Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

Appendix WCA

United States Department of Energy
Waste Isolation Pilot Plant

Carlsbad Area Office
Carlsbad, New Mexico

Waste Characterization Analysis

PREFACE

Appendix WCA of this application is a reproduction of a draft report that was reviewed by the Waste Characterization Analyses Peer Review panel. See Section 9.3.2 and Appendix PEER of this application for discussion of this peer review. Because of its draft status, the report reviewed by the peer review panel contained minor errors (for example, transuranic elements are incorrectly described in one location as those in atomic weights, rather than atomic numbers, greater than 92). These errors do not affect the technical content of the discussions, and have not been corrected in this reproduction although this appendix has undergone formatting to be consistent with other appendices in this application. Also, a preface has been added to Attachments WCA.8.1 and WCA.8.2 which describes the proper context of the attachment(s) with regard to the Compliance Certification Application. These prefaces are included here for completeness and clarification, but were not in the draft report reviewed by the peer review panel. Exact copies of all materials provided to the peer review panel are contained in the appropriate WIPP files.

In the case of the discussion of the temperature rise in the disposal region that may occur as a result of exothermic reactions, technical information presented to the peer panel has been superseded. The original discussion is reproduced here for historical accuracy. The updated discussion of temperature rise is provided in a memorandum by Bennett et al. (1996), contained in Appendix PEER of this application. Conclusions of Appendix WCA are not affected by the change, which results in a lowering of the maximum possible temperature rise from the 7°C reported here as 6°C, as reported by Bennett et al.

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LIST OF ACRONYMS

BID	Background Information Document (for an EPA regulation)
BIR	Baseline Inventory Report
BRAGFLO	BRine And Gas FLOw code
CCA	Compliance Certification Application
CCDF	complementary cumulative distribution function
CFR	Code of Federal Regulations
CH-TRU	contact-handled transuranic (waste)
CUTTINGS_S	code that models radionuclide release from drilling, caving, spalling
DOE, USDOE	United States Department of Energy
EDTA	ethylene diamine tetra-acetate
EPA, USEPA	United States Environmental Protection Agency
FEP	feature, event, or process
FFCA	Federal Facilities Compliance Act of 1992 (PL 102-386)
IDB	(USDOE) Integrated Data Base
INEL	Idaho National Engineering Laboratory
INGRES	name of performance assessment database
K_d	equilibrium constant for distribution of a solute between solution and adsorption
LANL	Los Alamos National Laboratory
NUTS	NUclide Transport System code
PA	performance assessment
PANEL	code that decays and dissolves radionuclides
PCB	polychlorinated biphenyl
PIC	passive institutional control
pH	the negative $\log_{10}$ of the hydrogen ion concentration
PL	Public Law
RCRA	Resource Conservation and Recovery Act
RFETS	Rocky Flats Environmental Technology Site
RH-TRU	remote-handled transuranic (waste)
RTR	real-time radiography
SEIS	Supplementary Environmental Impact Statement (for the WIPP)
SNL	Sandia National Laboratories
SRS	Savannah River Site
TOC	total organic carbon
TRU	transuranic (waste)
TWBIR	TRU Baseline Inventory Report
TWBID	TRU Waste Baseline Inventory Data Base
WIPP	Waste Isolation Pilot Plant

WCA.1 INTRODUCTION

WCA.1.1 Scope

The objective of this appendix is to satisfy the requirements specified in 40 CFR 194.24(b):

> *40 CFR 194.24(b) The Department shall submit in the compliance certification application the results of an analysis which substantiates:*
> *(1) That all waste characteristics influencing containment of waste in the disposal system have been identified and assessed for their impact on disposal system performance. The characteristics to be analyzed shall include, but shall not be limited to: solubility; formation of colloidal suspensions containing radionuclides; production of gas from the waste; shear strength; compactability; and other waste-related inputs into the computer models that are used in the performance assessment.*
> *(2) That all waste components influencing the waste characteristics identified in paragraph (b)(1) of this section have been identified and assessed for their impact on disposal system performance. The components to be analyzed shall include, but shall not be limited to: metals; cellulosics; chelating agents; water and other liquids; and activity in curies of each isotope of the radionuclides present.*
> *(3) Any decision to exclude consideration of any waste characteristic or waste component because such characteristic or component is not expected to significantly influence the containment of the waste in the disposal system.*

This appendix identifies those waste components and waste characteristics that can influence the containment of waste and that are included as inputs to the computer models and codes used in performance assessment. Waste components are the elements that make up the waste (for example, 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 nutrient for microbes in the repository. The property of the paper to act as a substrate for microbial gas production is a characteristic of the paper. Microbes metabolizing paper will produce CO_2, methane, and other gaseous metabolic products, which can increase the pressure in a waste panel and potentially impact the performance of the repository.

This appendix represents a step in the process of using sensitivity analysis to specify limiting values and associated uncertainties in the waste characteristics and components as required in 40 CFR Part 194.24 (c). Initial evaluations, based on previous sensitivity analyses, calculations related to features, events, and processes (FEPs) (Appendix SCR), and reasoned arguments, have identified those waste characteristics that are included or excluded from performance assessment. These preliminary evaluations will be refined once sensitivity studies with the final performance assessment (PA) model for the Compliance Certification Application (CCA) are completed.

The repository performance considered in this appendix is only with respect to the movement of radionuclides to the accessible environment. More specifically, disposal system performance means the ability of the Waste Isolation Pilot Plant (WIPP) to comply with 40 CFR Part 191 (b) and (c). This appendix does not discuss Resource Conservation and Recovery Act (RCRA) related matters; the Department of Energy (DOE) has submitted a No-Migration Variance Petition to the Environmental Protection Agency (EPA) and a RCRA Part B Permit Application to the State of New Mexico that cover issues related to hazardous waste.

WCA.1.2 History of Identification of Components and Characteristics Affecting Performance

The waste components and characteristics affecting repository performance have evolved as understanding about repository processes and disposal system performance has increased. Development of 40 CFR Parts 191 and 194 have also influenced this process. Three major changes that have occurred during the historical development of WIPP conceptual models are as follows:

(1) the change from assuming an essentially dry repository to consideration of brine inflow and outflow, and

(2) promulgation of 40 CFR Part 191 in 1985; Part 191 required consideration of human intrusion, set release limits at defined boundaries, and established a regulatory time period of 10,000 years, and

(3) promulgation of 40 CFR Part 194 in 1996. Part 194 requires that all well types be included in calculations of the future intrusion rate, that mining within the controlled area be considered in performance assessment, and that performance assessment calculations may take credit for passive institutional controls (PICs).

WCA.1.2.1 Initial Estimate of Significant Waste Characteristics

During the 1975-1976 site selection period, the Salado Formation (hereafter referred to as the Salado) was thought to be dry; gas generation by microbial action on the waste was recognized as a possible pressure-building mechanism, and radiolysis of host rock salts could occur. At that time, the emplacement of heat-emitting high-level radioactive waste in a separate repository in the same salt formation was also envisioned, and thermal effects were considered to be significant. Postulated breach of the repository was only by natural processes, which were deemed sufficiently unlikely that repository performance would not be affected.

Experimental activities at the WIPP site focused on characterizing the Salado host rock, microbial gas generation, and migration of intra-granular brine in a thermal gradient. Radionuclides from the repository could be transported in aquifers above the Salado if they reached those aquifers, but a fluid connection between the repository and these aquifers was not established. Measured permeability of the Salado rock matrix proved to be such that microbially generated gas would dissipate in the rock, rather than building to high pressure. Consequently, the program to analyze gas generation was canceled in 1981.

A new gas generation program began in 1988 (Brush 1990) because Salado permeability had been overestimated. Observed brine seepage into the repository suggested the potential for gas generation by corrosion of iron compounds in the waste and waste containers. Thus, gas generation by both corrosion and microbial reaction remains a moderately significant influence on repository performance. In addition, microbially produced CO_2 has a significant effect on actinide solubility, although this effect will be mitigated by MgO backfill. The hydrogen gas produced by corrosion has no effect on repository chemistry.

WCA.1.2.2 Impact of 40 CFR Part 191 on Identification of Significant Characteristics

Promulgation of 40 CFR Part 191 in 1985 required the consideration of human intrusion into the repository, raising the possibility of multiple boreholes into and through the repository, thus allowing brine saturation. Several new release mechanisms were then possible: gas spallation, drill cuttings and cavings, and brine flow, both directly to the surface and to the overlying aquifers.

Mobilization of radionuclides by dissolution of waste added actinide solubility to microbial gas generation and corrosion as a characteristic to be considered, as well as the characteristics that affect solubility, like complexants and pH and redox determinants. Carbon dioxide generation was a characteristic of concern, in addition to total gas generation, because of its effect on pH and actinide solubility. With the increase in importance of dissolved actinide transport in overlying aquifers, identification of the Culebra member of the Rustler Formation (hereafter referred to as the Culebra) as the predominant groundwater route, possible retardation in the Culebra was considered, and waste characteristics that can influence such retardation were studied.

In the late 1980s, transport of actinides in colloidal forms was recognized as potentially significant, adding colloid formation as a waste characteristic to be studied. In 1989, a literature review and analysis resulted in a very large range of estimated actinide solubility (Trauth et al. 1992; Hobart et al. 1996), resulting in an experimental program to study these solubilities more intensively (Novak 1995a). This program also showed the importance of dissolved iron as a corrosion product for actinide solubility.

WCA.1.2.3 Interaction of Performance Assessment and Identification of Significant Waste Characteristics

Since 1989, performance has been (and continues to be) assessed by constructing cumulative distribution functions (CDFs) of releases under various probable scenarios and comparing the complement of this function (CCDFs) with the EPA criteria of 40 CFR 191.13. Before 1996, there were three complete cycles of performance assessment calculations (Lappin et al. 1989; WIPP PA Division 1991; WIPP PA Dept. 1992, 1993). After each of these cycles, the results of a sensitivity analysis were used to refine both waste characterization procedures and experimental work related to the waste characteristics and their expected influence on repository performance. Some examples of this use of sensitivity analysis are:

(1) Estimates of brine inflow from the 1989 performance assessment prompted studies of brine inflow rates and volumes, leading ultimately to the laboratory studies of humid and inundated anoxic corrosion and microbial reaction (Brush 1990). These studies, in turn, highlighted the importance of cellulosics, plastic, and rubber in the emplaced waste as microbial substrates. The latter studies led to assessment of nitrates, sulfates, and phosphates in the waste because these compounds supply microbes with necessary nutrients.

(2) Systems analyses carried out by Lappin et al. (1989) demonstrated that gas would affect repository performance if present in significant quantities. Laboratory studies of gas generation were restarted in February of 1989, and focused on single-process experiments on anoxic corrosion, microbial activity, and radiolysis. Between 1989 and 1995, the DOE project developed gas generation models.

(3) Assessment of brine inflow and brine volumes in the waste prompted the combined modeling and experimental study of actinide solubilities, described in Appendix SOTERM. Modeling actinide solubility revealed the need to assess the impact of waste components on the redox environment of both the Castile and Salado brine.

(4) Calculation of actinide activity through the 10,000-year regulatory period identified those radionuclides that make up less than 1 percent of the EPA release limit (WIPP PA Dept. 1993, 7-12). This information was used in waste characterization and in the actinide source term program to identify the radionuclides that do not need complete characterization and transport and is illustrated by the graphs in Section WCA.8.3.

(5) Studies of the Culebra transmissivity suggested that both physical and chemical retardation could occur, and separate conceptual models were analyzed for cases with and without chemical retardation (WIPP PA Dept. 1993, Section 8.4.3). As a result, the dissolved actinide chemical retardation research program has studied the sorption of dissolved and colloidally sorbed actinides and the components of the waste, primarily organic ligands, that would affect retardation.

(6) Results from the solubility model (Novak 1995a, b) that actinide solubility was pH-dependent led to an evaluation of the influence of cementitious materials in the waste on pH.

WCA.1.3 Organization

This appendix is organized as follows:

Section WCA.1.0 Introduction

The introduction includes a discussion of the overall approach to compliance with 40 CFR 194.24 (b) and the organization of the appendix. This section also discusses the history of using performance assessment to identify the waste components and characteristics that affect performance.

Section WCA.2.0 Summary of Waste Components and Characteristics: Waste Characterization Analysis

This section includes lists of the components and characteristics that are important to performance, as well as those that are not.

Section WCA.3.0 Characteristics That Affect Performance: Curie Content

Section WCA.3.0 considers all of the radionuclides inventoried in the TRU Baseline Inventory Report (TWBIR) (USDOE 1996) and identifies those radionuclides that will affect performance. The only characteristic discussed in Section WCA.3.0 is radioactivity.

Section WCA.4.0 Characteristics of Radionuclides: Solubility and Colloid Formation

Section WCA.4.0 has two subsections devoted to characteristics that affect performance: subsection WCA.4.1 discusses solubility, while subsection WCA.4.2 discusses colloid formation.

Section WCA.5.0 Nonradioactive Waste Components and Characteristics

Section WCA.5.0 has four subsections: subsection WCA.5.1 discusses components and characteristics affecting gas generation; subsection WCA.5.2, those affecting mechanical properties of the repository; and subsection WCA.5.3, those affecting heat generation.

Section WCA.6.0 Summary

Section WCA.7.0 References

Section WCA.8.0 Supplemental Documents

WCA.1.4 Terminology

WCA.1.4.1 Terms Used to Refer to Radioactive Materials

The terms "actinide," "radionuclide" or "nuclide," and "isotope" have particular, but often overlapping, meanings. "Actinide" is used as a general term for an element in the actinium series of the periodic table: for example, thorium, uranium, neptunium, plutonium, americium, and curium are all actinides. This term is used in connection with the chemical properties of these elements and generally not in connection with radiological properties. "Radionuclide" (or "nuclide") is used when referring to one of the class of radioactive elements. "Isotopes" of an element have the same atomic number and chemical properties, but different atomic masses. The term is used most often in conjunction with radiological properties.

WCA.1.4.2 The Waste Unit Factor and EPA Units

The "waste unit factor" is the number of millions of curies of α-emitting transuranic (TRU) radionuclides with half-lives longer than 20 years (40 CFR Part 191, Appendix A). In the WIPP, 4.07 million curies of TRU waste will be in the repository at closure, so the waste unit factor is 4.07.

The number of EPA units of a radionuclide is the activity (in curies) 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.

As an example of EPA units, the Pu-239 inventory at closure is 7.95×10^5 curies (TWBIR; USDOE 1996), and the release limit for Pu-239 is 407 curies, so the number of EPA units is calculated as:

$$\frac{7.95 \times 10^5 \text{ curies}}{407 \text{ curies}} = 1{,}954 \text{ EPA units.}$$

The release limit for Pu-239 is given by the waste unit factor (4.07) multiplied by the release limit per million curies of TRU. The release limit per million curies is given in Table WCA-1, a copy of Table 1 in Appendix A, 40 CFR Part 191. The value for Pu-239 is 100 curies, giving a release limit of 407.

WCA.1.4.3 Normalized Release for All Radionuclides

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

Table WCA-1. Table 1 of Appendix A, 40 CFR Part 191

Radionuclide	Release Limit per Million Curies of TRU Radionuclides* (Curies)	Release Limit for the WIPP Normalized By Total from Table WCA-5 (Curies)
Americium: Am-241 or -243	100	407
Carbon: C-14	100	407
Cesium: Cs-135, or -137	1,000	4,070
Iodine: I-129	100	407
Neptunium: Np-237	100	407
Plutonium: Pu-238, -239, -240, or -242	100	407
Radium: Ra-226	100	407
Strontium: Sr-90	1,000	4,070
Technetium: Tc-99	10,000	40,700
Thorium: Th-230 or -232	10	40.7
Tin: Sn-126	1,000	4,070
Uranium: U-233, -234, -235, -236, or -238	100	407
Any other α-emitting radionuclide with a half-life greater than 20 years	100	407
Any other radionuclide with a half-life greater than 20 years that does not emit α particles	1,000	4,070

* In Appendix A of 40 CFR Part 191, this column is in terms of metric tons heavy metal (MTHM), and the equivalence to curies of TRU is presented in Footnote *e* to the table.

- 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

$$R_j = \frac{1}{f_w}\left[\frac{Q_{1j}}{L_1} + \frac{Q_{2j}}{L_2} + \ldots\right] = \sum_{i=1}^{nR} \frac{Q_{ij}}{f_w L_i} \leq \begin{Bmatrix} 1 \text{ with a probability of } 0.1 \\ 10 \text{ with a probability of } 0.001 \end{Bmatrix}$$

in which R_j is the total release in EPA units under scenario *j*, f_w is the waste unit factor, Q_{ij} is the cumulative release for radionuclide *I* under scenario *j*, L_i is the EPA release limit for radionuclide *I*, and the EPA release limit 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 Section WCA.8.2, and a comprehensive discussion of the background for these limits is provided in EPA (1985).

WCA.1.4.4 Chelating Agents

Although 40 CFR 194.24 refers to "chelating agents," this appendix uses the term "organic ligands." In general, organic ligands increase the solubility of the complexed substance. Chelating agents are a particular category of organic ligand that increases solubility by forming a cage around certain ligated (or chelated) substances. Although this mechanism is peculiar to chelators, performance assessment looks only at the effect — increase in solubility. Performance assessment, therefore, does not distinguish between chelators and other organic ligands.

WCA.2 SUMMARY OF WASTE COMPONENTS AND CHARACTERISTICS: WASTE CHARACTERIZATION ANALYSIS

Tables WCA-2, WCA-3, and WCA-4 summarize, in tabular form, all the waste characteristics and waste components considered in this appendix. These tables provide:

- a list of the waste characteristics retained as a result of the analysis,
- a list of the waste components influencing these characteristics,
- identification of specific waste-related inputs to computer models,
- a list of all waste characteristics and components that were considered and excluded.

Table WCA-2 lists the waste characteristics and components that are included in performance assessment and were expected prior to the analysis to have a significant impact on repository performance. Table WCA-3 lists the waste characteristics and components that are included in performance assessment, but were expected prior to the analysis to have a negligible impact on performance. The impact of microbially generated CO_2 on performance is insignificant because the CO_2 will react with the MgO backfill, forming Mg carbonate minerals that greatly reduce the impact of CO_2 on pH. Actual sensitivities of the analysis to waste characteristics and components are described in Appendix SA. The relationships between components, characteristics, and performance assessment codes is illustrated in Figure WCA-1.

