{213}Bi	×	*NA*	*NA*
^{214}Bi	×	*NA*	*NA*
^{249}Bk	×	*NA*	*NA*
^{250}Bk	×	*NA*	*NA*
^{14}C	*NA*	×	*NA*
^{109}Cd	×	*NA*	*NA*
^{113m}Cd	×	*NA*	*NA*
^{141}Ce	×	*NA*	*NA*
^{144}Ce	×	*NA*	*NA*
^{249}Cf	*NA*	×	×
^{250}Cf	×	*NA*	*NA*
^{251}Cf	*NA*	×	*NA*
^{242}Cm	×	*NA*	*NA*
^{246}Cm	*NA*	×	×
^{247}Cm	*NA*	*NA*	×
^{250}Cm	*NA*	*NA*	×
^{60}Co	*NA*	×	*NA*
^{134}Cs	×	*NA*	*NA*

Table TRU WASTE-10. Radionuclides Excluded From All Source Terms — Continued

Radionuclide	*Reason for Exclusion*[3]		
	Short Half-life and Progeny with Short Half-life[1]	*Small EPA Unit*	*Negligible*[2] *Ingrowth*
^{135}Cs	*NA*	×	*NA*
^{152}Eu	×	*NA*	*NA*
^{154}Eu	×	*NA*	*NA*
^{155}Eu	×	*NA*	*NA*
^{55}Fe	×	*NA*	*NA*
^{221}Fr	×	*NA*	*NA*
^{223}Fr	×	*NA*	*NA*
^{152}Gd	*NA*	×	*NA*
^{3}H	×	×	*NA*
^{129}I	*NA*	×	×
^{85}Kr	×	*NA*	*NA*
^{54}Mn	×	*NA*	*NA*
^{22}Na	×	*NA*	*NA*
^{93m}Nb	×	*NA*	*NA*
^{95}Nb	×	*NA*	*NA*
^{95m}Nb	×	*NA*	*NA*
^{144}Nd	*NA*	*NA*	×
^{59}Ni	*NA*	×	×
^{63}Ni	*NA*	*NA*	×
^{238}Np	×	*NA*	*NA*
^{239}Np	×	*NA*	*NA*
^{240m}Np	×	*NA*	*NA*
^{233}Pa	×	*NA*	*NA*
^{234}Pa	×	*NA*	*NA*
^{234m}Pa	×	*NA*	*NA*
^{209}Pb	×	*NA*	*NA*
^{211}Pb	×	*NA*	*NA*
^{212}Pb	×	*NA*	*NA*
^{214}Pb	×	*NA*	*NA*
^{107}Pd	*NA*	×	*NA*
^{210}Po	×	*NA*	*NA*
^{211}Po	×	*NA*	*NA*
^{212}Po	×	*NA*	*NA*
^{213}Po	×	*NA*	*NA*

Table TRU WASTE-10. Radionuclides Excluded From All Source Terms — Continued

Radionuclide	*Reason for Exclusion*[3]		
	Short Half-life and Progeny with Short Half-life[1]	*Small EPA Unit*	*Negligible*[2] *Ingrowth*
^{214}Po	×	*NA*	*NA*
^{215}Po	×	*NA*	*NA*
^{216}Po	×	*NA*	*NA*
^{218}Po	×	*NA*	*NA*
^{144}Pr	×	*NA*	*NA*
^{236}Pu	×	*NA*	*NA*
^{243}Pu	×	×	*NA*
^{223}Ra	×	*NA*	*NA*
^{224}Ra	×	*NA*	*NA*
^{225}Ra	×	*NA*	*NA*
^{106}Rh	×	*NA*	*NA*
^{219}Rn	×	*NA*	*NA*
^{220}Rn	×	*NA*	*NA*
^{222}Rn	×	*NA*	*NA*
^{106}Ru	×	*NA*	*NA*
^{125}Sb	×	*NA*	*NA*
^{126}Sb	×	*NA*	*NA*
^{126m}Sb	×	*NA*	*NA*
^{79}Se	*NA*	×	×
^{147}Sm	*NA*	×	*NA*
^{148}Sm	*NA*	*NA*	×
^{151}Sm	*NA*	*NA*	×
^{121m}Sn	*NA*	×	*NA*
^{126}Sn	*NA*	×	*NA*
^{99}Tc	*NA*	×	×
^{123}Te	*NA*	*NA*	×
^{123m}Te	×	*NA*	*NA*
^{125m}Te	×	*NA*	*NA*
^{227}Th	×	*NA*	*NA*
^{228}Th	×	*NA*	*NA*
^{231}Th	×	*NA*	*NA*
^{234}Th	×	*NA*	*NA*
^{207}Tl	×	×	*NA*
^{208}Tl	×	×	*NA*

Table TRU WASTE-10. Radionuclides Excluded From All Source Terms — Continued

Radionuclide	Reason for Exclusion[3]		
	Short Half-life and Progeny with Short Half-life[1]	Small EPA Unit	Negligible[2] Ingrowth
^{209}Tl	×	NA	NA
^{232}U	NA	×	×
^{237}U	×	NA	NA
^{240}U	×	NA	NA
^{90}Y	×	NA	NA
^{91}Y	×	NA	NA
^{65}Zn	×	NA	NA
^{93}Zr	NA	×	×
^{95}Zr	×	NA	NA

[1] "Short" half-life means $t_{½}$ < 20 years. Radionuclides with $t_{½}$ < 20 years are not regulated by 40 CFR Part 191 Subparts (b) and (c).
[2] Negligible ingrowth includes ingrowth of the progeny that are radionuclides already predominant in the inventory.
[3] NA indicates that the column heading does not apply to the particular isotope.

Solubility and colloid formation are discussed for thorium, uranium, neptunium, plutonium, and americium. The experimental determination and modeling of solubility and colloid formation, and the manner in which they are taken into account by PA, are discussed in detail in Appendix PA. Cesium and strontium are assumed to be extremely soluble and their concentrations will be limited by their inventories (see Appendix WCA, Section WCA.3.2.2, in the CCA). Thus, the two elements are not considered in this section. Radium is excluded from the source term because of its short half-life.

Actinide mobility depends on the particular chemical environment (brine pH, fugacity of CO_2, redox potential, organic ligand concentration, etc). That environment will be controlled by the MgO reacting with brine. Magnesium oxide is added to mitigate the effect of CO_2 generated by microbial degradation of organic materials and to control the pH of any brines in the repository. The mechanism of the control is discussed in Appendix BARRIERS and Appendix PA, Attachment SOTERM.

Actinide mobility also depends on the formation of colloids. Actinides can either form intrinsic colloids by condensation of hydrolyzed ions, or can be sorbed on to nonradioactive colloidal particles.

TRU WASTE-2.4.1 Components and Characteristics Influencing Solubility

In the absence of MgO, the factors that would most directly affect solubility in the repository are pH, CO_2 fugacity, redox conditions, the availability of complexing agents, and the source and composition of the brine (clearly not a waste characteristic). The important waste components that affect actinide solubility are steel, cellulosic, plastic, rubber, organic ligand, and cementitious materials. Actinide solubility also depends on temperature. However, the temperature in the repository will remain almost constant (about 300 K) and the thermal effect

of exothermal chemical reactions among brine, waste component, and MgO will be negligible (see Appendix WCA, Section WCA-5.3.1 in the CCA and Wang 1996b). Repository pressure does not influence solubility until it is at least an order of magnitude higher than lithostatic pressure and this will not occur (Butcher et al. 1991). The following subsections discuss the influence of waste characteristics and components on each of these factors, as well as those that have little or no influence on solubility.

TRU WASTE-2.4.1.1 Components Influencing Redox Environment

The components of the waste that greatly influence the redox environment in the inundated WIPP repository are steels and biodegradable organic materials (CPR materials). The radionuclides contributing to the brine release source terms are all actinides. Because of their electronic structure, these elements can form a wide variety of inorganic compounds that dissolve in aqueous solutions like brine in several different valence or oxidation states. In the WIPP environment, the solubilities of these compounds can vary from about 10^{-9} Molar (M) to about 10^{-5} M (see Appendix PA, Attachment SOTERM). In general, for both plutonium and the other actinides, the higher oxidation states (V and VI) are more soluble than the lower oxidation states (III and IV). The redox environment determines which of these oxidation states are likely to be stable in solution under WIPP conditions—an important determinant of solubility because of the differences among oxidation states. Although a detailed discussion of the experimental determination of oxidation state distribution is found in Appendix PA, Attachment SOTERM, a brief discussion is given here.

Anoxic conditions will be dominant during the whole time period of 10,000 years. At the time of the CCA, it was believed that anoxic steel corrosion would produce both hydrogen and $Fe(OH)_2$ (see Wang and Brush 1996). A small amount of oxygen, trapped at emplacement, will be used quickly by oxic corrosion and microbial action. Based on recent experimental work (described in Appendix PA, Attachment SOTERM), anoxic corrosion of steel could produce hydrogen, and Fe(II) or Fe(II,III)-bearing corrosion products. It has been shown that both metallic iron and Fe^{2+} ($Fe(OH)_2$) in simulated WIPP brine, under anoxic conditions, will reduce Pu(+VI) stoichiometrically to the much less soluble Pu(+IV). Plutonium(+V) is seen in this chemical reaction as an unstable intermediate. It is expected, therefore, that Pu(+VI) and Pu(+V) will not be stable in solution in WIPP brines. The iron in the drums and waste boxes is enough to provide several thousand-fold excess over what is needed stoichiometrically, even if all the emplaced plutonium existed in the +VI oxidation state. The other metals in the waste may also be able to reduce the actinides, but their effect would be negligible compared to the effect of iron, because they are present in smaller quantities.