Table WCA-4 lists the waste characteristics and components that are excluded from performance assessment. 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 performance assessment analyses.

Each waste characteristic shown in Tables WCA-2 and WCA-3 is reflected in one or more parameters that are used in performance assessment. The performance assessment parameters are compiled in the INGRES database (presented in Appendix PAR), and the INGRES material and parameter names are the variable names used by the performance assessment models.

Table WCA-2. Table of Waste Characteristics and Components Used in Performance Assessment: Characteristics Expected to Have Significant Effect on Disposal System Performance

Characteristic	Component	Effect on Performance	INGRES* Material Name (App. PAR)	INGRES* Parameter Name (App. PAR)	Section of WCA
radioactivity in curies of each isotope	radioactivity in curies of each isotope	used in calculating normalized releases	AM241 CM245 NP237 CS137 TH229 RA226 U238 PU239 PU240, etc	EPAREL ATWEIGHT INVCHD	3.1, 3.2
TRU radioactivity at closure	α-emitting TRU radionuclides, $t_{1/2} > 20$ years	determines waste unit factor	AM241 CM245 NP237 PU238 PU239 PU240, etc	HALFLIFE ATWEIGHT INVCHD INVRHD	3.1
solubility	radionuclides	actinide mobility	SOLAM3 SOLPU3 SOLPU4 SOLU4 SOLTH4 SOLU6, etc* CS RA SR	OXSTAT SOLSIM SOLCIM LOGSOLM	4.1
colloid formation	radionuclides, cellulose, soils, plastics, rubber	actinide mobility	PHUMOX3, etc* AM NP PU U, etc	PHUMCIM CAPHUM CAPMIC CONCINT CONCMIN PROPMIC	4.2
redox state	radionuclides	actinide mobility	U+6, U+4 PU+3, PU+4 TH+4, AM+3	MKD_U MKD_PU MKD_TH MKD_AM	4.1

* The material and parameter names given here are examples only.

Table WCA-2. Table of Waste Characteristics and Components Used in Performance Assessment: Characteristics Expected to Have Significant Effect on Disposal System Performance (Continued)

Characteristic	Component	Effect on Performance	INGRES* Material Name (App. PAR)	INGRES* Parameter Name (App. PAR)	Section of WCA
redox potential	ferrous metals	actinide oxidation state; actinide mobility	STEEL REFCON	STOIFX ASDRUM DRROOM	4.1.1
gas (H_2) generation	ferrous metals	increase in H_2 pressure	STEEL REFCON	STOIFX CORRMCO2 HUMCOR ASDRUM DRROOM	4.1.2, 5.1
microbial substrate: CH_4 generation	cellulose	increase in gas pressure	WAS_AREA	GRATMICI GRATMICH	4.1.2, 5.1
microbial substrate: CH_4 generation	plastics, rubber	increase in gas pressure	WAS_AREA	PROBDEG	4.1.2, 5.1
particle diameter	solid waste components	spalling release	BLOWOUT	PARTDIA	5.2
microbial nutrients: CH_4 generation	sulfates	increase in gas pressure	SULFATE	QINIT	5.1
microbial nutrients: CH_4 generation	nitrates	increase in gas pressure	NITRATE	QINIT	5.1
compressibility and shear strength	solid waste components	effect on creep closure, cuttings, caving, spalling	WAS_AREA	COMP_RCK	5.2

*The material and parameter names given here are examples only

Table WCA-3. Table of Waste Characteristics and Components Used in Performance Assessment: Characteristics Expected to Have A Negligible Effect on Disposal System Performance

Characteristic	Component	Effect on Performance	INGRES* Material Name	INGRES* Parameter Name	Section of WCA
permeability	solid waste components	negligible effect on brine movement, gas storage; see 2.4.1, SCR 2.3.8.1***	WAS_AREA	PRMX_LOG PRMY_LOG PRMZ_LOG	5.2
porosity	solid waste components	negligible effect on brine movement, see SCR 2.3.8***	WAS_AREA	SAT_WICK POROSITY	5.2
microbial nutrients, CO_2 generation	sulfates	negligible: MgO reacts with CO_2	SULFATE	QINIT**	4.1.2
microbial nutrients, CO_2 generation	nitrates	negligible: MgO backfill reacts with CO_2,	NITRATE	QINIT**	4.1, 5.1
microbial substrate: CO_2 generation	cellulose	negligible: MgO backfill reacts with CO_2	WAS_AREA	GRATMICI GRATMICH	4.1.2, 5.1
microbial substrate: CO_2 generation	plastics, rubber	negligible: MgO backfill reacts with CO_2	WAS_AREA	PROBDEG	4.1.2, 5.1
gas generation	water in the waste	enhances initial gas generation	WAS_AREA	SAT_RBRN	5.3.2

* The material and parameter names given here are examples only

** These parameters are significant to gas generation and are therefore also listed in Table WCA-2.

*** Appendix SCR

Table WCA-4. Table of Waste Characteristics and Components Not Used in Performance Assessment

Characteristic	Component	Effect on Performance	Section of SCR***	Section of WCA
cellulose radiolysis	radionuclides	negligible effect on total CO_2	2.2.4	**
explosivity	other organic compounds	none	2.3.3	
brine radiolysis	radionuclides	negligible effect on actinide valence	2.5.1.3.1	**
galvanic action	nonferrous metals	negligible	2.5.1.2.1	**
complexation with actinides*	soil and humic material*	actinide mobility	**	4.1.3
buffering action*	cement*	negligible: reacts with CO_2 and $MgCl_2$	2.5.4.5	4.1.2
heat of solution	cement	negligible	2.5.7	**
Ca^{2+} binding to organic ligands	cement	negligible compared to other metals	2.5.4.5	4.1.3
binding to organic ligands*	ferrous metals*	can reduce actinide mobility	**	4.1.3
buffering action*	ferrous metals*	actinide mobility	**	4.1.2
galvanic action	ferrous metals	negligible	2.5.1.2.1, 2.7.4	**
binding to organic ligands*	ferrous alloy components*	can reduce actinide mobility	**	4.1.3
redox reactions	nonferrous metals	negligible compared to iron	**	4.1.1
binding to organic ligands*	nonferrous metals*	can reduce actinide mobility	**	4.1.3
complexation with actinides	organic ligands	negligible	**	4.1.3
gas generation	Al and other nonferrous metals	negligible relative to steels	**	5.1
microbial nutrients, CO_2 generation	phosphates	negligible because MgO backfill reacts with CO_2	**	4.1.2
microbial nutrients: CH_4 generation	phosphates*	negligible	**	5.1
heat generation	RH-TRU	negligible	SCR 2.2.2, 2.3.7, 2.3.8.1	5.3.2
electrochemical processes	sulfate, nitrate, phosphate	negligible	SCR 2.7.4	**

* Waste characteristics and components that influence performance indirectly—by influencing components and characteristics listed in Table WCA-2.

** The waste characteristics and components in the table are either discussed in a section of this appendix or are the subject of a FEP.

*** Appendix SCR

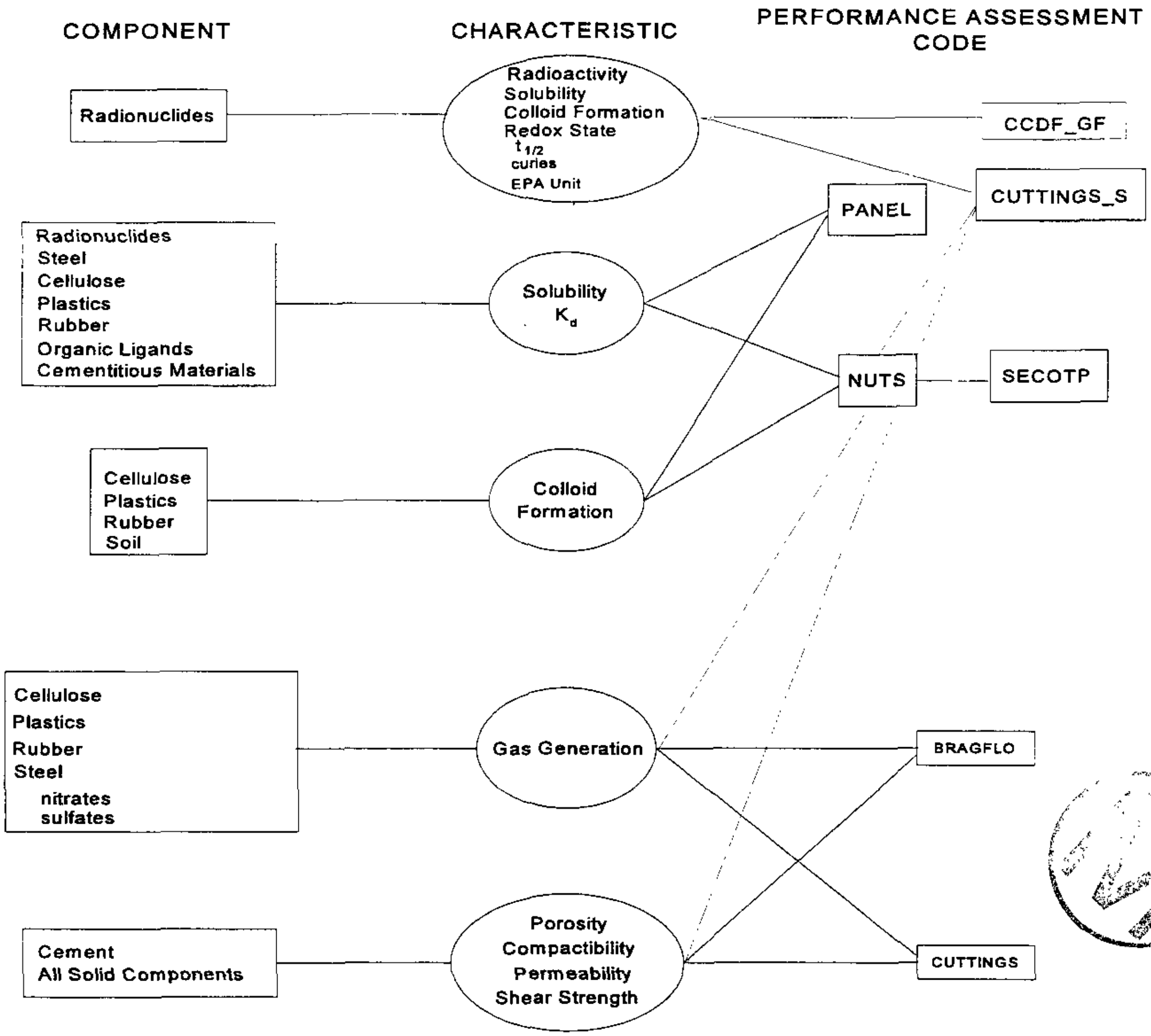

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Figure WCA-1. **Waste components, the associated waste characteristics, and a performance assessment code related to each characteristic.**

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WCA.2.1 Relationship Between Inventory Data and Performance Assessment

The TWBIR, Revision 3 (USDOE 1996) provides both site-level data and waste stream-level data on the radionuclide inventory for the WIPP. PA models generally use the site-level data, normalized to 1995 and scaled-up to the full WIPP capacity. The one exception to this approach is for the cuttings/caving model, which uses waste stream level data to capture potential inhomogeneities in the contact-handled (CH) TRU waste.

The relationship between TWBIR data and performance assessment is shown in Figure WCA-2. As Figure WCA-2 shows, the waste stream level data are used only in modeling direct release by cuttings and cavings (see Appendix CUTTINGS). This direct release scenario includes the probability of penetrating each of the 569 CH-TRU waste streams, and the single remote-handled (RH)-TRU waste stream, as discussed in Chapter 6, Section 6.4.12 of the CCA and in Sanchez et al. (1996).

This approach for cuttings and caving releases represents the potential inhomogeneities 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, 0.3112 meters (12.25 inches), which is less than the diameter of a 55-gallon drum. A cuttings and cavings intrusion will, therefore, extract waste from three specific drums (remember that drums are stacked three high in the disposal rooms), rather than sampling from a larger volume of waste.

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 will 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 total inventory from all generator sites, as shown in Figure WCA-2. In a similar fashion, spall releases use site-level data because this mechanism is assumed to release waste from a volume larger than several drums, averaging out any inhomogeneities in waste streams.

Radionuclide content will be evaluated in 2033, when the WIPP is decommissioned. Stored waste was decayed and grown in to a base year of 1995. Ingrowth occurs in a radioactive decay chain: as a nuclide decays, it produces a daughter, which is said to grow in. The memo of L. R. Sanchez, attached as Section WCA 8.1, includes decay calculations showing that application of the 1995 decayed values to 2033 does not make a significant difference in either the EPA unit or the waste unit factor. Discussions of the scaling of the stored waste inventory to WIPP capacity and of the renormalization of the waste stream data are in the TWBIR.

WCA.3 COMPONENTS THAT AFFECT PERFORMANCE: CURIE CONTENT

The radioactivity of a particular isotope, 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 WCA-1, and (2) inclusion in the source term for the compliance demonstration. The waste unit factor is based only on TRU wastes that are α-emitters with a half-life greater than 20 years, while the CCDF is based on the full inventory of all radioactive elements in the repository. This section, therefore, includes two subsections: WCA.3.1, components relevant to inclusion in the waste unit factor; and WCA.3.2, components relevant to inclusion in CCDFs for each applicable scenario.

WCA.3.1 Radioactivity Included in the Waste Unit Factor

The waste unit factor is the activity of TRU, α-emitting waste with a half-life greater than 20 years at the time of repository closure. The units for the waste unit factor are millions of curies.

Figure WCA-3 is a flow diagram for the selection of those radionuclides in the inventory that contribute to the waste unit factor. As noted above, not all radionuclides are included in this factor. For example, Sr-90 is excluded because it is not a transuranic and is a β-emitter. Even uranium is excluded because it is not a transuranic, which is defined as elements with atomic weight greater than 92.

The radionuclides that are included in the waste unit factor are listed in Table WCA-5. As noted in the table, the relevant inventory at closure is 4.07×10^6 curies, resulting in a waste unit factor of 4.07. Table WCA-5 is based on an analysis (see Section WCA.8.2) of the radionuclide inventory in Revision 3 of the TWBIR (USDOE 1996).

It is worthwhile to note that the inventory in Table WCA-5 is dominated by americium and plutonium. More specifically, the radionuclides Am-241, Pu-238, -239, -240, -242, and Cm-245 capture 99.9% of the waste unit factor. The combined activity at emplacement of Am-241, Pu-238, Pu-239, and Pu-240 is three orders of magnitude greater than the combined activity of the remaining 11 radionuclides.

WCA.3.2 Radioactivity Included in the Source Term for Performance Assessment

Unlike the waste unit factor, all radionuclides are potentially included in a demonstration of compliance and must therefore be considered for inclusion in the source term for performance assessment. An exhaustive list of radionuclides in the waste is presented in Table 3 of Section WCA.8.2. However, 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 negligable impact on compliance.

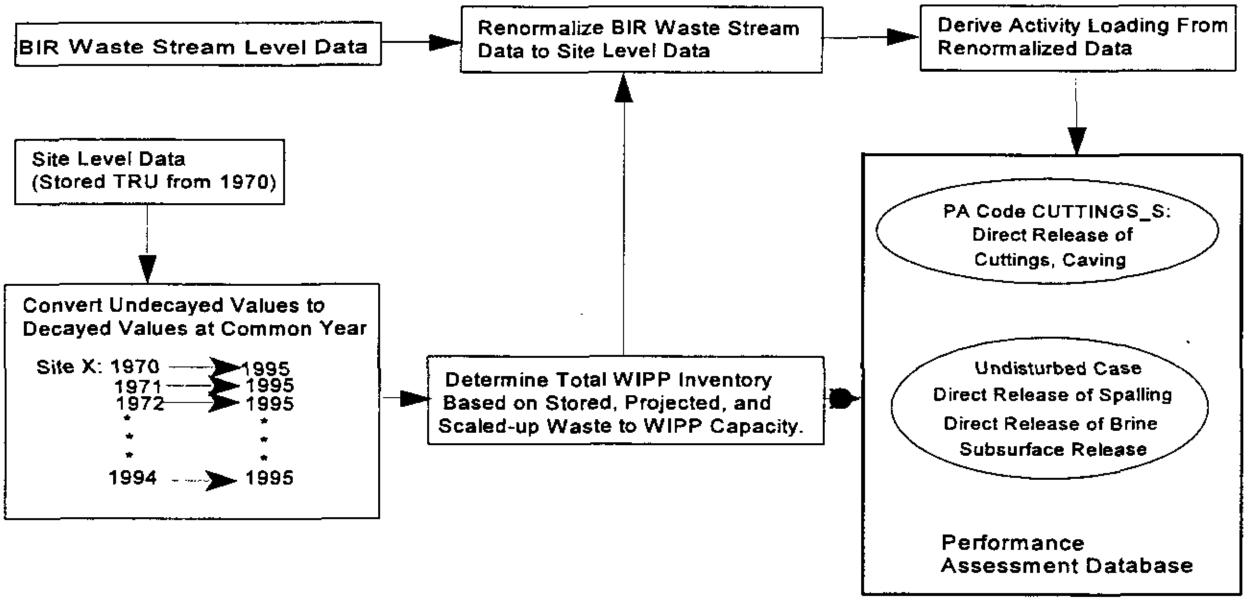

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Figure WCA-2. Flow chart for inventory input into performance assessment database. Data reported by the generator sites are decayed and grown in to the year 1995. These data are then scaled up to the capacity of the WIPP and used in performance assessment. Data for individual waste streams are renormalized and rolled up to site level data. Waste stream level data are unnormalized from this roll-up and used in performance assessment to calculate direct release of cuttings and cavings.

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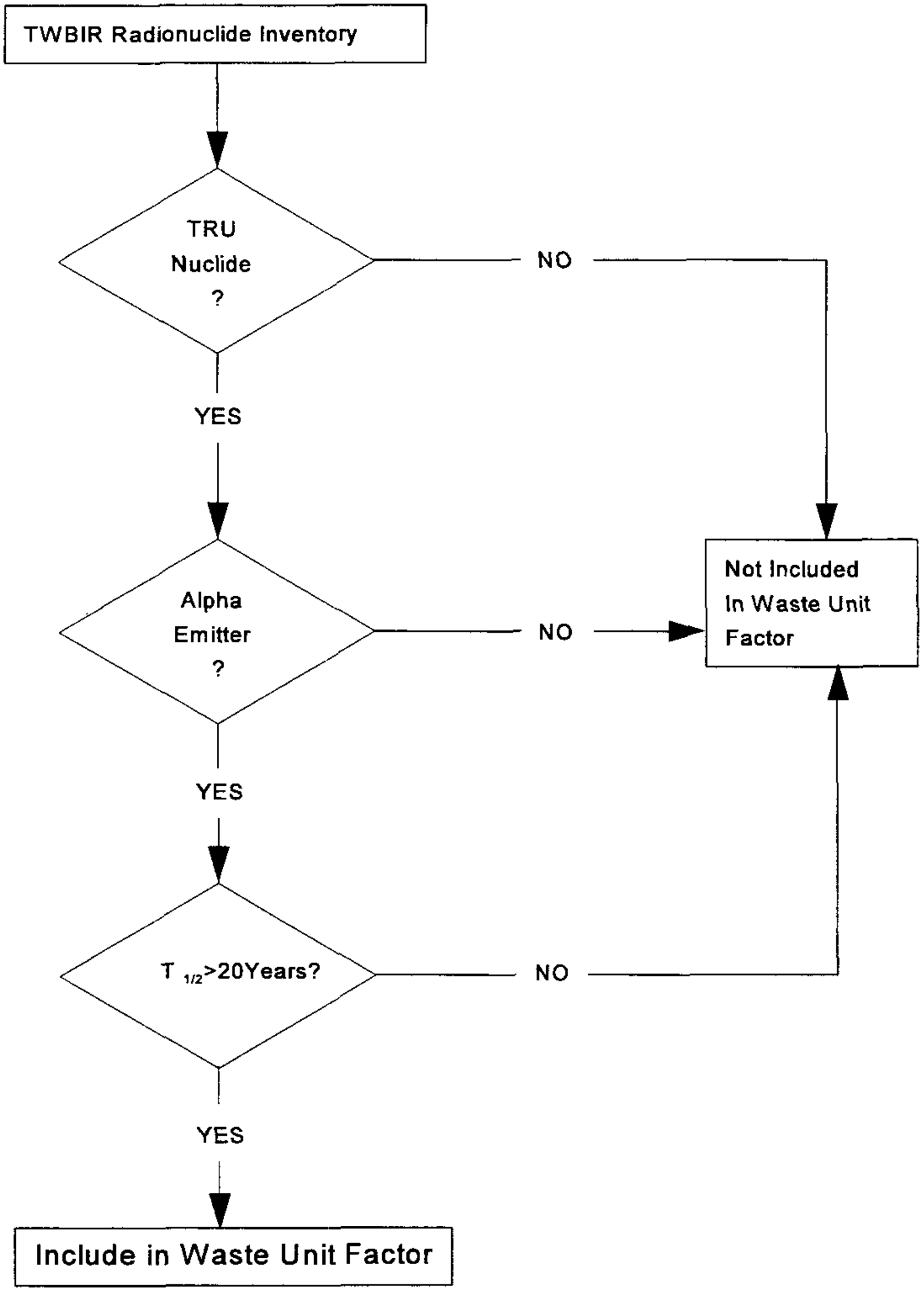

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Figure WCA-3. Flow diagram for including radionuclides in the waste unit factor.

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Table WCA-5. Radionuclides That Contribute to the Waste Unit Factor

Nuclide	Half-Life (years)	Inventory at Closure (curies)	% of Waste Unit
Am-241	432.7	4.48×10^{5}	11.0
Am-243	7370	32.6	8.01×10^{-4}
Cf-249	351	0.687	1.69×10^{-6}
Cf-251	900	3.78×10^{-3}	9.28×10^{-6}
Cm-243	29.1	101.7	2.50×10^{-3}
Cm-245	8500	115	2.82×10^{-3}
Cm-246	4760	0.102	2.51×10^{-6}
Cm-247	1.56×10^{7}	3.21×10^{-9}	7.88×10^{-14}
Cm-248*	3.48×10^{5}	0.0369	9.1×10^{-7}
Np-237	2.14×10^{6}	56.4	1.39×10^{-3}
Pu-238	87.7	2.61×10^{6}	64.1
Pu-239	2.41×10^{4}	7.95×10^{5}	19.5
Pu-240	6560	2.15×10^{5}	5.28
Pu-242	3.75×10^{5}	1170	2.87×10^{-2}
Pu-244	8.0×10^{7}	1.50×10^{-6}	3.68×10^{-11}
TOTAL		4.07×10^{6}	

*This number differs slightly from that in Section WCA.8.2 as a result of more recent information.

Two different release pathways are used in performance assessment: (1) direct releases comprised of (a) material brought to the surface by cuttings, caving, 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 WCA-4 is a flow diagram for selecting radionuclides for different release mechanisms according to the criteria of Table WCA-1. The result of applying these criteria to the radionuclides in the TWBIR is shown in Table WCA-6, which 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 WCA-6 because some nuclides experience considerable ingrowth, but not enough to affect the domination by the most prevalent radionuclides Pu-239 and Pu-240. Am-241 is also important for the first 3,000 years after closure.

WCA.3.2.1 Radionuclides Included in Direct Releases by Cuttings, Caving, and Spalling

The 10 isotopes listed in the column headed "Cuttings/Cavings/Spallings" (see Table WCA-6) are used to model direct release by cuttings, caving, 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 radionuclide 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 Sanchez et al. (1996). The direct release scenario is discussed in greater detail in Section 6.4.12.4 of the CCA.

Eight of the listed isotopes comprise more than 99.9 percent of the EPA units for the entire regulatory period. 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 1 percent would increase computational time and difficulty without any impact on compliance (see Section WCA.8.3). The lack of impact on compliance is clear because if 1 percent of the calculated release is significant, then the calculated release itself would be a much greater violation.

WCA.3.2.2 Radionuclides Included in Direct Releases of Brine to the Surface

Direct release of brine to the surface carries 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 U-238 (for example), 90 percent of the dissolved uranium in moles/liter will be U-238, even though 90 percent of the radioactivity will not be U-238. This phenomenon is illustrated for the uranium isotopes in Table WCA-7.

The EPA units of Sr-90 and Cs-137 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 Sr-90 and Cs-137 are initially large (about 55), rapid decay from a short half-life (about 30 years)

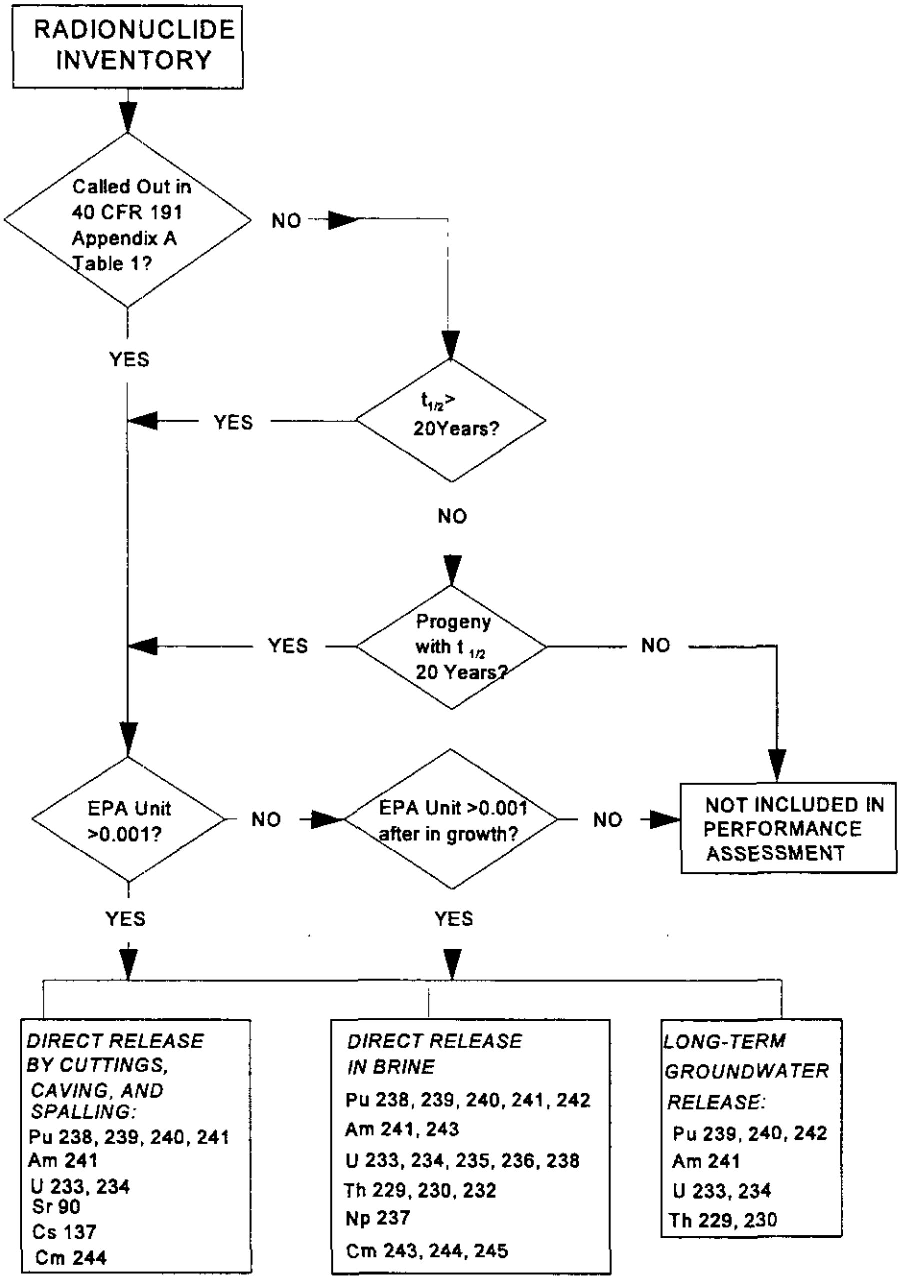

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Figure WCA-4. Flow diagram for selecting radionuclides for the release pathways conceptualized by performance assessment. The top part of the diagram describes the criteria for selecting radionuclides in Table WCA-6. The criteria for selecting specific radionuclides for each release mechanism are described in Sections WCA.3.2.1 through WCA.3.2.3.

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Table WCA-6. Radionuclides Included

Radionuclide	Inventory at Closure (curies)	EPA Unit at Closure***	EPA Unit at 10,000 Years	Releases		
				Cutting/ Cavings/ Spall Release	Direct Brine Release	Culebra Release
Pu-238	2.61×10^6	6416	0.00**	x	x	--
Pu-239	7.95×10^5	1954	1464	x	x	x
Am-241	4.48×10^5	1101	0.13	x	x	x
Pu-240	2.15×10^5	528	183	x	x	c
Cs-137	2.24×10^5	55.0	0.00	x	--	--
Sr-90	2.16×10^5	53.0	0.00	x	--	--
U-233	1.95×10^3	4.79	4.59	x	x	c
U-234	5.08×10^2	1.25	3.45	x	x	x
Th-230	0.0882	2.17×10^{-3}	2.99	--	x	x
Pu-242	1.17×10^3	2.88	2.82	--	x	c
Th-229	2.997	7.36×10^{-3}	2.86	--	x	c
Np-237	58.95	0.145	0.41	--	x	--
Cm-245	1.15×10^2	0.28	0.13	--	x	--
Ra-226	11.6	0.029	0.23	--	--	--
Cm-243	52.22	0.13	0.00	--	x	--
U-238	50.1	0.12	0.12	--	x	--
U-236	0.43	1.06×10^{-3}	0.10	--	x	--
Am-243	32.6	0.08	0.03	--	x	--
U-232	25.8	0.0634	0.00	--	--	--
U-235	17.4	0.0428	0.06	--	x	--
C-14	12.9	0.03	0.01	--	--	--
Th-232	1.006	0.0248	0.02	--	x	--
Pb-210	2.55	6.27×10^{-3}	0.023	--	--	--
Pa-231	0.453	1.1×10^{-3}	1.08×10^{-3}	--	--	--
Ac-227	0.61	1.5×10^{-3}	1.5×10^{-3}	--	x	--
Cm-248	0.090	2.2×10^{-4}	2.2×10^{-4}	--	x	--
Pu-241	2.45×10^6	*	*	x	x	--
Cm-244	3.18×10^4	*	*	x	x	--
% of EPA Units at closure represented by nuclides in source term				99.96%	98.93%	35.48%
% of EPA Units at 10,000 years represented by nuclides in source term				99.41%	99.98%	99.76%

* Pu-241 and Cm-244 are not regulated by 40 CFR Part 191, but are included because their daughters, Am-241 and Pu-242, respectively, are significant to PA.

** Pu-238 ($t_{1/2}$ = 87.8 years) dominates the initial EPA unit but will have decayed away, even with some ingrowth, by 10,000 years.

***The EPA units in this column are accurate. Calculating EPA units from the inventory may produce rounding errors

x indicates an isotope included in the source term

c indicates nuclides that are carried during transport with an isotope having similar characteristics

Table WCA-7. Activities and EPA Units of Uranium Isotopes

Radionuclide	Curies Emplaced	Half - Life (yr)	Moles	% of Total	% at 10,000 yr
U-232	25.8	70	5.05E-3	7.6E-7	1.43E-8
U-233	1948	1.59E5	867.4	0.13	0.122
U-234	507.5	2.46E5	349.3	0.05	6.45
U-235	17.43	7.04E8	3.43E4	5.18	4.84
U-236	0.4298	2.34E7	28.1	0.004	0.165
U-238	50.1	4.47E9	6.26E5	94.6	88.4

results in negligible impact on the performance assessment from those two isotopes. The lack of impact on compliance is explained below.

Sr-90 and Cs-137 decay by about 90 percent during the first 100 years after closure, when borehole intrusions are excluded by 40 CFR Part 191. During this time period, the EPA unit of either isotope decays from 55 down to 5.5 for the whole repository. At 200 years, the EPA unit for either isotope are down to 0.94, again for the whole repository.

In addition to the rapid decay, were an individual borehole intrusion to occur at 100 years, it would release 5.5 EPA units (Appendix SA) 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 is only 0.01 m^3. In summary, the rapid decay of Cs-137 and Sr-90 and the negligible volumes of brine release at early times provide the basis for excluding these isotopes from the inventory.

C-14 is not included in this (or any) source term. Any C-14 transported out of the repository will be diluted by the large excess of nonradioactive carbon. With the current inventory, there is 0.2 moles of C-14 (see Section WCA.8.9) out of 3×10^8 moles of carbon in the cellulosics (see TWBIR), or one part in 100 million.

WCA.3.2.3 Radionuclides Included in Releases to the Culebra Aquifer

Release of brine from the repository to the Culebra also carries dissolved and colloidal radionuclides. The eight 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 Rustler is sufficiently slow that shorter-lived radionuclides would decay to negligible amounts before reaching the accessible environment. The selection of the eight radionuclides is discussed in Section WCA.8.3.

Of the eight radionuclides, only Pu-239, Am-241, U-234, and Th-230 are transported separately in performance assessment. 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, as presented in detail in Section WCA.8.3:

- U-233 can be combined with U-234 for transport because their half-lives are similar.

- Similarly, Th-229 can be combined with Th-230, because they will be in a fixed ratio to each other. Th-232 can be dropped because it is a constant small fraction of the EPA unit throughout the regulatory period.

- Pu-240 and Pu-242 can be combined with Pu-239; their long half-lives also indicate a fixed ratio between them.

- Pu-238 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.

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

WCA.3.2.4 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 WCA-4. Table WCA-8 lists those excluded radionuclides that have not already been discussed, and indicates the reason for their exclusion.

Table WCA-8. Radionuclides Excluded From All Source Terms

Radionuclide	**Reason for Exclusion**		
	Short $t_{1/2}$ and Progeny With Short $t_{1/2}$*	**Small EPA Unit**	**Negligible** Ingrowth**
H-3	NA	x	NA
Cr-51	x	NA	NA
Mn-54	x	NA	NA
Fe-55	x	NA	NA
Co-58	x	NA	NA
Fe-59	x	NA	NA

Table WCA-8. Radionuclides Excluded From All Source Terms (Continued)

Radionuclide	Reason for Exclusion		
	Short $t_{1/2}$ and Progeny With Short $t_{1/2}$*	Small EPA Unit	Negligible** Ingrowth
Ni-59	NA***	x	NA
Co-60	NA	x	NA
Ni-63	NA	x	NA
Zn-65	x	NA	NA
Se-79	NA	x	NA
Kr-85	x	NA	NA
Sr-89	x	NA	NA
Y-90	x	NA	NA
Zr-93	NA	x	NA
Nb-95	x	NA	NA
Zr-95	x	NA	NA
Tc-99	NA	x	NA
Rh-106	x	NA	NA
Ru-106	x	NA	NA
Ag-109m	x	NA	NA
Cd-109	x	NA	NA
Ag-110	x	NA	NA
Pd-107	NA	x	NA
Cd-113m	x	NA	NA
Sn-119m	x	NA	NA
Sb-125	x	NA	NA
Te-125	x	NA	NA
Sn-126	NA	x	NA
Sb-126m	x	NA	NA
Te-127	x	NA	NA
Te-127m	x	NA	NA
I-129	NA	x	NA
Cs-134	x	NA	NA
Ba-137m	x	NA	NA
Ce-144	x	NA	NA

Table WCA-8. Radionuclides Excluded From All Source Terms (Continued)

Radionuclide	Reason for Exclusion		
	Short $t_{1/2}$ and Progeny With Short $t_{1/2}$*	Small EPA Unit	Negligible** Ingrowth
Pr-144	x	NA	NA
Sn-121m	NA	x	NA
Gd-150	NA	x	NA
Sm-151	x	NA	NA
Eu-152	x	NA	NA
Eu-154	x	NA	NA
Eu-155	x	NA	NA
Ta-182	x	x	NA
Tl-207	x	x	NA
Tl-208	x	x	NA
Tl-209	x	NA	NA
Pb-209	x	NA	NA
Pb-210	NA	x	NA
Pb-211	x	NA	NA
Pb-212	x	NA	NA
Ac-227	x	x	NA
Ra-225	x	NA	x
Ra-228	x	NA	NA
Pa-231	NA	x	NA
Pa-233	x	NA	x
Pa-234	x	NA	x
Pa-234m	x	NA	x
Th-231	x	NA	x
Np-238	x	x	x
Np-239	x	NA	x
Np-240m	x	NA	x
Pu-243	NA	x	NA
Cm-246	NA	x	NA
Cf-249	NA	x	NA

Table WCA-8. Radionuclides Excluded From All Source Terms (Continued)

Radionuclide	Reason for Exclusion		
	Short $t_{1/2}$ and Progeny With Short $t_{1/2}$*	Small EPA Unit	Negligible** Ingrowth
Cf-251	x	x	NA
Cf-252	x	NA	x

* "Short" half-life means $t_{1/2} < 20$ years. Radionuclides with $t_{1/2} < 20$ years are not regulated by 40 CFR Part 191(b) and (c).