The oxidation state distribution used in PA, based on experimental data as well as the published literature, is (Katz et al. 1986; Hobart 1990; Clark et al. 1995; Felmy et al. 1996; Rai and Strickert 1980; Rai et al. 1982; Kim et al. 1985; Pryke and Rees 1987; Nitsche and Edelstein 1985):

thorium:	*+IV*
uranium:	*+IV and +VI*
neptunium:	*+IV and +V*
plutonium:	*+III and +IV*

americium: +III

Curium exhibits essentially the same chemical behavior and oxidation state as americium. In PA, half of the realizations will include the lower oxidation states of uranium, neptunium, and plutonium; the other half will include the higher oxidation states (CCA Appendix SOTERM, Section 4.7; Katz et al. 1986; Weiner 1996).

TRU WASTE-2.4.1.2 Components Influencing pH and CO_2 Fugacity

In the absence of MgO, actinide solubility would be highly dependent on pH and CO_2 fugacity of the brine. Lower pH and higher CO_2 fugacity could result in higher actinide solubility. Original Salado and Castile brines exhibit pH values of about 6 and 7, respectively (Brush 1990, Tables 2-2 and 2-3). The production of CO_2 by microbial degradation in the repository would acidify the brine and lower the brine pH to about 4.5, if no MgO were added (CCA Appendix SOTERM, SOTERM.2). Microbial CO_2 production can be described by the following sequential reactions (Wang and Brush 1996):

$$C_6H_{10}O_5 + 4.8H^+ + 4.8NO_3^- \rightarrow 7.4H_2O + 6CO_2 + 2.4N_2 \quad (3)$$

$$C_6H_{10}O_5 + 6H^+ + 4.8SO_4^{2-} \rightarrow 5H_2O + 6CO_2 + 3H_2S \quad (4)$$

$$C_6H_{10}O_5 + H_2O \rightarrow 3CO_2 + 3CH_4. \quad (5)$$

Nitrate and sulfate are used as electron acceptors in these reactions and determine CO_2 yield per mole of organic carbon. Based on the inventory estimates for nitrate and sulfate, over 94% (see Appendix BARRIERS) of organic materials (CPR materials) would be biodegraded via the third reaction, methanogenesis, in which one mole of organic carbon will produce one half of a mole each of CO_2 and CH_4.

Based on the inventory estimate for organic carbon (Appendix DATA, Attachment F) and the estimated CO_2 yield per mole of organic carbon, to mitigate the negative effect of microbially produced CO_2, 1.41×10^9 moles of MgO will be added to the repository (see Appendix BARRIERS). At the time of the CCA, it was estimated that 2×10^9 moles of MgO would be required. However, as discussed below, DOE's understanding of the chemical interaction of MgO and components of the waste has evolved.

In the CCA, the waste components of organic carbon, nitrate, and sulfate were used to determine the amount of MgO needed. It was stated that hydrated MgO would react with CO_2:

$$Mg(OH)_2 + CO_2 \rightarrow MgCO_3 + H_2O. \quad (6)$$

The above reaction would buffer the pH at approximately 9.4 in Salado brine and 9.9 in Castile brine and CO_2 fugacity at 10^{-7} atm for both brines. Actinide solubility calculated for the brine in equilibrium with $Mg(OH)_2$ and $MgCO_3$ is minimal (CCA Appendix SOTERM, SOTERM.3). Now, however, the quantities of CPR materials, nitrate, and sulfate are used to determine the amount of MgO needed, based on the understanding that hydrated MgO will react with CO_2:

$$5Mg(OH)_2 + 4CO_2 \rightarrow Mg_5(CO_3)_4(OH)_2 + 4H_2O \quad (7)$$

under conditions in which microbial activity produces gas, and

$$Mg(OH)_2 + Ca^{2+} + CO_2 \rightarrow CaCO_3 + Mg^{2+} + H_2O \quad (8)$$

under conditions in which microbial activity does not occur (see Appendix BARRIERS).[2]

The above reactions will buffer pH at approximately 9 in both Salado and Castile brines, and CO_2 fugacity at $10^{-6.2}$ to $10^{-5.5}$ atm for both brines.

Cementitious waste (that contains calcium oxide and/or calcium hydroxide) could also be expected to raise the pH, and the waste is currently estimated to contain a total of about 1.2×10^7 kg cementitious material (Appendix DATA, Attachment F). This amount of cementitious material contains about 9×10^6 moles of $Ca(OH)_2$. However, this amount of $Ca(OH)_2$ would not be enough to affect pH or brine composition significantly. It was shown that $Ca(OH)_2$ could be consumed by reaction with microbial generated CO_2 or with $MgCl_2$ in the Salado brine and thus the repository chemistry would be dominantly controlled by the $Mg(OH)_2$ / Mg CO_3 buffer, rather than the $Ca(OH)_2$ / $CaCO_3$ buffer (CCA, Wang 1996a and Wang 1996c). Because of the additional MgO that will be added, other components of the waste are unlikely to affect the pH.

TRU WASTE-2.4.1.3 Waste Components That Directly Enhance Solubility

A number of organic compounds are capable of forming strong complexes with actinide ions, thereby stabilizing the actinide in the solution. Of the about 60 organic compounds in the waste (Drez and James-Lipponer 1989; Brush 1990; Drez 1996), 4 of these (acetate, citrate, oxalate, and ethylene diamine tetra-acetate [EDTA]) have been identified to have an effect on actinide mobility, because they are water-soluble and present in significant quantities (Appendix DATA, Attachment F).

Ligand concentrations in the repository were estimated using current inventory amounts of each ligand and a brine volume equal to 75 percent of the total repository brine volume of 29,841 m^3—the minimum brine for significant brine release to occur. The effect of these organic ligands on the solubility of actinides in both Salado and Castile brines has been studied, and is discussed in detail in Appendix PA, Attachment SOTERM.

To estimate the effectiveness of other metals in binding organic ligands and thereby reducing the free ligand concentrations, some simple competition calculations were performed (for the CCA) using parameters obtained in dilute solutions, because parameters for concentrated salt solutions like the WIPP brines were not available. These metal species included iron (Fe), nickel (Ni), chromium (Cr), vanadium (V), and manganese (Mn), because the steels used for the waste drums contain on average at least 0.001 weight percent of Ni, Cr, V, and Mn as

[2] *The conceptual model for the repository maintains a probability of significant microbial degradation of CPR materials of 0.5. Thus, there is no microbial activity and concomitant gas generation in about half of the PA vectors (Brush and Xiong 2003a; 2003b).*

minor constituents. Based on at least 1.9×10^9 moles of steels destined to be disposed of in the WIPP, there should be at least 1×10^4 moles of each of Ni, Cr, V, and Mn in the repository (CCA Appendix SOTERM). There are also expected to be more than 6×10^7 moles of lead (Pb). Additionally, several other metals that can sequester organic ligands will be present in small quantities.

Table TRU WASTE-11 presents complexation constants for several metals with EDTA. These values were measured in dilute solution. For comparison, for EDTA in 5 molal (moles of solute per kilogram of solvent) NaCl, the magnesium association constant is log $K_{Mg} = 6.6$ (Martell and Smith 1982).

Table TRU WASTE-11. Complexation Constants for Selected Metals[1]

Species	log K
Fe^{2+}	14.3
Cr^{2+}	13.6
Ni^{2+}	18.4
Mn^{2+}	13.9
V^{2+}	12.7
Cu^{2+}	18.9
Pb^{2+}	18

[1] From Martell and Smith (1982).

To assess the ability of these metals to sequester the organic ligands, the calculations for competition between these metals and actinides for organic ligands were performed by the DOE. The calculation results show that under expected WIPP conditions, 99.8% of the EDTA was complexed by Ni, effectively rendering it unavailable for complexation with the actinides (CCA, Appendix SOTERM).

TRU WASTE-2.4.2 Components and Characteristics Influencing Colloidal Actinide Mobility

The waste components that directly contribute to actinide colloid formation include mineral fragments, and humic substances (soil). CPR materials can contribute to the quantity of humic colloids. Actinides can form intrinsic colloids or can be sorbed on to nonradioactive colloidal particles. A complete discussion of colloid formation in the WIPP can be found in CCA Appendix SOTERM and Papenguth (1996a through 1996e). A summary of that discussion follows.

In principle, intrinsic colloids are formed by condensation (or polymerization) of hydrolyzed actinide ions. Examples of polymeric species of many of the actinides of importance to the WIPP have been found in the literature (see Papenguth and Behl (1996) for an extensive literature review). However, except for Pu, the intrinsic colloids of other actinides (Am, U, Th, and Np) do not develop to sizes large enough to affect transport behavior of these actinides relative to their dissolved form. Therefore, the intrinsic colloid concentrations for Am, U, Th,

and Np are modeled as zero in the disposal room and only intrinsic plutonium colloids have any impact on performance. Plutonium(IV) readily forms an intrinsic colloid; evidence suggests that the initial polymerization, or condensation, of hydrolyzed Pu(IV) produces a macromolecule that becomes progressively more crystalline with time. As the Pu polyelectrolytes mature, they are expected to be kinetically destabilized and immobilized by the high ionic strength of the WIPP brines, then coagulate and settle out of solution.

Within the repository, mineral fragment colloids could form from corrosion of iron-bearing waste, soils, and portland cement-based matrices. Because a wide range of mineralogies with different sorptive behavior are present at the WIPP, a bounding approach is used to estimate the maximum concentration of actinides bound to mineral fragment colloids. Mineral fragments are expected to be kinetically destabilized in the high-ionic strength brines present in the disposal room. Experimental information, combined with a conservative estimate of adsorption site density, provided a most likely value of 2.6×10^{-9} mole of colloidal mineral-fragment-bound actinides per liter of dispersion; the experimental results were increased by a factor of two to account for the possibility that the indigenous mineral fragment colloids in the Culebra could sorb dissolved actinides. This value is presumed to be the same for all five key actinides. Although mineral fragments contribute to actinide mobility and are included in PA, their contribution is negligible and they do not impact repository performance (see Appendix PA).