** Negligible ingrowth includes ingrowth of the progeny that are radionuclides already predominant in the inventory.

***NA indicates that the column heading does not apply to the particular isotope.

WCA.4 CHARACTERISTICS OF RADIONUCLIDES: 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 SCR, Section SCR 2.6.5).

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

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 performance assessment, are discussed in detail in Appendix SOTERM, Sections SOTERM.4 through SOTERM.6 when relevant to performance assessment. Cesium and strontium are assumed to be extremely soluble and their concentrations will be limited by their inventories (see Section WCA.3.2.2). 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 backfill reacting with brine, steels, cellulosics, plastics, and rubber. MgO backfill is added to mitigate the effect of CO_2 generated by microbial degradation of organic materials. The mechanism of the control is discussed in Sections WCA.8.9 and WCA.8.10, and in Section SOTERM.2 of Appendix SOTERM.

WCA.4.1 Components and Characteristics Influencing Solubility

In the absence of the MgO backfill, 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 of brine (brine composition) (clearly not a waste characteristic). The important waste components that affect actinide solubility are steels, cellulosics, plastics, rubber, organic ligands, 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 WCA.5.3.1 and WCA.8.15). 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.

WCA.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 (cellulosics, plastics, and rubber). 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} M to about 10^{-5} M (see Appendix 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 SOTERM.4, a brief discussion is given here. The bibliography of Appendix SOTERM also includes documentation of the experimental program.

Anoxic conditions will be dominant during the whole time period of 10,000 years. A small amount of oxygen, trapped at emplacement, will be used quickly by oxic corrosion and microbial action. Anoxic steel corrosion will produce both hydrogen and $Fe(OH)_2$ (Section WCA.8.17). Experimental work described in Appendix SOTERM.4 has 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). Pu(+V) is seen in this chemical reaction as an unstable intermediate. It is expected, therefore, that Pu(+VI) and P(+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 performance assessment, based on experimental data as well as the published literature, is (Katz et al. 1986, 917, 970, 1135 and following; 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 performance assessment, half of the realizations will include the lower oxidation states of uranium, neptunium, and plutonium; the other half will include the higher oxidation states (Appendix SOTERM 4.7; Katz et al. 1986; Weiner 1996).

WCA.4.1.2 Components Influencing pH and CO_2 Fugacity

In the absence of the MgO backfill, actinide solubility would be highly dependent on pH and CO_2 fugacity of the brine. Lower pH and higher CO_2 fugacity result in higher actinide solubility (Appendix SOTERM). 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 carbon dioxide by microbial degradation in the repository would acidify the brine and lower the brine pmH to about 4.5, if no MgO backfill were added (Appendix SOTERM.2). Microbial CO_2 production can be described by the following sequential reactions (Section WCA.8.17):

$$C_6H_{10}O_5 + 4.8H^+ + 4.8NO_3^- \rightarrow 7.4H_2O + 6CO_2 + 2N_2$$

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

$$C_6H_{10}O_5 + H_2O \rightarrow 3CO_2 + 3CH_4.$$

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 90% of organic materials (cellulosics, plastics, rubbers) will be biodegraded via the third reaction, methanogenesis, in which one mole of organic carbon will produce half a mole each of CO_2 and CH_4.

Based on the inventory estimate for organic carbon and the estimated CO_2 yield per mole of organic carbon, to mitigate the negative effect of microbially produced CO_2, 2×10^9 moles of MgO will be added to the repository as a backfill (USDOE 1996; WCA.8.17). The waste components of organic carbon, nitrate, and sulfate here are used to determine the amount of MgO needed. The hydrated MgO backfill will react with CO_2:

$$Mg(OH)_2 + CO_2 = MgCO_3 + H_2O.$$

The above reaction will buffer the pmH 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 (Appendix SOTERM.3).

Cementitious waste (that contains calcium oxide) could also be expected to raise the pH, and the waste is currently estimated to contain about a total of 8.54×10^6 kg cementitious material (Section WCA.8.13). This amount of cementitious material contains about 8×10^6 moles of $Ca(OH)_2$. However, this amount of $Ca(OH)_2$ will be not enough to affect pH or brine composition significantly. It is shown that $Ca(OH)_2$ will be consumed easily by reaction with microbial generated CO_2 or with $MgCl_2$ in the Salado brine and thus the repository chemistry will be dominantly controlled by the $Mg(OH)_2$ / Mg CO_3 buffer, rather than the $Ca(OH)_2$ / $CaCO_3$ buffer (Sections WCA.8.9 and WCA.8.10). Because the excess of MgO will be added, other components of the waste are unlikely to affect the pH in important ways.

WCA.4.1.3 Waste Components That Directly Enhance Solubility

A number of organic compounds are capable of forming strong complexes with actinide ions, thereby stablizing the actinide in the solution. The TWBIR (USDOE 1996) initially identified about 60 organic compounds in the waste (Drez and James-Lipponer 1989; Brush 1990; Section WCA.8.11). Four of these (acetate, citrate, oxalate, and EDTA) have been identified to have an effect on actinide mobility, because they are water-soluble and present in significant quantities (WCA.8.11).

Ligand concentration in the repository was estimated using inventory amounts of ligands and a brine volume equal to 75 percent of the total repository volume of 29841 m^3—the minimum brine for significant brine release to occur (Section WCA.8.12). The ligand concentrations are estimated to be: acetate : 8×10^{-4} M; oxalate : 2×10^{-4} M; citrate: 4×10^{-3} M; and EDTA: 2×10^{-6} M (Section WCA.8.12; Appendix SOTERM.5).

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 SOTERM.6. Modeling predicts that for the amount of these complexants expected to be emplaced in the repository, the concentration of americium and plutonium in solution is increased by less than 18 percent in the simulated Salado brine; in this brine, about 88 percent of the EDTA, 98 percent of the oxalate, 74 percent of the acetate, and 65 percent of the citrate is bound with Mg. In simulated Castile brines, which have much lower Mg concentrations, modeling predicts increases of americium and plutonium concentrations less than a factor of 8. Even so, about 40 percent of EDTA is bound with Mg (Novak and Moore 1996; Appendix SOTERM.6).

To estimate the effectiveness of other metals in binding organic ligands and thereby reducing the free ligand concentrations, some simple competition calculations were performed using parameters obtained in dilute solutions, because parameters for concentrated salt solutions like the WIPP brines are not available. These metal species include 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 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 (Appendix SOTERM). There are also expected to be more than 6×10^7 moles of Pb. Additionally, several other metals that can sequester organic ligands will be present in some of the waste forms.

Table WCA-9 presents complexation constants for several metals with EDTA. These values were measured in dilute solution. For comparison, for EDTA in 5 molal NaCl, the magnesium association constant is $\log K_{Mg} = 6.6$ (Martell and Smith 1982).

Table WCA-9. Complexation Constants for Selected Metals*

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

* 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 (Appendix SOTERM).

WCA.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). Cellulosic materials, plastic, and rubber 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 Appendix SOTERM and Sections WCA.8.4 through WCA.8.8.

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 (Appendix SOTERM.6). Therefore, the intrinsic colloid concentrations for Am, U, Th, and Np will be modeled as zero in the disposal room and only intrinsic plutonium colloid will have any impact on performance. Pu(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 (Appendix SOTERM).

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 was used to estimate the maximum concentration of actinides bound to mineral fragment colloids (Appendix SOTERM). 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 performance assessment, their contribution is negligible and they will not impact repository performance.

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 cellulosic, plastic, and rubber in the waste is 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 detailed ratios for the WIPP brines are given in (Papenguth 1996; Section WCA.8.4; Appendix SOTERM). 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 (Section WCA.8.7). The oxidation state analogy was also used to develop parameter values for actinides expected to have multiple oxidation states in the WIPP disposal room. 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 (Appendix SOTERM).

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; Francis and Gillow 1994). The waste material in the disposal room will 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 (Table WCA-2): proportionality constants (with performance assessment parameter designations PROPMIC, PHUMSIM, and PHUMCIM) describing 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 (Sections WCA.8.4 to 8.8; Appendix SOTERM) were performed to obtain the following values of performance assessment parameters for each actinide shown in Table WCA-10.

As evident in Table WCA-10, 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 performance assessment (details are discussed in Appendix SOTERM.7) and are expected to affect disposal system performance.

WCA.5 NONRADIOACTIVE WASTE COMPONENTS AND CHARACTERISTICS

WCA.5.1 Gas Generation

The waste components that contribute to gas generation are: (a) ferrous and nonferrous metals, (b) cellulosics, plastics, rubber, and (c) nitrate and sulfate.

The mechanisms and reactions for gas generation are discussed in Section WCA.8.17.

Metals contribute to gas generation through corrosion. The anoxic corrosion reaction of iron in the WIPP is

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

Table WCA-10. Colloid Concentration Factors

	Concentration on Mineral Fragments*	Concentration as Intrinsic Colloid*	Proportion Sorbed on Microbes**	Maximum Sorbed on Microbes*	Proportion Sorbed on Humics**		Maximum Sorbed on Humics*
					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}

* in units of moles total mobile actinide per liter

** in units of moles microbial actinide per moles dissolved actinide

The hydrogen gas produced by this reaction contributes to total gas pressure, but does not affect repository chemistry. In addition, steel corrosion will consume water in the repository; this effect is taken into account in computer code BRAGFLO. Nonferrous metals such as alumimum alloys also corrode, producing H_2, but their contribution to total gas pressure is negligible, because they are present in much smaller quantities than iron (TWBIR; USDOE 1996).

Cellulose materials, plastic, rubber, nitrate and sulfate control microbial gas generation. Cellulosics, plastics, and rubbers will be used as substrates by anaerobic microbes in the WIPP. Nitrate and sulfate will be used as electron acceptors by microbes to oxidize the organic materials. Organic materials will be biodegraded through reactions (Section WCA.8.17)

$$C_6 H_{10} O_5 + 4_1 8H^+ + 4.8\ NO_3^- \rightarrow + 7.4H_2O + 6CO_2 + 24N_{2(g)}$$

$$C_6 H_{10} O_5 + 6H^+ + 3SO_4^{2-} \rightarrow 5H_2O + 6CO_2 + 3H_2S(g)$$

$$C_6 H_{10} O_5 + H_2O \rightarrow 3CH_{4(g)} + 3CO_{2(g)}$$

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 the MgO backfill, the methane is a major 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 cellulosics biodegradation used in performance assessment 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 performance assessment (Francis and Gillow 1994).

Based on the inventories of steels and organic materials and the rates of gas generation estimated by Wang and Brush (Section WCA.8.17), microbially produced gases may dominate early in the repository's history. Gas pressure does 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 performance assessment through the specific variables identified in Table WCA-2 in BRAGFLO calculations.

WCA.5.1.1 Waste Fluid Content

The initial water content of the waste contributes to 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 performance assessment 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; Butcher 1996).

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.

WCA.5.2 Components and Characteristics Influencing Physical Properties

As noted in Tables WCA-2 and WCA-3, the following physical properties of the solid waste components are used in performance assessment:

- *Expected Significant Effect on Disposal System Performance*:

Compressibility: this affects the creep closure, and the porosity of the waste.

Shear Strength: the amount of material released directly on a drilling intrusion, calculated as cuttings, cavings and spalling, depends on the erosion and the spall strengths of the waste at the time of the intrusion, which in turn depend on the time-dependent extent of waste consolidation.

- *Expected Negligible Effect on Disposal System Performance*

Porosity: effects on brine movement in the waste. Also controls the maximum volume that can exist in the waste for potential saturation with radionuclides or gas storage

Permeability: effect on brine movement in the waste

WCA.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.

The condition of the waste at any time can be represented in terms of its porosity, which gives a measure of the pore volume available for storage of generated gas or brine. A subcategory of this issue is that release may depend on how much contaminated brine exists in the waste before the intrusion, which depends on the waste porosity.

The compressibility of the waste has been determined from a series of laboratory tests on simulated waste materials, which are described in detail in Butcher et al. 1991. These included small-scale compaction tests, as well as a number of tests on full-scale waste drums filled with simulated waste materials. In these tests the materials used were simulations of all of the main classes of waste anticipated at the WIPP, including metallics, combustibles, cellulosics, and sludges. Waste compressibility was determined by combining the individual compressibilities of the different waste types in the proportions expected at the WIPP.

The conceptual model for creep closure assumes that compaction takes place before complete degradation. This assumption is borne out by observation of microbial gas generation rates. Estimates of degraded waste response suggest that the porosity of the corroded and biodegraded waste would be comparable to that of the unreacted waste, even though the cellulosics have been totally consumed (Luker et al. 1991). A volumetric plasticity model of the waste is used (Weatherby et al. 1991). The model and the experimental data supporting it are described in Butcher et al. (1991) and Callahan (1993).

WCA.5.2.2 Strength

Strength of the waste is important in evaluating the potential for release due to caving or spalling following an inadvertent human intrusion. As described in Appendix CUTTINGS, solid waste can be released through a borehole by erosion of the borehole walls by circulating drilling mud (caving), and by suspension in gas released from the repository during a high pressure blowout (spalling). Cavings are controlled in large part by the erosional shear strength of the waste, which is based upon analogy to deep-sea sediment erosion, which provides a minimum, conservative estimate of this property. Spalling is controlled largely by the velocity of gas flow, and the particle diameter, but is limited by the tensile strength. As argued by Berglund et al. (1996), a tensile strength of the waste of 1 psi may be established from a study of analog materials, and a consideration of mechanisms in the repository, including salt precipitation.

WCA.5.2.3 Permeability

Fluid flow within a disposal room affects the fluid distribution in the waste and backfill, and the flow of brine and gas within the room and repository. Both waste permeability and liquid present in the waste can affect fluid flow.

The permeability of the waste at a given time can influence repository performance by controlling how rapidly gas or brine can flow through the waste. The WIPP waste region is confined between layers of very low permeability (intact halite permeability $<10^{-21}$ square meters). Therefore, the waste is much more permeable than the halite and may be expected to be the dominant path for fluids flowing into and through the repository. The flow path through the repository will be short in comparison to the external flow paths for brine migration (through seals and up shafts or boreholes, etc.). Thus, assuming a permeability of about 10^{-13} square meters is analogous to assuming that there is little restriction of flow of either gas or brine within the waste.

The mean permeability of waste on the scale of a drum is 1.7×10^{-13} square meters, based upon laboratory data reported in Luker et al. 1991. For the preliminary performance assessment (WIPP PA Dept. 1993) a median value of 1×10^{-13} square meters used, and was assumed to be independent of porosity (WIPP PA Dept. 1993, Table 3.4-1, 3-56, 3-57). Any time-dependent variation in permeability has been shown to have no significant effect on system performance.

WCA.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 (USDOE 1995) and the heat generated by MgO hydration and carbonization, steel corrosion, aluminum corrosion, and organic biodegradation.

WCA.5.3.1 Exothermal Reactions

MgO hydration and carbonization, steel corrosion, aluminum corrosion, 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 1996: WCA 8.15), as shown in Table WCA-11:

Table WCA-11. Maximum Temperature Increases

Reaction Number	Maximum Temperature Increase (K)
MgO hydration	5
Mg(OH$_2$) carbonization	0.8
Steel corrosion	2
Microbial degradation	1
Aluminum corrosion	7

In the worst case, a temperature increase of 7 K could be experienced. 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 has previously been screened out of the performance assessment on the basis of low consequence to factors such as creep closure, seal performance, transport, etc. (see Appendix SCR.2.5.7). 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 (the maximum temperature increase possible) would result in an approximately 3 percent change in the free energy of formation of any species contained within the model. This value is well within the model parameter bounds.

WCA.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 71 and 82 watts per cubic meter, which would result in a temperature rise near the "worst-case" RH-TRU canister between 2.85 K and 3.19 K. The expected WIPP average temperature increase from RH-TRU heat loading is between 0.38 K and 0.49 K. The RH-TRU thermal heat load is small enough that there is no anticipated impact on repository performance. A complete discussion and analysis is given in Section WCA.8.16.

WCA.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 WCA-12:

Table WCA-12. Waste Characteristics and Components Expected to be Most Significant to Performance

Characteristic/Component	Reason for Significance
Pu-239, Pu-240, Am 241, U-233, and U-234	99 percent of EPA unit after 2,000 years
Pu-238	dominates EPA unit at early times
solubility of Pu and Am	large EPA unit; mobility depends on solubility
U-238	very low activity; dilutes higher-activity uranium isotopes for brine-based releases
iron	1. maintains reducing environment so that lower, less soluble oxidation states of actinides predominate 2. corrodes to produce hydrogen, increasing gas pressure;
cellulose, plastic, rubber, nitrate, sulfate	microbial nutrients that are metabolized to methane and several other gases, increasing gas pressure; formation of colloids
humic materials, cellulose breakdown products	form humic colloids that sorb and transport actinides
nonferrous metals	prevent increase in actinide solubility by binding with ligands
waste shear strength	important to spalling and cavings

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 (WIPP PA Dept. 1992).

Table WCA-13 summarizes those characteristics and components with an insignificant impact on performance.