Humic colloids will be present in the repository, both (a) in soil and humic material that is part of the emplaced waste and (b) in colloids that will be formed if the CPR materials in the waste are microbially degraded. The contribution of humic colloids to repository performance is therefore calculated by quantifying humic-actinide complexation coupled with solubilities of humic substances in WIPP brines, and expressing the result as the ratio of moles of humic-bound actinide to moles of dissolved actinide. The range of ratios is from about 4.3×10^{-4} to about 6.3 in Castile brine and from about 5.3×10^{-5} to about 6.3 in Salado brine.

To compute the concentration of actinides bound to humic substances, several parameters, such as solubility of humic substances, site binding capacity, actinide complexation factors, and stability constants, were measured or obtained from published literature (Papenguth 1996c). The oxidation state analogy was also used to develop parameter values for actinides expected to have multiple oxidation states in the WIPP disposal rooms. In addition, the theoretical maximum concentration of actinides that can be bound to humic substances was also computed and found to be 1.1×10^{-5} M.

The other major source of colloidal material in the repository is the microbes themselves, though they are not necessarily waste components. Microbes are known to actively bioaccumulate actinides intercellularly, as well as act as substrates for passive extracellular sorption. Naturally occurring halophilic and halotolerant microbes have been observed in the Salado brines at the WIPP site (Brush 1990 and Francis and Gillow 1994). The waste material in the disposal room would serve as a nutrient and substrate for microbes, and consequently increase the microbe population, making them potentially important to actinide mobility.

The uptake of actinides by microbes and humic substances is quantified through two parameters for each actinide and substrate: proportionality constants (with PA parameter designations PROPMIC, PHUMSIM, and PHUMCIM) that describe the amount of each actinide bound to mobile microbes and humic colloids, respectively; and the maximum concentrations (CAPMIC and CAPHUM) of each actinide associated with mobile microbes and humics, respectively. As discussed above, the concentrations of mineral-fragment-bound actinides and intrinsic actinides are very small, and are presented as concentrations (CONCMIN and CONCINT) only. A series of bioaccumulation and toxicity experiments were performed to obtain the following values of PA parameters for each actinide shown in Table TRU WASTE-12.

Table TRU WASTE-12. Colloid Concentration Factors

	Concentration on Mineral Fragments[1]	Concentration as Intrinsic Colloid[1]	Proportion Sorbed on Microbes[2]	Maximum Sorbed on Microbes[1]	Proportion Sorbed on Humics[2]		Maximum Sorbed on Humics[1]
					Salado	Castile	
Th	2.6×10^{-8}	0.0	3.1	0.0019	6.3	6.3	1.1×10^{-5}
U(IV)	2.6×10^{-8}	0.0	0.0021	0.0023	6.3	6.3	1.1×10^{-5}
U(VI)	2.6×10^{-8}	0.0	0.0021	0.0023	0.12	0.51	1.1×10^{-5}
Np(IV)	2.6×10^{-8}	0.0	12.0	0.0027	6.3	6.3	1.1×10^{-5}
Np(V)	2.6×10^{-8}	0.0	12.0	0.0027	9.1×10^{-4}	7.1×10^{-3}	1.1×10^{-5}
Pu(III)	2.6×10^{-8}	0.0	0.3	6.8×10^{-5}	0.19	1.1	1.1×10^{-5}
Pu(IV)	2.6×10^{-8}	1.0×10^{-9}	0.3	6.8×10^{-5}	6.3	6.3	1.1×10^{-5}
Am	2.6×10^{-8}	0.0	3.6	NA	0.19	1.1	1.1×10^{-5}

[1] in units of moles total mobile actinide per liter
[2] in units of moles microbial actinide per moles dissolved actinide

As evident in Table TRU WASTE-12, microbial colloids can transport concentrations of actinides that are several multiples of the dissolved concentration, and thus increase the potential for actinide mobility considerably. Humic colloids are waste components, and microbial colloids increase in quantity as they metabolize waste components. Both types of colloids are incorporated in PA (details are discussed in Appendix PA) and are expected to affect disposal system performance.

The treatment of colloids in CRA-2004 is like that of the CCA. The only difference between the CCA colloid assumptions and values and CRA-2004 colloid assumptions and values is in relation to the microbial colloids. In the CCA, microbial colloids were present in all calculations as described above. For CRA-2004, in the absence of microbes (PA assumes that microbes are present in only 50 percent of the calculations), microbial colloids are not included in the calculations.

TRU WASTE-2.5 Nonradioactive Waste Components and Characteristics

TRU WASTE-2.5.1 Gas Generation

The waste components that contribute to gas generation are: (a) ferrous and nonferrous metal, (b) CPR materials, and (c) nitrate and sulfate. Water content of the waste also contributes to the generation of gas. The mechanisms and reactions for gas generation are discussed in Wang and Brush 1996.

Metal can contribute to gas generation through corrosion. The anoxic corrosion reaction of iron is:

$$Fe + 2H_2O \rightarrow Fe(OH)_2 + H_2(g) \quad (9)$$

The hydrogen gas produced by this reaction contributes to total gas pressure, but does not affect repository chemistry. In addition, steel corrosion is likely to consume water in the repository; this effect is taken into account in the computer code BRAGFLO. Nonferrous metals such as aluminum alloys can also corrode, producing H_2, but their contribution to total gas pressure is negligible, because they are present in much smaller quantities than iron (Appendix DATA, Attachment F).

CPR materials and nitrate and sulfate control microbial gas generation. CPR materials can be used as substrates by anaerobic microbes in the WIPP. Nitrate and sulfate can be used as electron acceptors by microbes to oxidize the organic materials. Organic materials are likely to be biodegraded through reactions:

$$C_6H_{10}O_5 + 4.8H^+ + 4.8NO_3^- \rightarrow + 7.4H_2O + 6CO_2 + 2.4N_2(g) \quad (10)$$

$$C_6H_{10}O_5 + 6H^+ + 3SO_4^{2-} \rightarrow 5H_2O + 6CO_2 + 3H_2S(g) \quad (11)$$

$$C_6H_{10}O_5 + H_2O \rightarrow 3CH_4(g) + 3CO_2(g) \quad (12)$$

The above reactions will proceed sequentially according to the energy yield per mole of carbon in each reaction. Based on the inventory estimates for nitrate and sulfate, the third reaction is expected to be dominant. Because the CO_2 produced by these reactions will be removed by reaction with MgO, methane is the primary, microbially generated gas that will contribute to the total gas in the repository.

Phosphate in the waste may enhance microbial activity in the repository. The rates of cellulosic material biodegradation used in PA are derived from the incubation experiments amended with nutrients including phosphate. Thus, the effect of phosphate on microbial reactions is captured indirectly in the parameters submitted to PA (Francis and Gillow 1994).

Based on the inventories of steels and organic materials and the rates of gas generation estimated, microbially produced gases may dominate early in the repository's history. Gas pressure can affect repository performance. Pressure in the repository may approach lithostatic, initiating or propagating fractures within the interbeds, and clay seams in the

Salado. Gas pressure will not exceed lithostatic (Butcher et al. 1991) because gas can leak out through the interbeds.

Gas pressure is incorporated into PA through parameters in BRAGFLO calculations.

The initial water content of the waste also contributes to the generation of gas because it defines how much brine is immediately available for the corrosion reaction. All of the liquid in the waste is assumed to be aqueous with no volume correction. A mean value of 0.06 percent is assumed in PA for the initial free unbound water saturation of the waste, based on waste characterization data and transportation restrictions on the amount of free liquid that the waste can contain (Appendix PAR, Table PAR-39 in the CCA).

Materials such as dry portland cement, vermiculite, and other sorbents have intentionally been added to the waste to absorb any excess water that may be present. Sorbed water is much less readily available than any brine available from the surrounding rock. Therefore, the effect of initial water content on gas generation is negligible.

TRU WASTE-2.5.2 Components and Characteristics Influencing Physical Properties

As noted in Tables TRU WASTE-4 and TRU WASTE-5, the following physical properties of the solid waste components are used in PA:

Compressibility: This property is a measure of deformational stress-strain response of the waste material. The response of the waste is modeled to represent the conventional 55-gallon drums, pipe overpack configurations, and the supercompacted waste.

Strength: Strength of the waste is only of concern in the highly degraded state. Strength properties enter directly into PA human intrusion scenarios, whereby a driller inadvertently intersects a repository room. If high pressures exist in the disposal room, a pressure gradient pulse could induce tensile failure and transport of waste particulate into the wellbore—the spalling event. In addition, the drill bit and drilling fluid circulate in the advancing wellbore and set up fluid shear stress in the degraded waste. The effects of waste strength on room closure are included in the discussion of compressibility.

Porosity: Initial porosity of the waste room is modified by salt creep. The waste inventory establishes the initial porosity as well as mechanical resistance to the impinging salt. Waste porosity is directly incorporated into the PA via a porosity surface.

Permeability: Permeability controls movement of fluids in the waste rooms, and therefore is an important parameter for the Salado fluid flow calculations. Permeability is also a key consideration within the human intrusion conceptual model, as it enters into the calculations of material transport to well bore.

TRU WASTE-2.5.2.1 Compressibility

An important characteristic of the WIPP repository is the closure of the disposal rooms over time due to the creep response of the surrounding salt in response to the presence of the mined openings. This ability of salt to deform with time, eliminate voids, and create an impermeable

salt barrier around waste is one of the principal reasons for locating the WIPP repository in a bedded salt formation, as suggested by the National Academy of Sciences (NAS-NRC 1957). This closure process is rather complex, and the rate at which it occurs depends in large part on the balance of forces tending to close the repository (the far-field lithostatic stresses) and those resisting the closure. These resisting forces are the tendency of the waste to resist deformation, measured in terms of its compressibility, and the effect of any gas pressure within the rooms.

At the time of the CCA, the compressibility of the waste was determined from laboratory experiments on 55-gallon drums (Butcher et al. 1991). Waste containers other than the 55-gallon drum package have been delivered to WIPP and other forms, such as supercompacted waste, are anticipated to be sent. Therefore, the response model incorporated into the CRA-2004 calculations was enhanced to account for a range of structural responses. Updated coefficients developed for the volumetric plasticity model were based on modeling analysis of other waste forms (Weatherby et al. 1991; Park and Hansen 2003). The wastes were characterized by their general structural form, which predominantly depends on the packaging. Appendix PA describes the calculations that were used to evaluate the competing conditions of creep closure, waste rigidity, and gas generation to yield porosity histories that are compiled into a porosity surface for incorporation into PA calculations.

TRU WASTE-2.5.2.2 Strength

Shear and tensile strength are important parameters in the models for cavings and spallings releases, respectively. It is likely that alternative waste forms, such as the pipe overpacks and the supercompacted wastes, will be less likely to degrade and corrode than standard waste forms, and as such their mechanical strengths may be expected to be equal to or higher than standard waste.

Degraded material property estimates were recently summarized for the spallings model peer review (Hansen et al. 2003). The authors assert that degraded waste properties determined for the new spall model, DRSPALL, represent extreme bounds of the future possible states of the waste because strengthening processes are not included in the minimal shear and tensile strength properties determined for surrogate degraded waste. It is likely that the new waste forms, such as the pipe overpacks, would render the waste less vulnerable to collapse and more resistant to massive corrosion.

Shear Strength. The shear strength implemented in PA is used to calculate the volume of cavings release, hence, it is a measure of erosional shear resistance. In the CCA, the waste shear strength was sampled from a uniform distribution from 0.05 to 10 Pascal (Pa) Pa, which is conservatively based on properties of marine clays (Appendix PA, Attachment MASS, Table MASS-1). For the PAVT, the waste shear strength was estimated based on particle size distribution determined by an expert elicitation panel. With this approach, the calculated critical shear strength ranged from 0.64 to 77 Pa. The EPA then retained the original lowest value and assigned a log-uniform distribution ranging from 0.05 to 77 Pa. Based on work by Jepsen et al. (1998), the lower value of 0.05 Pa is considered to be extremely conservative. Using the 50 percent degraded waste surrogates that represent the extreme possibilities for degradation of the WIPP waste (Hansen et al. 1997, Hansen et al. 2003), an average critical

shear strength of 1.4 Pa was determined. The minimal critical shear strength could approach this measured value only if massive degradation of waste ensues and no cementation or compaction of degraded waste occurs. The current minimum value sampled for the waste shear strength is thus at least 30 times smaller than the minimum value supported by empirical data.

Tensile Strength. Tensile strength is used in the calculation of spall volumes following a drilling intrusion. In the CCA, spall volumes were computed by a model of gas flow through fractures. Tensile strength entered the calculation of spall volumes by defining an effective gravity coefficient, which resisted particle mobilization in the flowing gas. The CCA calculations used a constant tensile strength of 0.0069 megapascal (MPa) (1 psi) (Helton et al. 1998). In response to EPA's review of the CCA, a new mechanistic model for spallings was developed in which gas flow in the waste may induce tensile failure of the waste material, and thus lead to spallings. The mechanistic model, called DRSPALL, served as the basis for a replacement for the CCA spallings model. In support of DRSPALL, a separate analysis determined an appropriate distribution for tensile strength would range from 0.12 MPa to 0.17 MPa (Hansen et al. 2003).

The range of tensile strength reported by Hansen et al. (2003) assumes that the waste is a weakly consolidated particulate material, representing an extreme case of waste degradation. The characteristics of the more robust waste forms (supercompacted and pipe overpack waste) would tend to less degradation, so the tensile strength of these waste forms would certainly be greater than the minimal values currently used in DRSPALL (Hansen et al. 2003). Therefore, the current range of tensile strength proposed for the DRSPALL model and for the CRA-2004 is conservative.

TRU WASTE-2.5.2.3 Permeability

The likely mechanical and physical form of the supercompacted and pipe overpack wastes over time indicates that the permeability of these waste forms will be at least as great as that of standard waste, and may be higher.

In the CCA, the waste permeability was assigned a value of 1.7×10^{-13} m^2 (Butcher 1996) based on the value used in the 1991 PA. The 1991 PA value was a composite value based on the relative quantities of three different types of materials (combustible, metals/glass, and sludges) each with an inherent range of permeabilities, which had previously been determined for compressed surrogate wastes (Luker et al. 1990). In their review of the data used in the CCA, the EPA recalculated this value as 2.4×10^{-13} m^2, although they conceded that the difference was small enough to be inconsequential (EPA 1997). This revised value is being used in the current PA calculations.

A constant value for permeability is used in PA, even though it is expected that there will be some variability in this parameter. The reason for this single value being acceptable is primarily because this permeability value is much higher than the surrounding salt and the disturbed rock zone, as discussed in 1991 PA. In addition, the coefficient of variation for the uncertainty in measured permeabilities is too small to justify treating waste permeability as an uncertain parameter (Rechard and Tierney 2003). Finally, Vaughn et al. (1995) discuss

whether permeability should be a function of porosity, since porosity is treated as a time-varying quantity in BRAGFLO while permeability is a constant. Their analysis concluded that including a dynamic model for permeability had an insignificant effect on waste room conditions (pressure and saturation), and an insignificant effect on resulting releases.

Waste Permeability of the New Waste Forms. The underlying assumption with respect to the new waste forms is that the pipe overpacks and supercompacted wastes will be more durable than the original baseline package of the 55-gallon drum. The rigidity of the waste and its packaging, such as the pipe overpack and supercompacted waste, tends to hold the room open and preserve the structural integrity of the waste stack. The logical evolution involved with disposal of a more rigid and armored waste package would be preservation of a large portion of the waste in its original, intact form as it will deform only modestly as compared to the standard waste form. Thus, the architecture of the waste comprises bulky, compressed steel containers that envelope the waste, and the rigid structure would tend to maintain the open channels between individual drums and packages, so that much of the original porosity inherent in the three-dimensional disposal configuration would be preserved. Permeability of this future state of the waste would tend to be high relative to the values implemented in the CCA and PAVT. This conclusion is reinforced by the results of the porosity surface calculations, which show that in the absence of gas generation the long-term porosity of the supercompacted and pipe overpack wastes is considerably higher than for standard waste, while with high gas generation rates the porosities are essentially the same (Park and Hansen 2003).

Waste Permeability in Process Models. Other conclusions can be drawn about the possible effects of waste heterogeneity on brine and gas flow in the repository. Vaughn et al. (1995, DR6) discuss how heterogeneity in the waste may cause flow to follow channels or preferential paths, and result in spatially varying saturations referred to as "puddling." Their analysis demonstrated that inclusion of puddling in the BRAGFLO model had an insignificant effect on waste room conditions (pressure and saturation), and an insignificant effect on resulting releases.

Waste Permeability in Direct Release Models. Waste permeability can affect the models for spallings and for direct brine releases. A pertinent study of the effects of spatially variable waste permeability was conducted as part of the spalling model investigations reported in Hansen et al. 1997. Calculations of gas flow through the porous waste regions were conducted to evaluate the influence of model assumptions on the predicted two-phase pressure response of the disposal rooms during a drilling intrusion. Results of the modeling indicated that the effect of waste heterogeneity is to reduce the pore pressure gradient close to the intruded wellbore; because this gradient is the major cause of tensile failure, any possible spall volumes are reduced.

TRU WASTE-2.5.3 Components and Characteristics Affecting Heat Generation

Heat generation is a characteristic of some components of the waste, or of their interactions. The WIPP includes two possibly significant sources of heat: the heat generated by RH-TRU waste (DOE 1995), and the heat generated by MgO hydration and carbonation, aluminum corrosion, cement hydration, and organic biodegradation.

TRU WASTE-2.5.3.1 Exothermal Reactions

MgO hydration and carbonation, aluminum corrosion, cement hydration, and organic biodegradation are all exothermal reactions. Evaluation of the ability of each of these reactions to produce heat while conservatively accounting for the repository's ability to dissipate the resulting heat generated has provided the following maximum temperature increases (Wang 1996d and Appendix PA, Attachment SCR), as shown in Table TRU WASTE-13:

Table TRU WASTE-13. Maximum Temperature Increases

Reaction Number	Maximum Temperature Increase (K)
MgO hydration	4.7
MgO carbonation	0.7
Cement hydration	2.5
Microbial degradation	1.4
Aluminum corrosion	6.8

In the worst case, a temperature increase of 6.8 K could be experienced (Appendix PA, Attachment SCR). However, these temperature extremes will not persist, if they are ever reached at all. Because all but one reaction consume brine, possible reactions will be competing with each other for what brine may enter the repository and will therefore temper the heat increase that could be predicted based on the most exothermic reaction alone. To evaluate the worst case possible, for the maximum temperature increase to be realized from the corrosion of aluminum, all of the aluminum would have to be corroded within 2.5 years, after which the heat would be dissipated very rapidly. Therefore, if such a condition were to be created, it would be transitory on the repository time scale and its influence inconsequential.

The effect of small temperature increases arising from exothermal reactions was previously screened out of the PA on the basis of low consequence to factors such as creep closure, seal performance, transport, etc. (see Appendix PA, Attachment SCR). The effect of heat generated by radiolysis has been considered as part of the repository conditions (Brush 1990) and utilized in the specification of experimental parameters, thus yielding data consistent with the anticipated conditions. Additionally, the small temperature increases cited above for exothermic reactions are insignificant to the thermodynamic modeling of solubility. For example, a temperature increase of 7°K would result in an approximately three percent change in the free energy of formation of any species contained within the model. This value is well within the model parameter bounds.