Table WCA-13. Waste Characteristics and Components Expected to be Not Significant

Characteristics/Component	Reason for insignificant impact
Radionuclides other than those in Table WCA-12	EPA unit is negligible fraction of total, even with ingrowth
substances that may affect pH*	pH is buffered by MgO backfill
substances that produce CO_2*	CO_2 is removed by reaction with MgO backfill
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	Heats of formation are small and thermal mass of repository is large so that temperature rise is negligible.
Fluid in the waste	negligible compared to brine volume

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

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WCA.8 SUPPLEMENTARY DOCUMENTS

WCA.8.1	Memo from L. C. Sanchez to M. Martell, April 24, 1996, "Justification for Choice of CCA Radionuclide Values." WPO# 37428
WCA.8.2	Memo From L. C. Sanchez: "Identification of Important Radionuclides Used in 1996 CCA WIPP Performance Assessment", April 25, 1996 WPO# 37432
WCA.8.3	Memo From James Garner to Christine Stockman "Radioisotopes to Be Used in the 1996 CCA Calculations", March 15, 1996 WPO# 35202
WCA.8.4	H. W. Papenguth to Christine T. Stockman: "Colloidal Actinide Source Term Parameters" March 29, 1996 WPO# 36771
WCA.8.5	H. W. Papenguth to Christine T. Stockman: "Parameter Record Package for Colloidal Actinide Source Term Parameters" May 7, 1996: Attachment A: Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids." WPO# 35852.
WCA.8.6	H. W. Papenguth to Christine T. Stockman: "Parameter Record Package for Colloidal Actinide Source Term Parameters" May 7, 1996: Attachment A: Rationale for Definition of Parameter Values for Microbes." WPO# 35856
WCA.8.7	H. W. Papenguth to Christine T. Stockman: "Parameter Record Package for Colloidal Actinide Source Term Parameters" May 7, 1996: Attachment A: Rationale for Definition of Parameter Values for Humic Substances." WPO# 35855
WCA.8.8	H. W. Papenguth to Christine T. Stockman: "Parameter Record Package for Colloidal Actinide Source Term Parameters" May 7, 1996: Attachment A: Rationale for Definition of Parameter Values for Mineral Fragment Type Colloids." WPO# 35850
WCA.8.9	Yifeng Wang, "Estimate of repository pH and f(CO_2) Distribution of the Long-Term WIPP Performance Assessment," March 29, 1996 WPO# 37415
WCA.8.10	Yifeng Wang, "Define Chemical Conditions for FMT Actinide Solubility Calculations," March 22, 1996. PDD# 3O819
WCA.8.11	P. Drez to J. Harvill, "Final Estimate of Complexing Agents in TRU Solidified Waste Forms Scheduled for Disposal in WIPP" March 20, 1996 WPO# 35552

WCA.8.12 R. Weiner to C. F. Novak, March 27, 1996, “Dissolved Ligand Concentrations” WPO# 36163

WCA.8.13 D. Watkins to L. E. Shephard, April 4, 1996, “Estimate of Cement Content in TRU Solidifed Waste Forms Schedules for Disposal in WIPP” WPO# 37064

WCA.8.14 P. E. Drez, “Preliminary Estimate for SNL/NM Performance Assessment Calculations of Nitrate, Sulfate, and Phosphate Content in Transuranic Solidified Wastes Destined for Disposal in WIPP,” January 26, 1996. WPO# 31379

WCA.8.15 Yifeng Wang, May 9, 1996. “Evaluation of the Thermal Effect of MgO Hydration for the Long-term WIPP Performance Assessment.” WPO# 37743

WCA.8.16 L. C. Sanchez and H. R. Trellue, January 17, 1996. “Estimation of Maximum RH-TRU Thermal Heat Load for WIPP.” WPO# 31165

WCA.8.17 Yifeng Wang and Larry Brush, January 26, 1996, “Estimates of Gas-Generation Parameters for the Long-Term WIPP Performance Assessment. WPO# 31943

WCA.8.18 Kurt Larson to R. V. Bynum, March 13, 1996, “Brine-Waste Contact Volumes for Scoping Analysis of Organic Ligand Concentration” WPO# 36044

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Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.1

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PREFACE TO ATTACHMENT WCA.8.1

Title 40 of the Code of Federal Regulations (CFR) § 194.31 states that

The release limits shall be calculated according to part 191, appendix A of this chapter, using the total activity, in curies, that will exist in the disposal system at the time of disposal.

Making an exact assessment of the total activity (the radionuclide inventory) at the time of disposal (2033) requires assessing the total activity, in 2033, of three categories of contact-handled transuranic (CH-TRU) waste.

Category 1: the stored, "legacy" waste; CH-TRU waste that currently exists, is packaged, and has been inventoried and decayed to the year 1995.

Category 2: future waste that has already been generated; CH-TRU waste that currently exists and has been identified, is not packaged, and has not been inventoried for shipment to the Waste Isolation Pilot Plant (WIPP).

Category 3: future to-be-generated waste; CH-TRU waste that has not been identified.

Categories 2 and 3, the projected waste, comprise 66% of the WIPP waste by volume (Transuranic Waste Baseline Inventory Report [TWBIR], DOE 1995, p. 3-1).

Category 1 waste has already been inventoried and the inventory data can be readily decayed to any common base year (that is, to 1995, as is done in the TWBIR). Category 2 waste is expected to be similar to Category 1 waste, and could thus also be assessed at any common base year (for example, 1995). The Category 1 and 2 inventories can also be decayed to any other common year such as the year of closure, 2033. However, Category 3 waste is not necessarily similar to the other two categories and therefore should be estimated separately on a year-by-year basis as it is generated. Then each yearly contribution should be decayed separately to the closure year (2033).

TWBIR data collection methods estimated Category 3 data in the same manner as Category 2 data, and prorated Category 3 data accordingly. Thus, Category 3 data are estimated at 1995 instead of the later years during which the waste would be generated. Additional decay calculations of Category 3 data would result in over-decay of the inventory. For example, waste assayed in 2030 should be decayed for only three years to 2033; decaying such waste for the 38 years from 1995 to 2033 would result in an underestimate, particularly since the fraction of projected waste that is Category 3 cannot be determined. 40 CFR § 194.31 requires assessing the radionuclide inventory at the time of closure, that is, the year 2033. This can be done readily for Category 1 and Category 2 data. Because the Category 3 data were not separated from the Category 2 data, decaying from 1995 to 2033 underestimates portions of the Category 3 inventory by between one and 37 years of decay.

Because Category 3 wastes cannot currently be assessed separately from Category 2 wastes, there are two alternatives for calculating the waste unit factor: (1) calculation on the basis of the entire inventory decayed to 1995 or (2) calculation on the basis of the entire inventory decayed to 2033. The first yields a waste unit factor of 4.07×10^6, and the second, a waste unit factor of 3.44×10^6. The waste unit factor determines the normalization factor used in calculating the release limit, according to Table 1 of 40 CFR Part 191 Appendix A. The curies of radionuclides are divided by the release limit to determine the EPA units. All else being equal, a smaller release limit (and thus a smaller waste unit factor) is the more conservative of the two possibilities. Therefore, the entire inventory is decayed to 2033 for the performance assessment calculations as specified in 40 CFR § 194.31 above.

Attachment WCA.8.1 states that the inventory decayed to 1995 is used. However, as described above, in keeping with the specification of 40 CFR § 194.31 the inventory decayed to 2033 is used instead.

Reference:

DOE (U. S. Department of Energy). 1995. *Transuranic Waste Baseline Inventory Report, Rev. 2,* DOE/CAO 95-1121, Carlsbad, NM.

WPO 37428

INFORMATION ONLY

Sandia National Laboratories

Managed and Operated by Sandia Corporation
a Lockheed Martin Corporation
Albuquerque, New Mexico 87185-1328

date : April 24, 1996

to : M. Martell, Org 6749, MS-1328

from : L. C. Sanchez, Org 6741, MS-1328, PH-(505)848-0685, Fax-848-0705

subject : **Justification For Choice of CCA Radionuclide Values**

This memo gives the justification for the choice of the radionuclide data and their corresponding "Unit of Waste" value to be used in the 1996 WIPP CCA PA calculations. These data are obtained directly from the Transuranic Waste Baseline Inventory Database (TWBID). These values supersede the published values in Rev. 2 of the Transuranic Waste Baseline Inventory Report (TWBIR, Ref. BIR-2) and are intended for use in WIPP PA calculations until Rev. 3 TWBIR data are available.

The concern that arose while generating the "Unit of Waste" value was: At what calendar year should the radionuclide decay values and the "Unit of Waste" correspond to? Obviously, the answer is that they should be evaluated at the year that WIPP is decommissioned, which is expected to be the year 2033. The problem at hand is that the TWBID data is all evaluated at the year 1995 and these data values are comprised of two key components: 1) stored (legacy) and 2) future (projected and scaled) waste. The stored radionuclide inventory data are comprised of data values from many individual years (representing annual assessment made from 1970 → 1995). The stored values are easy to deal with because they have already been "decayed" to a common base year of 1995 (i.e., 1970 values are decayed to 1995, and 1971 values independently decayed to 1995, and so on). These decay calculations (SNL-3) were performed prior to the projection and scaling operations for future generated waste (see discussions in Ref. BIR-2). Thus, they can easily be decayed to any future base year. The problem, therefore, resides only with the future waste. Unfortunately, the TWBID does not contain sufficient data from the waste generation sites to predict radionuclide inventories in the future. However, the waste generator sites can make some predictions of the volumes of waste that may be expected to be generated in the future based on process knowledge available at the sites. The methodology used within the TWBIR is to estimate the future radionuclide inventories by multiplying the future volumes by the curie density (Ci/vol) of the stored radionuclides. This approach makes it impossible to properly decay these data values to the base year of 2033. This is because TWBID future values are already decayed from as far back as 1970 to the base year of 1995. Added decay of this data to the year 2033 would result in a portion of the data being decayed in excess of 38 years. Thus, this approach would yield non-conservative estimates (under-estimated values) for key radionuclides. An additional complication is that the majority of the radionuclide inventory is dominated by future generated radionuclides and each radionuclide has different breakdown of stored versus future inventory values (see Tables 1 and 2). The preferred approach would be to identify future radionuclide inventories on a yearly basis using curie densities based only on the last year production (undecayed) rates. Thus 1996 values could be decayed to the base year of 2033 independently of the 1997 values (plus later yearly values). Since this is not currently possible within the TWBID, it was decided to apply the 1995 (stored and future) data to the year 2033. Thus, radionuclide inventory data will be slightly conservative. This will only be of some importance in the early human intrusion scenarios. At later years the difference in radionuclide estimates due to the delta time of 38 years will be minuscule.

To identify if there are any significant impacts of applying 1995 data to the base year of 2033, a set of ORIGEN2 (Ref. OR-1) decay calculations were performed. These calculations decayed the 1995 TWBID values to the year 2033 and then values for the Unit of Waste and EPA Units calculated. Detailed calculations for the Unit of Waste and the EPA Units for 1995 data are showned in Tables 3 and 4. Results of ORIGEN2 decay calculations are showned in Table 5 (slight differences in 1995 curie values presented in Table 5 versus those presented in Tables 3 and 4 are due to conversion errors when translating input curie values into mass units for ORIGEN2 and also in the translating output mass values into curies). The most important finding from Table 5 is that the cumulative EPA Unit for 2033 base year is nearly the same as that for a base year of 1995. The reason for this is that over the first 38 years, the cumulative inventory of the key radionuclides that contribute to the EPA Unit decay at a rate comparable to that of the Unit of Waste. This is more easily observable at the bottom of Table 5 which shows the top four radionuclides of importance. As can be seen, while some radionuclides decay rapidly with time, some increase due to in growth. And the overall effect is that during this small time period the EPA Unit is essentially constant.

REFERENCES

[BIR-1]

DOE (U.S. Department of Energy); Waste Isolation Pilot Plant Transuranic Waste Baseline Inventory Report; CAO-94-1005; Revision 1; February 1995, Volume 1, Table 4-2, pg. 4-6.

[BIR-2]

DOE (U.S. Department of Energy); Transuranic Waste Baseline Inventory Report; DOE/CAO-95-1121; Revision 2; printed December 1995.

[BIR-2d]

Ibid., Table 3-4, pp. 3-27 → 29 (Volume 1).

[CCA-1]

S. Chakraborti (SAIC/CTAC); Letter to: J. Harvill (ASI/CTAC), Subject: "Revised Radionuclide Data In Support Of The CCA", Dated: April 12, 1996.

[CCA-2] SAIC LGS 4-25-96

S. Chakraborti (SAIV/CTAC); Letter to: J. Harvill (ASI/CTAC), Subject: "Final Radionuclide Data In Support Of The CCA", Dated: April 19, 1996. [This letter gives radionuclide data that supersedes Rev. 2 of the TWBIR and should be used in the 1996 CCA calculations for the WIPP facility. This letter also supersedes Ref. CCA-1, which had preliminary values. The reason that that this reference was generated was that after publication of Ref. BIR-2 it was identified that inventory data for several key radionuclides needed to be modified in accordance to new information obtained from the waste generation sites (this information was deemed important enough that the updated information was needed for the 1996 CCA calculations).]

[DOE-1]

DOE (U.S. Department of Energy); Remote-Handled Transuranic Waste Study; DOE/CAO-1095, DOE Carlsbad Area Office; Carlsbad, NM, October 1995.

[DOE-2]
DOE (U.S. Department of Energy), Waste Isolation Pilot Plant (WIPP); Record of Decision, **Federal Register** , Vol. 46, No. 18, pg. 9163, January 28, 1981 (46 FR 9162), Office of Environmental Restoration and Waste Management, Washington, D.C.

[DOE-3]
DOE (U.S. Department of Energy), Final Supplement Environmental Impact Statement, Waste Isolation Pilot Plant; DOE/EIS-0026-FS, January 1990., Volume 2, pg. B-4, Office of Environmental Restoration and Waste Management, Washington, D.C.

[DOE-4]
DOE (U.S. Department of Energy) and State of New Mexico (1981 originally); Agreement for Consulation and Cooperation Between Department of Energy and the State of New Mexico on the Waste Isolation Pilot Plant, Updated April 18, 1988; Article VI (WIPP Mission), pg. 7.

[EPA-1]
EPA (Environmental Protection Agency). 1985a. :40 CFR Part 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radionactive Waste: Final Rule," *Federal Register,* **Vol. 50,** No, 182, 38066-38089 (1985).

[EPA-1b]
Ibid., Appendix A to Part 191, Subpart B, Table 1, Note 1 (e).

[GE-1]General Electric Company (Nuclear Energy Operations), **Nuclides and Isotopes** , Fourteenth Edition, 1989.

[LWA-1]
Public Law 102-579, 102d Congress, October 30, 1992; *Waste Isolation Pilot Plant Land Withdrawal Act.;* 1992. Section 7, subparts (a)(1)(A) and (a)(3). [Note, the WIPP LWA in addition to limiting the RH-TRU canister surface dose equivalent rate to 1,000 rem/hr also limits the design capacity of (all) transuranics to 6.2 million cubic feet of volume of which no more than 5.1 million curies (Ci) may be RH-TRU. The volume limit for the RH-TRU is identified in the WIPP ROD (Record of Decision) to be 0.25 million cubic feet of volume [Ref. DOE-2]. Also, prior to the WIPP LWA 6.2 million cubic feet volume was assign to CH-TRU waste only (for instance, Ref. DOE-3 identifies that the total volume of WIPP was to be 6.45 million cubic feet -- 6.2 for CH-TRU and 0.25 for RH-TRU) and not CH-TRU plus RH-TRU. The WIPP LWA seems to be patterned after the WIPP C&C agreement [DOE-4]. It is in the WIPP C&C that a misquote was made to the WIPP ROD. The WIPP C&C quotes the WIPP ROD as applying the 6.2 million cubic meters to (all) transuranic waste. Even though the WIPP LWA is technically incorrect, the volumes identified there are to be used for WIPP calculations. More thorough discussion can be found in Ref. SA-1.]

[OR-1]Croff, A.G.; "ORIGEN2: A Users Manual for ORIGEN2 Computer Code," Oak Ridge National Laboratory, July 1980. (Further generalized discussion on ORIGEN2 can be found in Ref. OR-2.) (Detailed information on the validation (as applied to analysis of PWR spent fuel) and functional requirements (related to long-term storage of LWR spent fuel) of ORIGEN2 can be found in Refs. OR-3 and OR-4.)

[OR-2]Croff, A.G.; "ORIGEN2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials," **Nuclear Technology,** Vol. 62, September 1983.

[OR-3]Hermann, O.W., S.M. Bowman, M.C. Brady and C.V. Parks; "Validation of the Scale System for PWR Spent Fuel Isotropic Composition Analyses," ORNL/TM-12667, Oak Ridge National Laboratory, March 1995.

[OR-4]Broadhead, B.L., M.D. DeHart, J.C. Ryman, J.S. Tang and C.V. Parks; "Investigation of Nuclide Importance to Functional Requirements Related to Transport and Long-Term Storage of LWR Spent Fuel," Oak Ridge National Laboratory, June 1995. ORNL/TM-12742,

[SA-1]L.C. Sanchez (SNL Org 6741) and S.G. Bertram (SNL Org 6747); Memo to: L.E. Shephard (SNL Org 6800), Subject: "WIPP Capacity", dated: October 6, 1995.

[SNL-1]
J.W. Garner (SNL Org 6749); Memo to: C.T. Stockman (SNL Org 6749), Subject: "Radioisotopes to be used in the 1996 CCA Calculations", dated: 3/15/96

[SNL-2]
L.C. Sanchez (SNL Org 6741); Memo to: M. Martell (SNL Org 6747), Subject: "Radionuclide Half-lives and Specific Activities Obtained From ORIGEN2 Data", dated: March 28, 1996.

[SNL-3]
J. Powell, R. Carter, and H. Trellue; "WIPP PA Analysis Report for ORIGEN2 Suite", Sandia National Laboratories, April 1996.

[YMP-1]
Sandia YMP Project. 1994. *Total-System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993), Volume 1.* (SAND93-2675), Albuquerque, NM; Sandia National Laboratories.

[YMP-1b]
Ibid., Table 5-1, pg. 5-1 (Volume 1).

[YMP-1c]
Ibid., Table 5-2, pp. 5-2 → 5-3 (Volume 1).

[YMP-1d]
Ibid., Table 5-7, pg. 5-6 (Volume 1).

LCS:6741:lcs/(96-2108)

Copy to:
MS-1328, Day File [Dept. 6741]
MS-1328, L.C. Sanchez [Dept. 6741]
File - SWCF-A WBS 1.1.6.2;PA;PBWAC - WIPP ACTIVITY

Table 1.
WIPP CH TOTAL (1995 DECAYED) CURIES (a)

Nuclide (b)	Stored	Projected	Total Ci	Stored (%)	Projected (%)
Ac225	1.94E+00	9.37E-01	2.88E+00	67 %	33 %
Ac227	2.80E-01	3.27E-01	6.07E-01	46 %	54 %
Ac228	3.76E-01	3.70E-01	7.46E-01	50 %	50 %
Ag109m	6.56E+00	9.12E+00	1.57E+01	42 %	58 %
Ag110	4.14E-09	2.92E-09	7.06E-09	59 %	41 %
Ag110m	3.11E-07	2.19E-07	5.31E-07	59 %	41 %
Am241	**2.39E+05**	**2.02E+05**	**4.42E+05**	**54 %**	**46 %**
Am242	2.34E-01	1.51E+00	1.74E+00	13 %	87 %
Am242m	2.35E-01	1.52E+00	1.75E+00	13 %	87 %
Am243	**1.79E+01**	**1.46E+01**	**3.25E+01**	**55 %**	**45 %**
Am245	1.27E-09	6.13E-11	1.33E-09	95 %	5 %
At217	1.94E+00	9.37E-01	2.88E+00	67 %	33 %
Ba137m	2.96E+03	4.66E+03	7.62E+03	39 %	61 %
Bi210	1.64E+00	9.12E-01	2.55E+00	64 %	36 %
Bi211	2.81E-01	3.27E-01	6.08E-01	46 %	54 %
Bi212	2.66E+01	4.59E-01	2.70E+01	98 %	2 %
Bi213	1.94E+00	9.37E-01	2.88E+00	67 %	33 %
Bi214	7.69E+00	3.93E+00	1.16E+01	66 %	34 %
Bk249	8.73E-05	4.23E-06	9.15E-05	95 %	5 %
Bk250	4.20E-11	1.64E-12	4.37E-11	96 %	4 %
C14	1.77E+00	9.06E+00	1.08E+01	16 %	84 %
Cd109	6.55E+00	9.12E+00	1.57E+01	42 %	58 %
Cd113m	7.81E-07	1.04E-06	1.82E-06	43 %	57 %
Ce144	3.70E-02	2.54E-02	6.25E-02	59 %	41 %
Cf249	5.08E-02	1.33E-02	6.41E-02	79 %	21 %
Cf250	3.20E-01	1.03E-02	3.30E-01	97 %	3 %
Cf251	1.58E-03	2.20E-03	3.77E-03	42 %	58 %
Cf252	**3.61E+01**	**2.03E+02**	**2.39E+02**	**15 %**	**85 %**
Cm242	1.54E-01	9.84E-01	1.14E+00	14 %	86 %
Cm243	**1.11E+00**	**1.61E+00**	**2.71E+00**	**41 %**	**59 %**
Cm244	**6.31E+03**	**2.51E+04**	**3.14E+04**	**20 %**	**80 %**
Cm245	**1.76E-03**	**9.70E-03**	**1.15E-02**	**15 %**	**85 %**
Cm246	4.28E-02	5.92E-02	1.02E-01	42 %	58 %
Cm247	1.34E-09	1.87E-09	3.21E-09	42 %	58 %
Cm248	**3.35E-02**	**5.59E-02**	**8.94E-02**	**37 %**	**63 %**
Co58	1.34E-13	1.70E-13	3.04E-13	44 %	56 %
Co60	6.27E+01	1.78E+00	6.45E+01	97 %	3 %
Cs134	6.09E-03	7.32E-03	1.34E-02	45 %	55 %
Cs135	2.15E-04	2.87E-04	5.01E-04	43 %	57 %
Cs137	**3.12E+03**	**4.93E+03**	**8.05E+03**	**39 %**	**61 %**
Es254	4.11E-11	1.25E-12	4.23E-11	97 %	3 %
Eu150	3.50E-05	0.00E+00	3.50E-05	100 %	0 %
Eu152	1.22E+00	3.30E-02	1.26E+00	97 %	3 %
Eu154	1.10E+00	4.89E-02	1.14E+00	96 %	4 %
Eu155	6.18E-01	3.27E-01	9.45E-01	65 %	35 %
Fe55	1.91E-05	0.00E+00	1.91E-05	100 %	0 %
Fe59	1.87E-07	7.68E-08	2.64E-07	71 %	29 %
Fr221	1.94E+00	9.37E-01	2.88E+00	67 %	33 %

Table 1 Continued.
WIPP CH TOTAL (1995 DECAYED) CURIES (a)

Nuclide (b)	Stored	Projected	Total Ci	Stored (%)	Projected (%)
Fr223	3.87E-03	4.51E-03	8.38E-03	46 %	54 %
H3	8.66E-01	1.96E-03	8.68E-01	100 %	0 %
I129	1.17E-07	5.87E-07	7.04E-07	17 %	83 %
Kr85	1.96E-01	5.96E-03	2.02E-01	97 %	3 %
Mn54	8.49E-04	7.67E-08	8.50E-04	100 %	0 %
Nb95	2.41E-09	1.26E-10	2.54E-09	95 %	5 %
Nb95m	8.06E-12	4.22E-13	8.49E-12	95 %	5 %
Ni59	1.25E-03	6.27E-03	7.52E-03	17 %	83 %
Ni63	1.53E-01	7.66E-01	9.18E-01	17 %	83 %
Np237	**1.08E+01**	**4.52E+01**	**5.60E+01**	**19 %**	**81 %**
Np238	1.18E-03	7.58E-03	8.76E-03	13 %	87 %
Np239	1.79E+01	1.46E+01	3.25E+01	55 %	45 %
Np240m	1.20E-06	3.04E-07	1.50E-06	80 %	20 %
Pa231	**3.16E-01**	**1.34E-01**	**4.50E-01**	**70 %**	**30 %**
Pa233	1.08E+01	4.52E+01	5.60E+01	19 %	81 %
Pa234	7.90E-03	4.35E-02	5.14E-02	15 %	85 %
Pa234m	6.08E+00	3.35E+01	3.95E+01	15 %	85 %
Pb209	1.94E+00	9.37E-01	2.88E+00	67 %	33 %
Pb210	**1.64E+00**	**9.12E-01**	**2.55E+00**	**64 %**	**36 %**
Pb211	2.81E-01	3.27E-01	6.08E-01	46 %	54 %
Pb212	2.66E+01	4.59E-01	2.70E+01	98 %	2 %
Pb214	7.69E+00	3.93E+00	1.16E+01	66 %	34 %
Pd107	3.17E-05	4.23E-05	7.41E-05	43 %	57 %
Pm147	**4.79E+00**	**3.06E+00**	**7.86E+00**	**61 %**	**39 %**
Po210	1.64E+00	9.12E-01	2.55E+00	64 %	36 %
Po211	7.86E-04	9.17E-04	1.70E-03	46 %	54 %
Po212	1.70E+01	2.94E-01	1.73E+01	98 %	2 %
Po213	1.90E+00	9.17E-01	2.81E+00	67 %	33 %
Po214	7.69E+00	3.93E+00	1.16E+01	66 %	34 %
Po215	2.81E-01	3.27E-01	6.08E-01	46 %	54 %
Po216	2.66E+01	4.59E-01	2.70E+01	98 %	2 %
Po218	7.69E+00	3.94E+00	1.16E+01	66 %	34 %
Pr144	3.66E-02	2.52E-02	6.18E-02	59 %	41 %
Pu236	1.04E-02	7.47E-17	1.04E-02	100 %	0 %
Pu238	**5.54E+05**	**2.06E+06**	**2.61E+06**	**21 %**	**79 %**
Pu239	**3.51E+05**	**4.33E+05**	**7.84E+05**	**45 %**	**55 %**
Pu240	**6.87E+04**	**1.41E+05**	**2.10E+05**	**33 %**	**67 %**
Pu241	**1.07E+06**	**1.23E+06**	**2.30E+06**	**47 %**	**53 %**
Pu242	**4.93E+02**	**6.79E+02**	**1.17E+03**	**42 %**	**58 %**
Pu243	1.34E-09	1.87E-09	3.21E-09	42 %	58 %
Pu244	**1.20E-06**	**3.04E-07**	**1.50E-06**	**80 %**	**20 %**
Ra223	2.81E-01	3.27E-01	6.08E-01	46 %	54 %
Ra224	2.66E+01	4.59E-01	2.70E+01	98 %	2 %
Ra225	1.94E+00	9.37E-01	2.88E+00	67 %	33 %
Ra226	**7.69E+00**	**3.94E+00**	**1.16E+01**	**66 %**	**34 %**
Ra228	**3.76E-01**	**3.70E-01**	**7.46E-01**	**50 %**	**50 %**
Rh106	1.52E-02	1.37E-02	2.89E-02	53 %	47 %
Rn219	2.81E-01	3.27E-01	6.08E-01	46 %	54 %

Table 1 Continued.
WIPP CH TOTAL (1995 DECAYED) CURIES (a)

Nuclide (b)	Stored	Projected	Total Ci	Stored (%)	Projected (%)
Rn220	2.66E+01	4.59E-01	2.70E+01	98 %	2 %
Rn222	7.69E+00	3.94E+00	1.16E+01	66 %	34 %
Ru106	1.52E-02	1.37E-02	2.89E-02	53 %	47 %
Sb125	5.22E-02	6.84E-02	1.21E-01	43 %	57 %
Sb126	5.78E-05	7.72E-05	1.35E-04	43 %	57 %
Sb126m	4.12E-04	5.51E-04	9.64E-04	43 %	57 %
Se 79	1.86E-04	2.49E-04	4.35E-04	43 %	57 %
Sm151	6.28E-01	8.40E-01	1.47E+00	43 %	57 %
Sn119m	2.44E-06	1.69E-06	4.14E-06	59 %	41 %
Sn121m	1.14E-02	1.52E-02	2.66E-02	43 %	57 %
Sn126	4.12E-04	5.51E-04	9.64E-04	43 %	57 %
Sr90	**2.22E+03**	**4.62E+03**	**6.84E+03**	**32 %**	**68 %**
Tc99	1.78E+01	7.33E+00	2.51E+01	71 %	29 %
Te125m	1.27E-02	1.67E-02	2.94E-02	43 %	57 %
Te127	1.07E-07	2.34E-08	1.30E-07	82 %	18 %
Te127m	1.09E-07	2.39E-08	1.33E-07	82 %	18 %
Th227	2.77E-01	3.23E-01	6.00E-01	46 %	54 %
Th228	2.66E+01	4.59E-01	2.70E+01	98 %	2 %
Th229	**1.94E+00**	**9.37E-01**	**2.88E+00**	**67 %**	**33 %**
Th230	**3.04E-02**	**5.01E-02**	**8.05E-02**	**38 %**	**62 %**
Th231	2.31E+00	1.05E+01	1.28E+01	18 %	82 %
Th232	**4.22E-01**	**4.90E-01**	**9.12E-01**	**46 %**	**54 %**
Th234	6.08E+00	3.35E+01	3.95E+01	15 %	85 %
Tl207	2.80E-01	3.27E-01	6.07E-01	46 %	54 %
Tl208	9.55E+00	1.65E-01	9.72E+00	98 %	2 %
Tl209	4.19E-02	2.02E-02	6.21E-02	67 %	33 %
U232	2.56E+01	1.20E-01	2.58E+01	100 %	0 %
U233	**1.20E+03**	**5.88E+02**	**1.79E+03**	**67 %**	**33 %**
U234	**9.23E+01**	**3.72E+02**	**4.64E+02**	**20 %**	**80 %**
U235	**2.31E+00**	**1.05E+01**	**1.28E+01**	**18 %**	**82 %**
U236	**6.74E-02**	**2.65E-01**	**3.33E-01**	**20 %**	**80 %**
U237	2.63E+01	3.02E+01	5.65E+01	47 %	53 %
U238	**6.08E+00**	**3.35E+01**	**3.95E+01**	**15 %**	**85 %**
U240	1.20E-06	3.04E-07	1.50E-06	80 %	20 %
Y90	2.22E+03	4.62E+03	6.85E+03	32 %	68 %
Zr93	2.41E-03	3.21E-03	5.62E-03	43 %	57 %
Zr95	1.09E-09	5.69E-11	1.14E-09	95 %	5 %
Total	2.31E+06	4.11E+06	6.41E+06	36 %	64 %

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-1.

Table 2.
WIPP RH TOTAL (1995 DECAYED) CURIES (a)

Nuclide (b)	Stored	Projected	Total Ci	Stored (%)	Projected (%)
Ac225	8.55E-02	3.18E-02	1.17E-01	73 %	27 %
Ac227	2.08E-04	5.49E-04	7.57E-04	27 %	73 %
Ac228	2.51E-02	5.26E-02	7.77E-02	32 %	68 %
Ag110	1.45E-09	2.92E-10	1.74E-09	83 %	17 %
Ag110m	1.09E-07	2.20E-08	1.31E-07	83 %	17 %
Am241	**1.36E+02**	**5.83E+03**	**5.96E+03**	**2 %**	**98 %**
Am243	**2.23E-04**	**5.10E-06**	**2.28E-04**	**98 %**	**2 %**
Am245	2.43E-16	4.40E-17	2.87E-16	85 %	15 %
At217	8.55E-02	3.18E-02	1.17E-01	73 %	27 %
Ba137m	5.02E+03	1.99E+05	2.04E+05	2 %	98 %
Bi210	1.33E-07	7.03E-06	7.16E-06	2 %	98 %
Bi211	2.08E-04	5.49E-04	7.58E-04	27 %	73 %
Bi212	2.45E-02	4.92E-02	7.36E-02	33 %	67 %
Bi213	8.55E-02	3.18E-02	1.17E-01	73 %	27 %
Bi214	7.97E-07	3.50E-05	3.58E-05	2 %	98 %
Bk249	1.68E-11	3.03E-12	1.98E-11	85 %	15 %
C14	1.74E+00	3.13E-01	2.05E+00	85 %	15 %
Cd113m	2.83E-07	2.63E-07	5.46E-07	52 %	48 %
Ce144	4.51E+00	6.17E-01	5.13E+00	88 %	12 %
Cf249	3.79E-03	6.85E-04	4.47E-03	85 %	15 %
Cf252	**1.09E+00**	**1.97E-01**	**1.29E+00**	**85 %**	**15 %**
Cm243	**4.19E+01**	**7.58E+00**	**4.95E+01**	**85 %**	**15 %**
Cm244	**2.67E+02**	**4.83E+01**	**3.15E+02**	**85 %**	**15 %**
Cm245	**1.24E-06**	**2.24E-07**	**1.46E-06**	**85 %**	**15 %**
Cm248	**1.73E-04**	**3.14E-05**	**2.05E-04**	**85 %**	**15 %**
Co58	1.24E-11	0.00E+00	1.24E-11	100 %	0 %
Co60	2.75E+02	1.02E+04	1.04E+04	3 %	97 %
Cr51	3.04E-06	0.00E+00	3.04E-06	100 %	0 %
Cs134	1.79E+01	4.96E-01	1.84E+01	97 %	3 %
Cs135	6.07E-05	5.66E-05	1.17E-04	52 %	48 %
Cs137	**5.31E+03**	**2.11E+05**	**2.16E+05**	**2 %**	**98 %**
Eu152	1.04E+03	1.87E+02	1.22E+03	85 %	15 %
Eu154	5.00E+02	9.05E+01	5.91E+02	85 %	15 %
Eu155	9.96E+01	1.84E+01	1.18E+02	84 %	16 %
Fe55	1.69E-01	0.00E+00	1.69E-01	100 %	0 %
Fr221	8.55E-02	3.18E-02	1.17E-01	73 %	27 %
Fr223	2.87E-06	7.58E-06	1.04E-05	27 %	73 %
H3	6.21E-02	3.94E-03	6.60E-02	94 %	6 %
Kr85	1.68E+00	0.00E+00	1.68E+00	100 %	0 %
Mn54	2.35E-02	0.00E+00	2.35E-02	100 %	0 %
Nb95	5.66E-01	1.02E-01	6.69E-01	85 %	15 %
Nb95m	1.90E-03	3.43E-04	2.24E-03	85 %	15 %
Ni63	9.88E-01	0.00E+00	9.88E-01	100 %	0 %
Np237	**2.37E+00**	**4.76E-01**	**2.85E+00**	**83 %**	**17 %**
Np239	2.23E-04	5.10E-06	2.28E-04	98 %	2 %
Np240m	1.87E-11	3.39E-12	2.21E-11	85 %	15 %
Pa231	**4.15E-05**	**1.87E-03**	**1.91E-03**	**2 %**	**98 %**
Pa233	2.37E+00	4.76E-01	2.85E+00	83 %	17 %

Table 2 Continued.
WIPP RH TOTAL (1995 DECAYED) CURIES (a)