TRU WASTE-2.5.3.2 RH-TRU Thermal Heat Load

The "worst case" heat load from RH-TRU emplaced in the WIPP is estimated to be between 47 and 54 watts per cubic meter, which would result in a temperature rise near the canister of between 1.87°K and 2.09 K (2.85 – 3.19 K in the CCA). The expected WIPP average

temperature increase from RH-TRU heat loading is between 0.23 K and 0.29 K (0.38 – 0.49 K in the CCA). The RH-TRU thermal heat load is small enough that there is no impact on repository performance. A more complete discussion and analysis is given in Djordjevic (2003) and Appendix PA, Attachment SCR.

TRU WASTE-2.6 Summary

The waste characteristics and components expected to be most significant to performance are the predominant radionuclides and those characteristics and components affecting actinide mobility. The waste characteristics and components expected to be significant to performance are summarized in Table TRU WASTE-14.

It should be noted that these components and characteristics have both positive and negative effects on performance. Iron has a beneficial effect because it reduces actinides to lower, less soluble oxidation states. Nonferrous metals are beneficial because they bind organic ligands, thereby sequestering them. Mobility enhancers like colloidal substrates, on the other hand, have a detrimental effect. Gas buildup can both enhance and detract from repository performance. Although gas can open fractures, it can also keep brine from entering the repository, thereby reducing transport of soluble actinides (SNL 1991).

Table TRU WASTE-15 summarizes those characteristics and components with an insignificant impact on performance.

Table TRU WASTE-14. Waste Characteristics and Components Expected to be Most Significant to Performance

Component	Characteristic	Reason for Significance
^{239}Pu, ^{240}Pu, ^{241}Am, ^{233}U, and ^{234}U	Activity	99 percent of EPA unit after 2,000 years
^{238}Pu	Activity	Dominates EPA Unit at early times
Pu and Am	Solubility	Large EPA Unit; mobility depends on solubility
^{238}U	Activity	Very low activity; dilutes Higher-Activity Uranium Isotopes For Brine-Based Releases
Iron	Corrosion	1. Maintains reducing environment; lower, less soluble oxidation states of actinides predominate 2. Corrosion produces hydrogen, increasing gas pressure
CPR Materials, Nitrate, Sulfate	Nutrient for microbes	Microbial nutrients are metabolized to methane and other gases, increasing gas pressure; formation of colloids
Humic Materials, Cellulosic Materials breakdown products	Colloid formation	Form humic colloids that sorb and transport actinides
Organic Complexation	Nonferrous metals	Prevent increase in actinide solubility by binding with ligands
Tensile and Shear strength	Waste strength	Important to spalling and cavings

Table TRU WASTE-15. Waste Characteristics and Components Expected to be Not Significant

Characteristics/Component	*Reason for insignificant impact*
Radionuclides (other than those in Table TRU WASTE-14)	*EPA Unit is negligible fraction of total, even with ingrowth*
Substances that may affect pH[1]	*pH is buffered by MgO*
Substances that produce CO_2[1]	*CO_2 is removed by reaction with MgO*
Intrinsic and mineral fragment colloids	*Fraction of actinides mobilized by these colloids is insignificant*
Organic ligands	*Removed by binding with Mg and nonferrous metal*
Heat generated by exothermic reactions	*Temperature rise is negligible; heats of formation are very small paired with a large thermal mass of the repository*
Fluid in the waste	*Negligible compared to brine volume*

[1] *These components are significant for gas generation, but not for actinide solubility.*

TRU WASTE-3.0 WASTE COMPONENTS LIMITS

The objective of this section is to satisfy the requirements specified in 40 CFR.194(c)(1) as stated in Section TRU WASTE-1.1.

This section updates Appendix WCL in the CCA by presenting the rationale for the upper and lower limits for waste components identified as potentially significant to disposal system performance (Table TRU WASTE-4). The sensitivity analysis in Appendix PA supports the conclusions that the disposal system performance is not sensitive to most properties of the emplaced waste and limits remain unnecessary for the components identified in Tables TRU WASTE-5 and TRU WASTE-6.

Table TRU WASTE-16 shows:

- *Waste components listed as potentially significant in Table TRU WASTE-4,*
- *Waste characteristics these components influence,*
- *Constituents of the components for which assaying during emplacement is required, and*
- *Limits for emplacement of each component, if necessary.*

This table illustrates that most components, associated characteristics, assay requirements, and emplacement limits have not changed since the CCA. The following discussion provides the rationale for the proposed assaying and emplacement limits for each component listed in Table TRU WASTE-16. All of the components listed in Tables TRU WASTE-5, TRU WASTE-6 and TRU WASTE-15 were found to be insignificant to disposal system performance, as was true for the CCA. Therefore, it is not necessary to establish emplacement limits for them other than limits based on the current TRU waste inventory or imposed on waste through limitations in the Contact Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant (DOE 2002a).

The emplacement limits identified in Table TRU WASTE-16 provide an envelope of fixed inventory values on a repository scale, without an associated uncertainty. That is, the limiting values are imposed to ensure compliance, and in fact represent the upper "end" of an uncertain range. To ensure these waste component limits are not exceeded, inventory quantities and uncertainty in those quantities will be tracked during the operational phase of the repository. This tracking is accomplished using the WWIS. If inventory estimates change over the operational life of the WIPP, new inventory estimates will be used in PA and revised limits for waste components will be developed based on the PA results in a future recertification application.

TRU WASTE-3.1 Radionuclide Components

As discussed in Section TRU WASTE-2.3, the following radionuclides have activities greater than one EPA unit at closure: ^{241}Am, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{233}U, ^{234}U, ^{90}Sr, and ^{137}Cs.

Table TRU WASTE-16. Emplacement Limits for Waste Components

Components	*Associated Characteristics*	*Constituent Components Requiring Assaying*	*Emplacement Limits*
Radionuclides	*Radioactivity at closure* *Radioactivity after closure* *Solubility* *Colloid formation* *Redox state*	*^{241}Am* *^{238}Pu* *^{239}Pu* *^{240}Pu* *^{242}Pu* *^{233}U* *^{234}U* *^{238}U* *^{90}Sr* *^{137}Cs*	*none[1]*
Ferrous metals (iron)	*Redox potential* *H_2 gas generation* *complexing with organic ligands*	*None*	*Minimum = 2.0×10^7 kg (amount from containers)[2]*
CPR materials	*Gas generation* *Humic colloids (see below)*	*Sum*	*Maximum = 2.2×10^7 kg[3]*
Sulfates	*Gas generation*	*None*	*None[4]*
Nitrates	*Gas generation*	*None*	*None[4]*
Solid components	*Particle size* *Effective shear resistance to erosion* *Tensile strength*	*None*	*None*
Free water emplaced with waste	*Gas generation*	*None*	*Maximum = 1684 m^3 (limit of one percent total waste volume as set by the WAC)[5]*
Humic substances	*Radionuclide-bearing humic colloids*	*None*	*None*
Nonferrous metals (metals other than iron)	*Bind with organic ligands and prevent increased solubility*	*None*	*Minimum = 2.0×10^3 kg[6]*
Organic ligands	*Solubility*	*None*	*None[4]*

[1] Inventory curie content will be tracked.
[2] Minimum sets to ensure sufficient reactants for reducing radionuclides to lower and less soluble oxidation states.
[3] Maximum set to ensure sufficient MgO is available to react with CO_2 produced.
[4] For the current waste generation processes that are documented in Appendix DATA.
[5] One percent of the design basis values for CH-TRU of 168,485 m^3.
[6] Minimum quantity for complexing with organic ligands (see Appendix PA, Attachment SOTERM).

The total activity of the waste at emplacement and during the entire 10,000-year performance period is dominated by the activities of four emplaced radionuclides: ^{241}Am, ^{238}Pu, ^{239}Pu, and ^{240}Pu. The radionuclides, ^{242}Pu, ^{233}U and ^{234}U, have significantly less total activity than the other Am and Pu components, but since their activities exceed one EPA unit they are not excluded from assaying requirements. The ^{238}U component is to be assayed as well, because its large mass fraction and low activity dilutes the overall activity of transported uranium species. The ^{90}Sr and ^{137}Cs components can contribute to direct releases at the surface resulting from inadvertent intrusion during the first several hundred years or so after closure.

Because of radioactive decay and ingrowth, the major contributors to the overall activity of the repository among these radionuclides change during 10,000 years. For the first several hundred years, ^{241}Am, ^{238}Pu, ^{239}Pu, and ^{240}Pu are important contributors to the total activity of the waste. At the present and projected inventory level, ^{90}Sr and ^{137}Cs may be important for about 200 years. The ^{241}Am component continues to be important for about 3,000 years. At 10,000 years, ^{239}Pu and ^{240}Pu remain as the only significant contributors to the total activity of the waste. Because the activities of these radionuclides in existing and projected waste overwhelmingly exceed the activities of all other radionuclides combined, they are the most important for repository performance modeling.

The total activity of the waste is not important for compliance with the criteria at 40 CFR § 194.24(c) because the containment requirements are normalized to the initial inventory. However, the PA is sensitive to relative changes in inventory curie content as a function of radionuclide decay and ingrowth over time. The magnitude of change in the total curie content depends on the initial ratios of the total activities of the assayed radionuclides at the time of repository closure. Accordingly, the results of the PA are conditional on the initial ratios in the inventory. The criteria in 40 CFR § 194.15(a)(5) state that:

> *In submitting documentation of continued compliance pursuant to section 8(f) of the WIPP LWA,….. Updated documentation shall include:… A description of all waste emplaced in the disposal system since the most recent compliance certification or recertification application.*

The PA for this and future recertifications must therefore incorporate the adjusted inventory curie content reflecting any significant changes relative to projected values for the important radioisotopes (plus ^{238}U) that are being accumulated. At repository closure, the ratios of the activities of the ten listed radionuclides (Table TRU WASTE-15) may or may not be similar to those ratios used in this assessment, but compliance with the containment requirements of 40 CFR §191.13 will be maintained for the full capacity of emplaced waste at the WIPP.

TRU WASTE-3.2 Ferrous and Ferrous Alloy Components

Ferrous and ferrous-alloy metal components in the waste have two significant effects on the repository. Ferrous and ferrous-alloy metal may corrode, thus creating gas, and they provide reducing conditions in the repository (see Section TRU WASTE-2.4.1).

The results of the CRA-2004 PA demonstrate that total normalized release from the repository is relatively insensitive to gas generation by corrosion. As shown in Figures PA-97 through PA-99 in Appendix PA, at probabilities greater than 0.01, total normalized release is dominated by cuttings and cavings releases. The cuttings and cavings release mechanism is completely independent of repository hydrologic conditions, such as gas pressure or brine saturation, at the time of the intrusion. This independence from repository pressure leads to the conclusion that total normalized release will be insensitive to gas generation. The other two direct release mechanisms for the CRA-2004 PA, spallings and direct brine release, are dependent on the quantity of gas generated. These two release mechanisms occur only if the pressure in the repository exceeds 8 MPa (Appendix PA, Sections PA.4.6 and PA.4.7.1). This pressure (8 MPa) corresponds to the hydrostatic pressure at the repository depth in a column of drilling mud.

The waste inventory contains sufficient ferrous and ferrous-alloy components that gas could be generated sufficiently in excess of that required to reach 8 MPa in the repository. In fact, there is always an excess of ferrous and ferrous-alloy metals, in the sense that the inventory of these metals is never depleted in any of the 300 realizations for the CRA-2004 PA (Stein and Zelinski 2003b). In this situation, PA already uses an extreme value for the mass of ferrous and ferrous-alloy metals, so that a maximum value for the mass of ferrous and ferrous-alloy metals would be extraneous (have no impact) on PA.

In summary, the dominance of the cuttings/cavings mechanism for total normalized release, and the excess mass of ferrous and ferrous-alloy metals in the initial inventory imply that it is unnecessary to place restrictions on the quantity of ferrous and ferrous-alloy metals emplaced for the purpose of controlling the quantity of gas generated.

On the other hand, ferrous and ferrous-alloy metals (and their corrosion products) provide the reactants that reduce radionuclides to lower and less-soluble oxidation states. As discussed in Section TRU WASTE-2.4.1.1, the anticipated quantity of these metals, principally from waste containers, to be emplaced in the WIPP is orders of magnitude in excess of the quantity required to assure reducing conditions. Therefore, no upper or lower limit need be established for the quantity of ferrous and ferrous-alloy metals that may be emplaced, beyond the CCA projection of the ferrous and ferrous-alloy metals in the waste containers.

TRU WASTE-3.3 CPR Materials, Nitrate, and Sulfate Components

The CPR materials, nitrate, and sulfate components of the waste influence the production of CH_4 gas in the repository by microbial action. Although the PA assigns a probability of 0.5 that microbial degradation will produce significant quantities of gas, the lower limit for these materials is effectively zero. As discussed in the preceding section, releases are dominated by cuttings/cavings, which is independent of repository pressure at the time of the intrusion. In addition, direct brine release and spallings are not sensitive to the quantity of gas generated, and the inventory of ferrous and ferrous-alloy metals is in excess of that required to produce a significant amount of gas (pressures of 8 MPa, or greater). Therefore, the additional components influencing microbial degradation have negligible impact on performance, and it is unnecessary, with respect to gas generation, to assign an upper limit on the amount of these materials that may be emplaced in the repository.

However, an upper limit on the total amount of CPR materials is still necessary to ensure that the amount of emplaced MgO is adequate. The current waste inventory indicates that there will be 2.19×10^7 kg of CPR materials disposed in WIPP. Since the amount of MgO currently projected for the WIPP is greater than the amount needed to react with the CO_2, the upper limit for CPR materials is set to 2.2×10^7 kg. Additional information on the safety factor for MgO relative to the emplaced mass of CPR materials is provided in Appendix BARRIERS-2.5.

TRU WASTE-3.4 Solid Components

Solid components in the waste affect the waste characteristics of effective shear resistance to erosion, particle size, and tensile strength. These properties affect releases from cavings and spallings during a drilling intrusion. The basic conceptualization for the assignment of these

properties is that fully degraded waste will have the least favorable properties, and will eventually be similar to granular materials whose properties can be measured today. The actual properties of the waste over the 10,000-year regulatory period are unknown, since the physical nature of the degraded waste is unknown. For these reasons, the parameter values assigned are chosen to conservatively reflect measured properties of natural and constructed materials.

These properties are reasonable analogs for degraded waste. The effective shear resistance to erosion used to calculate cavings is based on the erodibility of unconsolidated marine clays and other easily eroded materials, and is considered to be near a physical limit for the minimum value of this property (Parameter 58 in Attachment PAR to Appendix PA). The minimum particle size used in the range for the spallings model is based on assuming an average pore diameter consistent with an average waste permeability; this value is considered conservative because waste will not have a uniform distribution of permeability. The larger particles will define the more permeable pathways, along which most gas will flow during a spalling event, and larger particles are less likely to spall than smaller particles. Last, the tensile strength of the waste assigned for the spalling process is uncertain, ranging from 0.12 MPa to 0.17 MPa (Hansen et al. 2003 - DRSPALL parameter report). Tensile strength was developed from laboratory experiments on surrogate materials, which represented highly degraded residuals from typical waste inventory. These values are felt to represent extreme, low-end tensile strengths because they do not account for several strengthening mechanisms, such as MgO hydration and halite precipitation/cementation (see Hansen et al. 1997).

The properties assumed for solid components in PA bound the least favorable behavior of these components. Therefore, the PA analysis is not conditional on the quantities and kinds of solid components that will be emplaced. Upper or lower limits are not necessary for solid waste components because parameter values have been chosen conservatively.

TRU WASTE-3.5 Water Components

The amount of water emplaced with the waste can affect the rate at which gas is generated for a short period soon after closure, but the small quantity of water acceptable in the waste is not a concern for long-term performance. Consequently, there is no need to monitor water in the waste for compliance with 40 CFR § 194.24(c). In fact, the quantity of water in the waste used for PA calculations is greater than the Waste Acceptance Criteria allows, so the only limit on free water content of the waste is set by the Waste Acceptance Criteria. The FEPs screening analysis (Appendix PA, Attachment SCR) assumes no more than one percent volume of free liquid by container.

TRU WASTE-3.6 Humic Substances Components

Humic substances are likely to be introduced into the repository as a component of wastes containing soils or may form in situ from reactions involving microbial metabolites produced during degradation of cellulosic materials. Humic substances will dissolve until a solubility limit is reached. Dissolved humic substances are colloidal in nature and may complex radionuclides. The radionuclide-bearing humic colloids may be transported in moving liquid and contribute to a radionuclide release.

In PA, a steady-state concentration of humic colloids is assumed to exist in the repository during the performance period. This concentration is not inventory limited; in other words, it is assumed in PA that sufficient source materials exist that a constant concentration of humic colloids will be present at all times. Because it is assumed that there is sufficient solid material present for a steady-state concentration to exist at all times in the repository, PA results are not conditional on the quantity of total humic substances present, and there is no need to provide a maximum or minimum limit for the quantity of humic substances that may be emplaced in the repository.

TRU WASTE-3.7 Nonferrous Metal Components

The nonferrous metals present in the waste stream impact PA because they will dissolve and bind to organic ligands, thereby reducing the impact of organic ligands on the solubility of radionuclides (see Section TRU WASTE-2.4.1.3). According to the existing and projected inventory and composition of waste canister steels, these components will be emplaced in considerable excess of that required to sequester organic ligands. Therefore, no upper or lower limit need be established for the quantity of non-ferrous metals beyond the present projection of the non-ferrous metals in waste containers, and assay is not required for these metals.

TRU WASTE-3.8 Organic Ligands Components

The effects of organic ligands are directly considered in the CRA-2004 PA (Appendix PA, Attachment SCR, Section SCR-6.5.6). Since the organic ligand inventory has increased over that evaluated in the CCA, organic ligand concentrations were included in the actinide solubility calculations for recertification. Including the organic ligand concentrations in the solubility calculations had an insignificant impact on actinide solubility (see Appendix PA, Attachment SOTERM-5.0). Therefore, no upper or lower limit need be established for the quantity of organic ligands in the waste.

TRU WASTE-4.0 WASTE CHARACTERIZATION

The regulation 40 CFR § 194.24(c)(2) and (3) require that the DOE identify and describe the methods used to quantify the limits presented in Section TRU WASTE-3.0 for the waste components identified as potentially significant to the long-term performance of the disposal system. These waste components are radionuclides, free water, ferrous metals, nonferrous metals and CPR materials. The repository limits and the associated approved characterization methods for each of these components is summarized below:

- *Although Section TRU WASTE-3.0 does not specify limiting values for the activities and masses of specific radionuclides, the cumulative total activities of the specified radionuclides (^{241}Am, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{233}U, ^{234}U, ^{238}U, ^{90}Sr, and ^{137}Cs) must be reported and tracked to ensure that the total radionuclide inventory of the repository is consistent with the levels used for the current PA. The presence of these specific radionuclides, in terms of activities and masses, including associated total measurement uncertainties, is determined from acceptable knowledge (AK) and radioassay.*

- *The acceptance criterion specified in the CH-WAC states that there shall be no more than 2.5 cm (1 in) in the bottom of internal containers and the total residual liquid in any payload container shall not exceed 1% by volume of that payload container. The FEPs screening analysis (Appendix PA, Attachment SCR) assumes no more than one percent volume of free liquid by container. Therefore, the repository limit for free liquid is a maximum of 1,684 m^3 (1% by volume liquid per container × the expected number of containers). The qualitative methodologies of AK, radiography, or visual examination, used either singly or in combination, verify adherence to the compliance limits.*

- *The repository limit for ferrous metals is a minimum of 2.0×10^7 kg. This limit will be met in the total repository inventory by the quantity of ferrous metals that make up the payload containers alone; thus, the number and type of payload containers emplaced in the repository are tracked.*

- *The repository limit for nonferrous metals is a minimum of 2.0×10^3 kg (which was already met with the waste emplaced in the repository as of September 30, 2002). This limit will be met in the total repository inventory by the quantity of nonferrous metals that make up the payload containers alone; thus the number and type of payload containers emplaced in the repository are tracked.*

- *The repository limit for CPR materials is a maximum of 2.2×10^7 kg. The TRU waste sites are required to determine the CPR material weights in the waste by AK supplemented by radiography and/or visual examination.*

The methods used to quantify the above waste components are summarized below with more detailed descriptions in the following documents:

- *Contact-Handled Transuranic Waste Acceptance Criteria (CH-WAC), Appendix A (DOE 2002a)*

- *WIPP Hazardous Waste Permit, Waste Facility Analysis Plan (WAP), Attachments B through B6 (DOE 2003a)*

This section does not repeat the provisions of the WAP and the CH-WAC. References to the WAP and WAC will direct the reader to more detailed information on the CH-TRU waste characterization methods, where appropriate. The RH-TRU waste characterization methods are pending EPA approval and are not discussed here. Information on the proposed RH-TRU waste characterization program is contained in DOE (2002b).