Nuclide (b)	Stored	Projected	Total Ci	Stored (%)	Projected (%)
Pa234	1.12E-02	2.43E-03	1.36E-02	82 %	18 %
Pa234m	8.61E+00	1.87E+00	1.05E+01	82 %	18 %
Pb209	8.55E-02	3.18E-02	1.17E-01	73 %	27 %
Pb210	**1.33E-07**	**7.03E-06**	**7.16E-06**	**2 %**	**98 %**
Pb211	2.08E-04	5.49E-04	7.58E-04	27 %	73 %
Pb212	2.45E-02	4.92E-02	7.36E-02	33 %	67 %
Pb214	7.97E-07	3.50E-05	3.58E-05	2 %	98 %
Pd107	8.97E-06	8.37E-06	1.73E-05	52 %	48 %
Pm147	**7.40E+00**	**3.34E+00**	**1.07E+01**	**69 %**	**31 %**
Po210	1.33E-07	7.03E-06	7.16E-06	2 %	98 %
Po211	5.83E-07	1.54E-06	2.12E-06	27 %	73 %
Po212	1.57E-02	3.15E-02	4.72E-02	33 %	67 %
Po213	8.36E-02	3.11E-02	1.15E-01	73 %	27 %
Po214	7.97E-07	3.49E-05	3.57E-05	2 %	98 %
Po215	2.08E-04	5.49E-04	7.58E-04	27 %	73 %
Po216	2.45E-02	4.92E-02	7.36E-02	33 %	67 %
Po218	7.97E-07	3.50E-05	3.58E-05	2 %	98 %
Pr144	4.46E+00	6.09E-01	5.07E+00	88 %	12 %
Pu238	**3.95E+01**	**1.41E+03**	**1.45E+03**	**3 %**	**97 %**
Pu239	**1.57E+02**	**1.01E+04**	**1.03E+04**	**2 %**	**98 %**
Pu240	**5.06E+01**	**5.01E+03**	**5.07E+03**	**1 %**	**99 %**
Pu241	**1.33E+03**	**1.40E+05**	**1.42E+05**	**1 %**	**99 %**
Pu242	**1.67E-03**	**1.48E-01**	**1.50E-01**	**1 %**	**99 %**
Pu244	**1.87E-11**	**3.39E-12**	**2.21E-11**	**85 %**	**15 %**
Ra223	2.08E-04	5.49E-04	7.58E-04	27 %	73 %
Ra224	2.45E-02	4.92E-02	7.36E-02	33 %	67 %
Ra225	8.55E-02	3.18E-02	1.17E-01	73 %	27 %
Ra226	**7.97E-07**	**3.50E-05**	**3.58E-05**	**2 %**	**98 %**
Ra228	**2.51E-02**	**5.26E-02**	**7.77E-02**	**32 %**	**68 %**
Rh106	9.18E+00	1.74E+00	1.09E+01	84 %	16 %
Rn219	2.08E-04	5.49E-04	7.58E-04	27 %	73 %
Rn220	2.45E-02	4.92E-02	7.36E-02	33 %	67 %
Rn222	7.97E-07	3.50E-05	3.58E-05	2 %	98 %
Ru106	9.18E+00	1.74E+00	1.09E+01	84 %	16 %
Sb125	1.06E+00	8.25E-01	1.89E+00	56 %	44 %
Sb126	1.63E-05	1.52E-05	3.16E-05	52 %	48 %
Sb126m	1.17E-04	1.09E-04	2.25E-04	52 %	48 %
Se79	5.27E-05	4.91E-05	1.02E-04	52 %	48 %
Sm151	1.85E-01	1.72E-01	3.57E-01	52 %	48 %
Sn119m	8.05E-07	1.54E-07	9.59E-07	84 %	16 %
Sn121m	3.47E-03	3.23E-03	6.69E-03	52 %	48 %
Sn126	1.17E-04	1.09E-04	2.25E-04	52 %	48 %
Sr90	**1.23E+04**	**1.96E+05**	**2.09E+05**	**6 %**	**94 %**
Ta182	4.21E-08	0.00E+00	4.21E-08	100 %	0 %
Tc99	3.03E-03	2.82E-03	5.85E-03	52 %	48 %
Te125m	2.62E-01	2.03E-01	4.65E-01	56 %	44 %
Te127	1.67E-09	3.87E-11	1.71E-09	98 %	2 %
Te127m	1.71E-09	3.95E-11	1.75E-09	98 %	2 %

Table 2 Continued.
WIPP RH TOTAL (1995 DECAYED) CURIES (a)

Nuclide (b)	Stored	Projected	Total Ci	Stored (%)	Projected (%)
Th227	2.05E-04	5.42E-04	7.47E-04	27 %	73 %
Th228	2.45E-02	4.92E-02	7.36E-02	33 %	67 %
Th229	**8.55E-02**	**3.18E-02**	**1.17E-01**	**73 %**	**27 %**
Th230	**2.56E-04**	**7.30E-03**	**7.56E-03**	**3 %**	**97 %**
Th231	2.01E-01	4.43E+00	4.63E+00	4 %	96 %
Th232	**2.86E-02**	**6.39E-02**	**9.25E-02**	**31 %**	**69 %**
Th234	8.61E+00	1.87E+00	1.05E+01	82 %	18 %
Tl207	2.08E-04	5.48E-04	7.56E-04	27 %	73 %
Tl208	8.79E-03	1.77E-02	2.65E-02	33 %	67 %
Tl209	1.85E-03	6.88E-04	2.53E-03	73 %	27 %
U233	**1.23E+02**	**3.47E+01**	**1.58E+02**	**78 %**	**22 %**
U234	**3.30E+00**	**3.94E+01**	**4.27E+01**	**8 %**	**92 %**
U235	**2.01E-01**	**4.43E+00**	**4.63E+00**	**4 %**	**96 %**
U236	**7.97E-02**	**1.70E-02**	**9.68E-02**	**82 %**	**18 %**
U237	3.27E-02	3.45E+00	3.48E+00	1 %	99 %
U238	**8.61E+00**	**1.87E+00**	**1.05E+01**	**82 %**	**18 %**
U240	1.87E-11	3.39E-12	2.21E-11	85 %	15 %
Y90	1.23E+04	1.96E+05	2.09E+05	6 %	94 %
Zr93	6.81E-04	6.35E-04	1.32E-03	52 %	48 %
Zr95	2.56E-01	4.63E-02	3.02E-01	85 %	15 %
Total	3.91E+04	9.76E+05	1.02E+06	4 %	96 %

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-1.

Table 3.
40CFR191 Unit of Waste for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] **(d)**		Transuranic Inventory [α-Curies] (e)		% of Unit of Waste
			CH	RH	CH	RH	(%)
Ac225	α,γ	10.0 d	2.88E+00	1.17E-01			
Ac227	α,β^-,γ	21.77 a	6.08E-01	7.57E-04			
Ac228	α,β^-,γ	6.15 h	7.46E-01	7.77E-02			
Ag109m	ITe^-	39.8 s	1.57E+01	NR			
Ag110	$\beta^-,\gamma,\varepsilon$	24.6 s	7.07E-09	1.74E-09			
Ag110m	β^-,γ,ITe^-	249.8 d	5.31E-07	1.31E-07			
Am241	α,γ,SF	432.7 a	4.42E+05	5.96E+03	**4.42E+05**	**5.96E+03**	**11.0**
Am242	$\beta,\gamma,\varepsilon e^-$	16.02 h	1.75E+00	NR			
Am242m	α,ITe^-	141. h	1.75E+00	NR			
Am243	α,β^-,γ	7.37E+03 a	3.26E+01	2.28E-04	**3.26E+01**	**2.28E-04**	**8.01E-04**
Am245	β^-,γ	2.05 h	1.33E-09	2.87E-16			
At217	α,β^-,γ	32 ms	2.88E+00	1.17E-01			
Ba137m	IT	2.552 m	7.63E+03	2.04E+05			
Bi210	α,β^-,γ	5.01 d	2.55E+00	7.16E-06			
Bi211	α,β^-,γ	2.14 m	6.09E-01	7.58E-04			
Bi212	α,β^-,γ	1.009 h	2.71E+01	7.36E-02			
Bi213	α,β^-,γ	45.6 m	2.88E+00	1.17E-01			
Bi214	α,β^-,γ	19.9 m	1.16E+01	3.58E-05			
Bk249	α,β^-,γ	3.2E+02 d	9.16E-05	1.98E-11			
Bk250	β^-,γ	3.217 h	4.37E-11	NR			
C14	β^-	5730 a	1.08E+01	2.05E+00			
Cd109	γ,ε	462.0 d	1.57E+01	NR			
Cd113m	β^-,IT	14.1 a	1.82E-06	5.46E-07			
Ce144	β^-,γ	284.6 d	6.26E-02	5.13E+00			
Cf249	α,γ,SF	351 a	6.42E-02	4.47E-03	6.42E-02	4.47E-03	1.69E-06
Cf250	α,γ,SF	13.1 a	3.30E-01	NR			
Cf251	α,γ	9.0E+02 a	3.78E-03	NR	3.78E-03	NR	9.28E-08
Cf252	α,γ,SF	2.638 a	2.39E+02	1.29E+00			
Cm242	α,γ,SF	162.8 d	1.14E+00	NR			
Cm243	$\alpha,\gamma,SF,\varepsilon$	29.1 a	2.72E+00	4.95E+01	**2.72E+00**	**4.95E+01**	**1.28E-03**
Cm244	α,γ,SF	18.1 a	3.15E+04	3.15E+02			
Cm245	α,γ,SF	8.5E+03 a	1.15E+02	1.46E-06	**1.15E+02**	**1.46E-06**	**2.82E-03**
Cm246	α,γ,SF	4.76E+03 a	1.02E-01	NR	1.02E-01	NR	2.51E-06
Cm247	α,γ	1.56E+07 a	3.21E-09	NR	3.21E-09	NR	7.88E-14
Cm248	α,SF	3.48E+05 a	8.95E-02	2.05E-04	**8.95E-02**	**2.05E-04**	**2.20E-06**
Co58	$\beta^+,\gamma,\varepsilon$	70.88 d	3.05E-13	1.24E-11			
Co60	β^-,γ	5.271 a	6.46E+01	1.04E+04			
Cr51	$\varepsilon\gamma$	27.70 d	NR	3.04E-06			
Cs134	$\beta^-,\gamma,\varepsilon$	2.065 a	1.34E-02	1.84E+01			
Cs135	β^-	2.3E+06 a	5.02E-04	1.17E-04			
Cs137	β^-,γ	30.17 a	8.06E+03	**2.16E+05 (g)**			
Es254	α,γ	276 d	4.24E-11	NR			

Table 3 Continued.
40CFR191 Unit of Waste for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (**b**)	Decay Mode (**c**)	Half-Life (**c**)	Total Inventory [Curies] (**d**)		Transuranic Inventory [α-Curies] (**e**)		% of Unit of Waste
			CH	RH	CH	RH	(%)
Eu150	γ,ε	36 a	3.51E-05	NR			
Eu152	$\beta^-,\gamma,\varepsilon\beta^+$	13.48 a	1.26E+00	1.22E+03			
Eu154	$\beta^-,\gamma,\varepsilon\gamma$	8.59 a	1.15E+00	5.91E+02			
Eu155	β^-,γ	4.71 a	9.46E-01	1.18E+02			
Fe55	ε	2.73 a	1.91E-05	1.69E-01			
Fe59	β^-,γ	44.51 d	2.64E-07	NR			
Fr221	α,γ	4.8 m	2.88E+00	1.17E-01			
Fr223	α,β^-,γ	21.8 m	8.39E-03	1.04E-05			
H3	β^-	12.3 a	8.69E-01	6.60E-02			
I129	β^-,γ	1.57E+07 a	7.05E-07	NR			
Kr85	β^-,γ	10.73 a	2.02E-01	1.68E+00			
Mn54	$\varepsilon\gamma$	312.2 d	8.51E-04	2.35E-02			
Nb95	β^-,γ	34.97 d	2.54E-09	6.69E-01			
Nb95m	β^-,γ,IT	3.61 d	8.50E-12	2.24E-03			
Ni59	ε	7.6E+04 a	7.52E-03	NR			
Ni63	β^-	100. a	9.19E-01	9.88E-01			
Np237	α,γ	2.14E+06 a	5.61E+01	2.85E+00	**5.61E+01**	**2.85E+00**	**1.45E-03**
Np238	β,γ	2.117 d	8.77E-03	NR			
Np239	β^-,γ	2.355 d	3.26E+01	2.28E-04			
Np240‡	β,γ	1.032 h	NR	NR			
Np240m	β^-,γ,IT	7.22 m	1.50E-06	2.21E-11			
Pa231	α,γ	3.28E+04 a	4.51E-01	1.91E-03			
Pa233	β^-,γ	27.0 d	5.61E+01	2.85E+00			
Pa234	β^-,γ	6.69 h	5.14E-02	1.36E-02			
Pa234m	β^-,γ,IT	1.17 m	3.96E+01	1.05E+01			
Pb209	β^-	3.25 h	2.88E+00	1.17E-01			
Pb210	α,β^-,γ	22.3 a	2.55E+00	7.16E-06			
Pb211	β^-,γ	36.1 m	6.09E-01	7.58E-04			
Pb212	β^-,γ	10.64 hr	2.71E+01	7.36E-02			
Pb214	β^-,γ	27 m	1.16E+01	3.58E-05			
Pd107	β^-,γ	6.5E+06 a	7.41E-05	1.73E-05			
Pm147	β^-,γ	2.6234 a	7.87E+00	1.07E+01			
Po210	α,γ	138.38 d	2.55E+00	7.16E-06			
Po211	α,γ	0.516 s	1.71E-03	2.12E-06			
Po212	α	0.298 μs	1.73E+01	4.72E-02			
Po213	α	4 μs	2.82E+00	1.15E-01			
Po214	α,γ	163.7 μs	1.16E+01	3.57E-05			
Po215	α,β^-,γ	1.780 ms	6.09E-01	7.58E-04			
Po216	α,γ	0.145 s	2.71E+01	7.36E-02			
Po218	α,β^-,γ	3.10 m	1.16E+01	3.58E-05			
Pr144	β^-,γ	17.28 m	6.18E-02	5.07E+00			
Pu236	α,γ,SF	2.87 a	1.04E-02	NR			

Table 3 Continued.
40CFR191 Unit of Waste for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (d)		Transuranic Inventory [α-Curies] (e)		% of Unit of Waste
			CH	RH	CH	RH	(%)
Pu238	α,γ,*SF*	87.7 a	**2.61E+06 (f)**	1.45E+03	**2.61E+06**	**1.45E+03**	**64.1**
Pu239	α,γ,*SF*	2.410E+04 a	7.85E+05	1.03E+04	**7.85E+05**	**1.03E+04**	**19.5**
Pu240	α,γ,*SF*	6.56E+03 a	2.10E+05	5.07E+03	**2.10E+05**	**5.07E+03**	**5.28**
Pu241	α,β^-,γ	14.4 a	2.31E+06	1.42E+05			
Pu242	α,γ,*SF*	3.75E+05 a	1.17E+03	1.50E-01	**1.17E+03**	**1.50E-01**	**2.87E-02**
Pu243	β^-,γ	4.956 h	3.21E-09	NR			
Pu244	α,*SF*	8.0E+07 a	1.50E-06	2.21E-11	**1.50E-06**	**2.21E-11**	**3.68E-11**
Ra223	α,γ	11.435 d	6.09E-01	7.58E-04			
Ra224	α,γ	3.66 d	2.71E+01	7.36E-02			
Ra225	β^-,γ	14.9 d	2.88E+00	1.17E-01			
Ra226	α,γ	1.60E+03 a	1.16E+01	3.58E-05			
Ra228	β^-,γ	5.76 a	7.47E-01	7.77E-02			
Rh106	β^-,γ	29.9 s	2.90E-02	1.09E+01			
Rn219	α,γ	3.96 s	6.09E-01	7.58E-04			
Rn220	α,γ	55.6 s	2.71E+01	7.36E-02			
Rn222	α,γ	3.8235 d	1.16E+01	3.58E-05			
Ru106	β^-	1.02 a	2.90E-02	1.09E+01			
Sb125	β^-,γ	2.758 a	1.21E-01	1.89E+00			
Sb126	β^-,γ	12.4 d	1.35E-04	3.16E-05			
Sb126m	γ,*εe*$^-$	19.0 m	9.65E-04	2.25E-04			
Se79	β^-	6.5E+04 a	4.35E-04	1.02E-04			
Sm151	β^-,γ	90 a	1.47E+00	3.57E-01			
Sn119m	γ,*ITe*$^-$	293 d	4.14E-06	9.59E-07			
Sn121m	β^-,γ,*ITe*$^-$	55 a	2.66E-02	6.69E-03			
Sn126	β^-,γ	1.0E+05 a	9.65E-04	2.25E-04			
Sr89†	β^-,γ	50.52 d	NR	NR			
Sr90	β^-	29.1 a	6.85E+03	2.09E+05			
Ta182	β^-,γ	114.43 d	NR	4.21E-08			
Tc99	β^-,γ	2.13E+05 a	2.52E+01	5.85E-03			
Te125m	γ,*ITe*$^-$	58 d	2.95E-02	4.65E-01			
Te127	β^-,γ	9.4 h	1.30E-07	1.71E-09			
Te127m	β^-,γ,*ITe*$^-$	109 d	1.33E-07	1.75E-09			
Th227	α,γ	18.72 d	6.01E-01	7.47E-04			
Th228	α,γ	1.913 a	2.71E+01	7.36E-02			
Th229	α,γ	7.3E+03 a	2.88E+00	1.17E-01			
Th230	α,γ	7.54E+04 a	8.06E-02	7.56E-03			
Th231	β^-,γ	1.063 d	1.28E+01	4.63E+00			
Th232	α,γ	1.4E+10 a	9.13E-01	9.25E-02			
Th234	β^-,γ	24.10 m	3.96E+01	1.05E+01			
Tl207	β^-,γ	4.77 m	6.07E-01	7.56E-04			
Tl208	β^-,γ	3.053 m	9.73E+00	2.65E-02			

Table 3 Continued.
40CFR191 Unit of Waste for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (**d**)		Transuranic Inventory [α-Curies] (e)		% of Unit of Waste
			CH	RH	CH	RH	(%)
Tl209	β^-,γ	2.2 m	6.22E-02	2.53E-03			
Tl210‡	β,γ	1.30 m	NR	NR			
U232	α,γ,SF	70 a	2.58E+01	NR			
U233	α,γ,SF	1.592E+05 a	1.79E+03	1.58E+02			
U234	α,γ,SF	2.46E+05 a	4.65E+02	4.27E+01			
U235	α,γ,SF	7.04E+08 a	1.28E+01	4.63E+00			
U236	α,γ,SF	2.342E+07 a	3.33E-01	9.68E-02			
U237	β^-,γ	6.75 d	5.66E+01	3.48E+00			
U238	α,γ,SF	4.47E+09 a	3.96E+01	1.05E+01			
U240	β^-,γ	14.1 h	1.50E-06	2.21E-11			
Y90	β^-,γ	2.67 d	6.85E+03	2.09E+05			
Zn65†	$\beta^+,\gamma,\varepsilon$	243.8 d	NR	NR			
Zr93	β^-,γ	1.5E+06 a	5.63E-03	1.32E-03			
Zr95	β^-,γ	64.02 d	1.15E-09	3.02E-01			
		Sum =	6.42E+06 (h)	1.02E+06 (i)	(4.048E+06) **4.048E+06 (j)**	(2.283E+04) **2.283E+04 (k)**	100.00 %
		Sum =	7.44E+06 (l)		(4.07E+06) **4.07E+06** **(Unit of Waste = 4.07) (m)**		
Top 5 Radionuclides							
Pu238	α,γ,SF	87.7 a	**2.61E+06 (f)**	1.45E+03	**2.61E+06**	**1.45E+03**	**64.1**
Pu239	α,γ,SF	2.410E+04 a	7.85E+05	1.03E+04	**7.85E+05**	**1.03E+04**	**19.5**
Am241	α,γ,SF	432.7 a	4.42E+05	5.96E+03	**4.42E+05**	**5.96E+03**	**11.0**
Pu240	α,γ,SF	6.56E+03 a	2.10E+05	5.07E+03	**2.10E+05**	**5.07E+03**	**5.28**
Pu242	α,γ,SF	3.75E+05 a	1.17E+03	1.50E-01	**1.17E+03**	**1.50E-01**	**2.87E-02**

NR Not Reported by sites (see Ref. CCA-2).