TRU WASTE-4.1 Acceptable Knowledge

AK is the compilation of process knowledge and available existing information to characterize a TRU waste stream. AK includes information regarding the physical form of the waste, the base materials composing the waste, and the process that generates the waste. AK is discussed in the WAP and CH-WAC. AK discussions in the WAP delineate waste streams and characterize the chemical and physical properties of the waste, such as the amount of free liquid and waste material parameters. The CH-WAC discusses AK characterization requirements for the nuclear properties (i.e., as radionuclide activity and the distribution of the 10 WIPP-tracked isotopes) that each TRU waste site must obtain.

TRU WASTE-4.2 Radioassay

The EPA requires radiological characterization data to track the WIPP radionuclide inventory, by isotopic distribution and activity, of the ten WIPP-tracked radionuclides (^{241}Am, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{233}U, ^{234}U, ^{238}U, ^{90}Sr, and ^{137}Cs). This requisite data is derived from AK, radioassay or both. DOE-approved radioassay techniques are discussed in Attachment A of the CH-WAC (DOE 2002a).

Nondestructive analysis is a noninvasive radioassay method allowing the radiological characteristics of a waste container to be determined without altering its physical or chemical form. A variety of nondestructive assay (NDA) methodologies are effective in meeting the requirements of the CH-WAC.

Radiochemical analysis, another approved radioassay method, is more time consuming and has an inherently higher risk of exposure to the personnel performing the assay. Exposure to radiation is minimized when NDA methods are employed in place of intrusive measurement methods, making NDA the preferred choice for waste assay.

TRU WASTE-4.3 Radiography

Radiography is a nondestructive technique that involves x-ray examination of waste containers to identify and verify waste container contents; specifically to verify the physical form of the waste to identify and assess the quantity of CPR materials.

TRU WASTE-4.4 Visual Examination

Visual examination consists of an evaluation of the waste container contents. It verifies and augments the description of waste container contents derived from AK or radiography by opening the container and physically inspecting the contents. TRU waste sites may opt to substitute visual examination in place of radiography as long as all waste containers are inspected.

TRU WASTE-5.0 WIPP WASTE INFORMATION SYSTEM

All TRU waste sites planning to ship TRU waste to WIPP will supply the required characterization data to the computerized data management system known as the WWIS. The system continues to be used to gather, store, and process information pertaining to TRU waste destined for or disposed at the WIPP and includes automatic certification-based compliance limit and quality assurance checks. The WWIS is designed, maintained and operated in compliance with nuclear quality assurance requirements for computer software for nuclear facility applications.

To ensure compliance with the data requirements, CBFO reviews the data package for each container of each shipment for completeness and adequacy before notifying the shipping site of acceptance. Thus, the WWIS becomes an integral part of the waste information screening process. DOE provides EPA with an annual report using information generated from the WWIS on waste parameters as identified in Table TRU WASTE-16.

REFERENCES

ASME (American Society of Mechanical Engineers). 1989. "Part 2.7 Quality Assurance Requirements of Computer Software for Nuclear Facility Applications," Quality Assurance Requirements for Nuclear Facility Applications. ASME NQA-2a-1990, Part 2.7. May 31, 1990. ASME, New York, NY.

Berglund, J.W., J. Myers, L.R. Lenke. Memo to M.S.Y. Chu. 1996. "Estimate of the Tensile Strength of Degraded Waste for Use in Solids Blowout." July 19, 1996. ERMS #239423.

Brush, L.H. 1990. Test Plan for Laboratory and Modeling Studies of Repository and Radionuclide Chemistry for the Waste Isolation Pilot Plant. SAND90-0266. Albuquerque, NM: Sandia National Laboratories.

Brush, L.H. and Y. Xiong. 2003a. Calculation of Actinide Solubilities for the WIPP Compliance Recertification Application, Analysis Plan AP-098, Rev. 1. AP-098, Revision 1. Carlsbad, NM: Sandia National Laboratories. ERMS #527714.

Brush, L.H. and Y. Xiong. 2003b. Calculation of Organic Ligand Concentrations for the WIPP Compliance Recertification Application. Carlsbad, NM: Sandia National Laboratories. ERMS #527567.

Butcher, B.M. 1990. Disposal Room Porosity and Permeability Values for Disposal Room Performance Assessment Memorandum to M.G. Marietta. Included in SAND89-2408. Albuquerque, NM: Sandia National Laboratories. ERMS #306803.

Butcher, B.M., T.W. Thompson, R.G. VanBuskirk, and N.C. Patti. 1991. Mechanical Compaction of Waste Isolation Pilot Plant Simulated Waste. SAND90-1206. Albuquerque, NM: Sandia National Laboratories.

Butcher, B.M. 1996. Memorandum to M. Tierney, "QAP 9-2 Documentation for the Overall Waste Permeability and Flow Property Values for the CCA." Sandia National Laboratories, Albuquerque, NM. ERMS #230921.Callahan, G.D. 1993. "Appendix A: Further Discussion of the TRU Waste Model," A Summary of the Models Used for the Mechanical Response of Disposal Rooms in the Waste Isolation Pilot Plant with Regard to Compliance to 40 CFR 191, Subpart B. B.M. Butcher and F.T. Mendenhall. SAND92-0427. Albuquerque, NM: Sandia National Laboratories. A-27 through A-30.

Clark, D.L., Hobart, D.E., and Neu, M.P. 1995. "Actinide Carbonate Complexes and Their Importance in Actinide Environmental Chemistry." Chem Revs. v. 95, pp. 25-48.

Djordjevic. 2003. Estimation of Maximum RH-TRU Thermal Heat Load for WIPP for the Compliance Recertification Application, Supercedes 529634, Revision 1. ERMS # 531593. Carlsbad, NM: Sandia National Laboratories.

Drez, P. 1996. Final Preliminary Estimate of Complexing Agents in TRU Solidified Waste Forms Scheduled for Disposal in WIPP. Carlsbad, NM: Sandia National Laboratories. ERMS # 235552.

Drez, P.E., and P. James-Lipponer. 1989. "Preliminary Nonradionuclide Inventory for CH-TRU Waste," unpublished report cited in Brush, L.H. 1990. Test Plan for Laboratory and Modeling Studies of Repository and Radionuclide Chemistry for the Waste Isolation Pilot Plant. SAND90-0266. Albuquerque, NM: Sandia National Laboratories.

Felmy, A.R., D. Rai, S.M. Sterner, M.J. Mason, N.J. Hess, and S.D. Conradson. 1996. "Thermodynamic Models for Highly Charged Aqueous Species: The Solubility of Th(IV) Hydrous Oxide in Concentrated $NaHCO_3$ and Na_2CO_3 Solutions."

Francis, A.J., and J.B. Gillow. 1994. Effects of Microbial Processes on Gas Generation Under Expected Waste Isolation Pilot Plant Repository Conditions. Progress Report through 1992. SAND93-7036. Albuquerque, NM: Sandia National Laboratories.

Garner, J. 1996. Radioisotopes to Be Used in the 1996 CCA Calculations. ERMS # 235202.

Hansen, F. D., M.K. Knowles, T.W. Thompson, M. Gross, J.D. McLennan and J.F. Schatz. 1997. Description and Evaluation of a Mechanistically Based Conceptual Model for Spall, SAND97-1369. Sandia National Laboratories, Albuquerque, NM.

Hansen, F.D., T. W. Pfeifle, and D.L. Lord. 2003. Parameters Justification Report for DRSPALL, SAND2003-2930, Sandia National Laboratories, Albuquerque, NM.

Helton, J.C., Bean, J.E., Berglund, J.W., Davis, F.J., Economy, K., Garner, J.W., Johnson, J.D., MacKinnon, R.J., Miller, J., O'Brien, D.G., Ramsey, J.L., Schreiber, J.D., Shinta, A., Smith, L.N., Stoelzel, D.M., Stckman, C., and P. Vaughn. 1998. Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant. SAND98-0365. Sandia National Laboratories, Albuquerque, NM.

Hobart, D.E. 1990. "Actinides in the Environment," in Proceedings of the Robert A. Welch Foundation Conference on Chemical Research, No. XXXIV: 50 Years With Transuranium Elements. October 22-23, 1990.

Jepsen, R., J. Roberts, and W. Lick. 1998. Development and Testing of Waste Surrogate Materials for Critical Shear Stress. Sandia National Laboratories, Albuquerque, NM. ERMS #252647.

Katz, J.J., G.T. Seaborg, and L.R. Morss. 1986. The Chemistry of the Actinide Elements, 2 volumes, New York: Chapman and Hall.

Kim, J.I., Ch. Apostolidis, G. Buckau, K. Bueppelmann, B. Kannellakopoulos, Ch. Lierse, S. Magirius, R. Stumpe, I. Hedler, Ch. Rahner, and W. Stoewer. 1985. "Chemisches Verhalten von Np, Pu und Am in verschiedenen konzentrierten Salzloesunger" RCM 01085. Munich, Germany: Institut fuer Radiochemie der Technische Universitaet Muenchen.

Fox, B. 2003. Analysis of EPA Unit Loading Calculation, Compliance Recertification Application, Superceded ERMS #530304, Revision 1. Carlsbad, NM: Sandia National Laboratories. ERMS #531582.

Leigh, C. 2003a. Calculation of the Waste Unit Factor in the Compliance Recertification Application, Supercedes ERMS #529148, Revision 1. Carlsbad, NM: Sandia National Laboratories. ERMS #531099.

Leigh, C. 2003b. Radionuclides Expected to Dominate Potential Releases in the Compliance Recertification Application, Supercedes ERMS #529245, Revision 1. Sandia National Laboratories. Carlsbad, NM. ERMS #531086.

Leigh, C. 2003c. Calculation of Radionuclide Inventories for Use in NUTS in the Compliance Recertification Application, Supercedes ERMS #529289, Revision 1. Sandia National Laboratories. Carlsbad, NM. ERMS #531090.

Luker, R.S., T.W. Thompson and B.M. Butcher. 1990. "Compaction and Permeability of Simulated Waste" Proc. 32nd U.S. Symposium on Rock Mechanics, Norman OK, 1990.

Martell, Arthur E. and Robert M. Smith. 1982. Critical Stability Constants, Volume 5: Other Organic Ligands, Plenum Press, New York.

NAS-NRC. 1957. Disposal of Radioactive Waste on Land. Report by the Committee on Waste Disposal, Division of Earth Sciences, National Academy of Sciences-National Research Council, Washington, DC.

Nitsche, H. and N.M. Edelstein. Radiochimica Acta 1985, 39, 22.

Papenguth, H.W. 1996a. "Colloidal Actinide Source Term Parameters." March 29, 1996. ERMS #36771.

Papenguth, H.W. 1996b. "Parameter Record Package for Colloidal Actinide Source Term Parameters - Attachment A: Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids." May 7, 1996. ERMS #35852.

Papenguth, H.W. 1996c. "Parameter Record Package for Colloidal Actinide Source Term Parameters - Attachment A: Rationale for Definition of Parameter Values for Microbes." May 7, 1996. ERMS #35856.

Papenguth, H.W. 1996d. "Parameter Record Package for Colloidal Actinide Source Term Parameters - Attachment A: Rationale for Definition of Parameter Values for Humic Substances." May 7, 1996. ERMS #235855.

Papenguth, H.W. 1996e. "Parameter Record Package for Colloidal Actinide Source Term Parameters - Attachment A: Rationale for Definition of Parameter Values for Mineral Fragment Type Colloids." May 7, 1996. ERMS #235850.

Papenguth, H.W., and Y.K. Behl. 1996. Test plan for evaluation of colloid-facilitated actinide transport at the Waste Isolation Pilot Plant. SNL Test Plan TP 96-01.

Park, B.Y. and F.D. Hansen. 2003. Determination of the Porosity Surfaces of the Disposal Room Containing Various Waste Inventories for the WIPP PA. Sandia National Laboratories. Albuquerque, NM.

Pryke, D.C. and J.H. Rees. 1987. "Understanding the Behavior of the Actinides Under Disposal Conditions: a Comparison between Calculated and Experimental Solubilities." Radiochimica Acta, v. 51 p. 27.

Rai, D. and Strickert, R.G. 1980. "Chemical Aspects of Medium and Long-term Radioactive Waste Disposal." Trans. Am. Nuclear Soc. and Eur. Nuclear Soc. v. 35, p. 185.

Rai, D., Strickert, R.G. and McVay, G.L. 1982. "Neptunium Concentration in Solutions Containing Actinide-Doped Glass." Nuclear Technology v. 58, p. 69.

Rechard, R.P., and M.S. Tierney. 2003. Assignment of Probability Distributions for Parameters in the 1996 Performance Assessment for the Waste Isolation Pilot Plant, Part 2: Application of Process. Sandia National Laboratories, Albuquerque, NM.

Sanchez, L.C. 1996. Identification of Important Radionuclides Used in 1996 CCA WIPP Performance Assessment, April 25, 1996.

Sandia WIPP (Sandia National Laboratories). 1991. Preliminary Comparison with 40 CFR 191, Subpart B for the Waste Isolation Pilot Plant, December 1991. SAND91-0893/3. Albuquerque, NM: Sandia National Laboratories. ERMS #226419.

Sandia WIPP (Sandia National Laboratories). 2003. Performance Assessment Parameters Database (PAPDB), Version 1.0. Carlsbad, NM: Sandia National Laboratories. ERMS #518612.

State of New Mexico, ex rel., Jeff Bingaman, Attorney General of the State of New Mexico, Plaintiff, v. The United States Department of Energy, et al., Defendants. 1981. Stipulated Agreement. Civil Action No. 81-0363 JB. (United States District Court for the District of New Mexico). July 1, 1981. (Copy on file at the Sandia WIPP Records Center, ERMS #242008.)

Stein, J. and Zelinski, W. 2003. "Analysis Package for BRAGFLO: Compliance Recertification Application." Sandia National Laboratories. Carlsbad, NM. Sandia WIPP Central Files ERMS # 530163.

U.S. Department of Energy (DOE). 1995. Remote-Handled Transuranic Waste Study. DOE/CAO95-1095, Carlsbad, NM. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.

U.S. Department of Energy (DOE). 1996. Title 40 CFR 191 Compliance Certification Application for the Waste Isolation Pilot Plant. DOE/CAO-1996-2184. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.

U.S. Department of Energy (DOE). 1997. Performance Assessment Verification Test. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Area Office.

U.S. Department of Energy (DOE). 2001, "WIPP Waste Information System User's Manual for Use by Shippers/Generators," DOE/CAO 97-2273, Carlsbad Field Office, Carlsbad, NM.

U.S. Department of Energy (DOE). 2002a. Contact Handled Transuranic Waste Acceptance Criteria for the Waste Isolation Pilot Plant, DOE/WIPP-02-3122, U.S. Department of Energy, Carlsbad Field Office, Carlsbad, NM.

U.S. Department of Energy (DOE). 2002b. "Notification of Planned Change to the EPA 40 CFR Part 194 Certification of the Waste Isolation Pilot Plant, Remote Handled TRU Waste Characterization Plan," Revision 0. December 16, 2002, U.S. Department of Energy, Carlsbad Field Office, Carlsbad, NM.

U.S. Department of Energy (DOE). 2003. WIPP Hazardous Waste Facility Permit Attachment B through B6, Waste Analysis Plan, January 30, 2003, Carlsbad Field Office, Carlsbad, NM.

U.S. Environmental Protection Agency (EPA). 1985. High-Level and Transuranic Radioactive Wastes: Background Information for Final Rule. EPA 520/1-85-023. U. S. Environmental Protection Agency, Washington, D.C.

U.S. Environmental Protection Agency (EPA). 1997. Response to comments, Section 5 Models and Codes – Section 194.23, Issue L: CCA parameters and PAVT parameter selection, Response to Comments 5.L.4 and 5.L.5.

U.S. Environmental Protection Agency (EPA). 1998. Technical Support Document for Section 194.24: Consolidated Compliance Review of Waste Characterization Requirements, Docket No: A-93-02, V-B-15.

U.S. Environmental Protection Agency (EPA). 2002. Letter from F. Marcinowski, Director, Radiation Protection Division, to Dr. I. Triay, Manager, Carlsbad Field Office, June 7, 2002.

Vaughn, P., Bean, J., Garner, J., Lord, M., MacKinnon, R., McArthur, D., Schreiber, J., and Shinta, A.. 1995. FEPs Screening Analysis DR2, DR3, DR6, DR7 and S6. Sandia National Laboratories, Albuquerque, NM. ERMS #238152.

Wang, F. and L.H. Brush. 1996. "Estimates of Gas-Generation Parameters for the Long-Term WIPP Performance Assessment." Albuquerque, NM: Sandia National Laboratories. ERMS# 231943.

Wang, Y. 1996a. Estimate of repository pH and f(CO2) Distribution for the Long-Term WIPP Performance Assessment. ERMS # 237415.

Wang, Y. 1996b. Evaluation of the Thermal Effect of MgO Hydration for the Long-term WIPP Performance Assessment. ERMS # 237743.

Wang, Y. 1996c. Define Chemical Conditions for FMT Actinide Solubility Calculations. ERMS # 230819.

Wang, Y. 1996d. Evaluation of the Thermal Effect of Exothermal Chemical Reactions for WIPP Performance Assessment. July 19, 1996. ERMS #239647.

Weatherby, J.R., W.T. Brown, and B.M. Butcher. 1991. "The Closure of WIPP Disposal Rooms Filled with Various Waste and Backfill Combinations," Rock Mechanics as a Multidisciplinary Science, Proceedings of the 32nd U.S. Symposium, University of Oklahoma, Norman, OK, July 10-12, 1991. Ed. J.C. Roegiers. SAND90-2399C. Brookfield, VT: A.A. Balkema. 919-928.

Weiner, R. 1996. "Dissolved Ligand Concentration." March 27, 1996. ERMS #236163.

WIPP PA (Performance Assessment) Division. 1991. Preliminary Comparison with 40 CFR Part 191, Subpart B for the Waste Isolation Pilot Plant, December 1991. Volumes 1 and 3: Reference Data. SAND91-0893/1 and SAND91-0893/3. Eds. R.P. Rechard, A.C. Peterson, J.D. Schreiber, H.J. Iuzzolino, M.S. Tierney, and J.S. Sandha. Albuquerque, NM: Sandia National Laboratories.