‡ Data values for radionuclides were previously reported in Rev. 1 of WTWBIR (BIR-1).

† Data values for radionuclides were previously reported in Rev. 2 of WTWBIR (BIR-2).

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-1.

(c) Decay mode and half-life information taken from the Chart of the Nuclides, 14th Ed. Ref. GE-1. [It is better for technical calculations, to use halflives that are extracted from the databases of ORIGEN2 [Ref. OR-1] because the ORIGEN2 data are of a later version than that of Ref. GE-1 (see Ref. SNL-2 for ORIGEN2 values).]

(d) Total inventory (curie) data taken from Ref. CCA-2. Values correspond to a "WIPP-Scale" design basis.

(e) Transuranic inventory data corresponds to the activity (curie) data only for radionuclides that are "transuranic waste" per definitions in 40CFR191 Inventory data in bold corresponds to those data incorporated into the WIPP PA database (see Ref. SNL-1).

(f) Isotope with dominate curie load for CH-TRU wastes.

(g) Isotope with dominate curie load for RH-TRU wastes.

(h) Note, the total CH-TRU curie load is 6.42 MCi (also, 86.3 % of the total curie load in WIPP). The average CH-TRU volumetric total curie load is 6.42E+06/5.95E+06 = 1.08 (Ci/cu. ft.) = **38.1 (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes – CH→5.95E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume. The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values are applicable to expected waste at WIPP (see Ref. BIR-2d).]

(i) Note, the total RH-TRU curie load is only 1.02 MCi (also, only 13.7 % of the total curie load in WIPP). This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1]. The average RH-TRU volumetric total curie load is 1.02E+06/0.25E+06 = 4.08 (Ci/cu. ft.) = **144. (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft.]

(j) Note, there are only 15 radionuclides that comprise the "transuranic waste" (see footnote e above). Eleven of these radionuclides are included in the WIPP PA data base and correspond to 99.99999% of the total CH "transuranic" inventory. The average CH-TRU volumetric "transuranic" curie load is 4.048E+06/5.95E+06 = **0.680 (TRU-Ci/cu. ft.)** = **24.0 (TRU-Ci/cu. m.)**.

(k) Note, there are only 15 radionuclides that comprise the "transuranic waste" (see footnote e above). Eleven of these radionuclides are included in the WIPP PA data base and correspond to 99.99998% of the total RH "transuranic" inventory. The average RH-TRU volumetric "transuranic" curie load is 2.283E+04/0.25E+06 = **0.0913 (TRU-Ci/cu. ft.)** = **3.22 (TRU-Ci/cu. m.)**. [The RH contribution to the WIPP-scale inventory of transuranic curie load is 2.283E+04*100%/(2.283E+04 + 4.048E+06)=**0.561% (very small)**.] Note, this value is an order of magnitude less than that presented for the CH-TRU wastes – since the majority of the curie content of the RH-TRU waste is due to shorter-lived non-transuranic radionuclides, this means that as the shorter-lived components decay away the remaining RH-TRU waste will have a lesser curie content than CH-TRU waste (i.e., as the RH-TRU waste decays, it becomes "wimpier" than CH-TRU waste). This is evident from the RH Study (Ref. DOE-1) which showed that after about 150 → 250 years that CH-TRU waste has a higher specific activity than that of RH-TRU waste.

(l) It is interesting to know that the Yucca Mountain Project (YMP) has approximately 12.4 billion curies of inventory (spent fuel -- 63,000 MTU [YMP-1b] × 1.57E+05 Ci/MTU [YMP-1c] + vitrified high-level waste -- 2.47E+09 Ci [YMP-1d]). Thus YMP is equivalent to 1660 WIPPs as far as curie load is concerned. Even though WIPP is less than one part in a thousand in comparison to YMP it still requires the same amount of work (with the exception of thermal effects) to demonstrate compliance for WIPP as it does for YMP because the EPA compliance requirements are based on a normalized basis (i.e., whether a repository has a radionuclide inventory on the order of millicuries, curies, millions of curies (like WIPP), or billions of curies (like YMP), the amount of work (with the exception of thermal effects) to show compliance is the same).

(m) Note, the unit of waste (UW, calculated to three significant figures) is the same whether the UW is calculated using all available information in the TWBID (Ref. CCA-2) or using the limited data within the WIPP PA database. [Also, only 4 radionuclides (Am241, Pu238, Pu239, and Pu240) make up 99.96% of the Unit of Waste value [see Ref. EPA-1b] -- using 5 radionuclides (adding Pu242) makes up 99.9936% of the Unit of Waste value].

Table 4.
40CFR191 Release Limits for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] **(d)**		Release Limits Inventory [α-Curies] **(e)**		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Ac225	α,γ	10.0 d	2.88E+00	1.17E-01			
Ac227	α,β^-,γ	21.77 a	6.08E-01	7.57E-04	100.	407.	1.50E-03
Ac228	α,β^-,γ	6.15 h	7.46E-01	7.77E-02			
Ag109m	ITe^-	39.8 s	1.57E+01	NR			
Ag110	$\beta^-,\gamma,\varepsilon$	24.6 s	7.07E-09	1.74E-09			
Ag110m	β^-,γ,ITe^-	249.8 d	5.31E-07	1.31E-07			
Am241	α,γ,SF	432.7 a	4.42E+05	5.96E+03	**100.**	**407.**	**1101.**
Am242	$\beta,\gamma,\varepsilon e^-$	16.02 h	1.75E+00	NR			
Am242m	α,ITe^-	141. h	1.75E+00	NR			
Am243	α,β^-,γ	7.37E+03 a	3.26E-01	2.28E-04	**100.**	**407.**	**8.01E-02**
Am245	β^-,γ	2.05 h	1.33E-09	2.87E-16			
At217	α,β^-,γ	32 ms	2.88E+00	1.17E-01			
Ba137m	IT	2.552 m	7.63E+03	2.04E+05			
Bi210	α,β^-,γ	5.01 d	2.55E+00	7.16E-06			
Bi211	α,β^-,γ	2.14 m	6.09E-01	7.58E-04			
Bi212	α,β^-,γ	1.009 h	2.71E+01	7.36E-02			
Bi213	α,β^-,γ	45.6 m	2.88E+00	1.17E-01			
Bi214	α,β^-,γ	19.9 m	1.16E+01	3.58E-05			
Bk249	α,β^-,γ	3.2E+02 d	9.16E-05	1.98E-11			
Bk250	β^-,γ	3.217 h	4.37E-11	NR			
C14	β^-	5730 a	1.08E+01	2.05E+00	100.	407.	3.16E-02
Cd109	γ,ε	462.0 d	1.57E+01	NR			
Cd113m	β^-,IT	14.1 a	1.82E-06	5.46E-07			
Ce144	β^-,γ	284.6 d	6.26E-02	5.13E+00			
Cf249	α,γ,SF	351 a	6.42E-02	4.47E-03	100.	407.	1.69E-04
Cf250	α,γ,SF	13.1 a	3.30E-01	NR			
Cf251	α,γ	9.0E+02 a	3.78E-03	NR	100.	407.	9.29E-06
Cf252	α,γ,SF	2.638 a	2.39E+02	1.29E+00			
Cm242	α,γ,SF	162.8 d	1.14E+00	NR			
Cm243	$\alpha,\gamma,SF,\varepsilon$	29.1 a	2.72E+00	4.95E+01	**100.**	**407.**	**0.128**
Cm244	α,γ,SF	18.1 a	3.15E+04	3.15E+02			
Cm245	α,γ,SF	8.5E+03 a	1.15E+02	1.46E-06	**100.**	**407.**	**0.283**
Cm246	α,γ,SF	4.76E+03 a	1.02E-01	NR	100.	407.	2.51E-04
Cm247	α,γ	1.56E+07 a	3.21E-09	NR	100.	407.	7.89E-12
Cm248	α,SF	3.48E+05 a	8.95E-02	2.05E-04	**100.**	**407.**	**2.20E-04**
Co58	$\beta^+,\gamma,\varepsilon$	70.88 d	3.05E-13	1.24E-11			
Co60	β^-,γ	5.271 a	6.46E+01	1.04E+04			
Cr51	$\varepsilon\gamma$	27.70 d	NR	3.04E-06			
Cs134	$\beta^-,\gamma,\varepsilon$	2.065 a	1.34E-02	1.84E+01			
Cs135	β^-	2.3E+06 a	5.02E-04	1.17E-04	1000.	4070.	1.52E-07
Cs137	β^-,γ	30.17 a	8.06E+03	**2.16E+05 (g)**	**1000.**	**4070.**	**55.1**
Es254	α,γ	276 d	4.24E-11	NR			

Table 4 Continued.
40CFR191 Release Limits for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] **(d)**		Release Limits Inventory [α-Curies] **(e)**		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Eu150	γ,ε	36 a	3.51E-05	NR			
Eu152	$\beta^-,\gamma,\varepsilon\beta^+$	13.48 a	1.26E+00	1.22E+03			
Eu154	$\beta^-,\gamma,\varepsilon\gamma$	8.59 a	1.15E+00	5.91E+02			
Eu155	β^-,γ	4.71 a	9.46E-01	1.18E+02			
Fe55	ε	2.73 a	1.91E-05	1.69E-01			
Fe59	β^-,γ	44.51 d	2.64E-07	NR			
Fr221	α,γ	4.8 m	2.88E+00	1.17E-01			
Fr223	α,β^-,γ	21.8 m	8.39E-03	1.04E-05			
H3	β^-	12.3 a	8.69E-01	6.60E-02			
I129	β^-,γ	1.57E+07 a	7.05E-07	NR	100.	407.	1.73E-09
Kr85	β^-,γ	10.73 a	2.02E-01	1.68E+00			
Mn54	$\varepsilon\gamma$	312.2 d	8.51E-04	2.35E-02			
Nb95	β^-,γ	34.97 d	2.54E-09	6.69E-01			
Nb95m	$\beta^-,\gamma,\mathit{IT}$	3.61 d	8.50E-12	2.24E-03			
Ni59	ε	7.6E+04 a	7.52E-03	NR	1000.	4070.	1.85E-06
Ni63	β^-	100. a	9.19E-01	9.88E-01	1000.	4070.	4.69E-04
Np237	α,γ	2.14E+06 a	5.61E+01	2.85E+00	**100.**	**407.**	**1.45E-01**
Np238	β,γ	2.117 d	8.77E-03	NR			
Np239	β^-,γ	2.355 d	3.26E+01	2.28E-04			
Np240‡	β,γ	1.032 h	NR	NR			
Np240m	$\beta^-,\gamma,\mathit{IT}$	7.22 m	1.50E-06	2.21E-11			
Pa231	α,γ	3.28E+04 a	4.51E-01	1.91E-03	**100.**	**407.**	**1.11E-03**
Pa233	β^-,γ	27.0 d	5.61E+01	2.85E+00			
Pa234	β^-,γ	6.69 h	5.14E-02	1.36E-02			
Pa234m	$\beta^-,\gamma,\mathit{IT}$	1.17 m	3.96E+01	1.05E+01			
Pb209	β^-	3.25 h	2.88E+00	1.17E-01			
Pb210	α,β^-,γ	22.3 a	2.55E+00	7.16E-06	**100.**	**407.**	**6.27E-03**
Pb211	β^-,γ	36.1 m	6.09E-01	7.58E-04			
Pb212	β^-,γ	10.64 hr	2.71E+01	7.36E-02			
Pb214	β^-,γ	27 m	1.16E+01	3.58E-05			
Pd107	β^-,γ	6.5E+06 a	7.41E-05	1.73E-05	1000.	4070.	2.25E-08
Pm147	β^-,γ	2.6234 a	7.87E+00	1.07E+01			
Po210	α,γ	138.38 d	2.55E+00	7.16E-06			
Po211	α,γ	0.516 s	1.71E-03	2.12E-06			
Po212	α	0.298 µs	1.73E+01	4.72E-02			
Po213	α	4 µs	2.82E+00	1.15E-01			
Po214	α,γ	163.7 µs	1.16E+01	3.57E-05			
Po215	α,β^-,γ	1.780 ms	6.09E-01	7.58E-04			
Po216	α,γ	0.145 s	2.71E+01	7.36E-02			
Po218	α,β^-,γ	3.10 m	1.16E+01	3.58E-05			
Pr144	β^-,γ	17.28 m	6.18E-02	5.07E+00			
Pu236	$\alpha,\gamma,\mathit{SF}$	2.87 a	1.04E-02	NR			

Table 4 Continued.
40CFR191 Release Limits for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (d)		Release Limits Inventory [α-Curies] (e)		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Pu238	α, γ, SF	87.7 a	**2.61E+06 (f)**	1.45E+03	**100.**	**407.**	**6416.**
Pu239	α, γ, SF	2.410E+04 a	7.85E+05	1.03E+04	**100.**	**407.**	**1954.**
Pu240	α, γ, SF	6.56E+03 a	2.10E+05	5.07E+03	**100.**	**407.**	**528.**
Pu241	α, β^-, γ	14.4 a	2.31E+06	1.42E+05			
Pu242	α, γ, SF	3.75E+05 a	1.17E+03	1.50E-01	**100.**	**407.**	**2.88**
Pu243	β^-, γ	4.956 h	3.21E-09	NR			
Pu244	α, SF	8.0E+07 a	1.50E-06	2.21E-11	**100.**	**407.**	**3.69E-09**
Ra223	α, γ	11.435 d	6.09E-01	7.58E-04			
Ra224	α, γ	3.66 d	2.71E+01	7.36E-02			
Ra225	β^-, γ	14.9 d	2.88E+00	1.17E-01			
Ra226	α, γ	1.60E+03 a	1.16E+01	3.58E-05	**100.**	**407.**	**2.85E-02**
Ra228	β^-, γ	5.76 a	7.47E-01	7.77E-02			
Rh106	β^-, γ	29.9 s	2.90E-02	1.09E+01			
Rn219	α, γ	3.96 s	6.09E-01	7.58E-04			
Rn220	α, γ	55.6 s	2.71E+01	7.36E-02			
Rn222	α, γ	3.8235 d	1.16E+01	3.58E-05			
Ru106	β^-	1.02 a	2.90E-02	1.09E+01			
Sb125	β^-, γ	2.758 a	1.21E-01	1.89E+00			
Sb126	β^-, γ	12.4 d	1.35E-04	3.16E-05			
Sb126m	$\gamma, \varepsilon e^-$	19.0 m	9.65E-04	2.25E-04			
Se79	β^-	6.5E+04 a	4.35E-04	1.02E-04	1000.	4070.	1.32E-07
Sm151	β^-, γ	90 a	1.47E+00	3.57E-01	1000.	4070.	4.49E-04
Sn119m	γ, ITe^-	293 d	4.14E-06	9.59E-07			
Sn121m	β^-, γ, ITe^-	55 a	2.66E-02	6.69E-03	1000.	4070.	8.18E-06
Sn126	β^-, γ	1.0E+05 a	9.65E-04	2.25E-04	1000.	4070.	2.92E-07
Sr89†	β^-, γ	50.52 d	NR	NR			
Sr90	β^-	29.1 a	6.85E+03	2.09E+05	**1000.**	**4070.**	**53.0**
Ta182	β^-, γ	114.43 d	NR	4.21E-08			
Tc99	β^-, γ	2.13E+05 a	2.52E+01	5.85E-03	10000.	40700.	6.19E-04
Te125m	γ, ITe^-	58 d	2.95E-02	4.65E-01			
Te127	β^-, γ	9.4 h	1.30E-07	1.71E-09			
Te127m	β^-, γ, ITe^-	109 d	1.33E-07	1.75E-09			
Th227	α, γ	18.72 d	6.01E-01	7.47E-04			
Th228	α, γ	1.913 a	2.71E+01	7.36E-02			
Th229	α, γ	7.3E+03 a	2.88E+00	1.17E-01	**100.**	**407.**	**7.36E-03**
Th230	α, γ	7.54E+04 a	8.06E-02	7.56E-03	**10.**	**40.7**	**2.17E-03**
Th231	β^-, γ	1.063 d	1.28E+01	4.63E+00			
Th232	α, γ	1.4E+10 a	9.13E-01	9.25E-02	**10.**	**40.7**	**2.48E-02**
Th234	β^-, γ	24.10 m	3.96E+01	1.05E+01			
Tl207	β^-, γ	4.77 m	6.07E-01	7.56E-04			
Tl208	β^-, γ	3.053 m	9.73E+00	2.65E-02			

Table 4 Continued.
40CFR191 Release Limits for (1995 Decayed) WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (d)		Release Limits Inventory [α-Curies] (e)		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Tl209	β⁻, γ	2.2 m	6.22E-02	2.53E-03			
Tl210‡	β, γ	1.30 m	NR	NR			
U232	α, γ, *SF*	70 a	2.58E+01	NR	100.	407.	6.34E-02
U233	α, γ, *SF*	1.592E+05 a	1.79E+03	1.58E+02	**100.**	**407.**	**4.79**
U234	α, γ, *SF*	2.46E+05 a	4.65E+02	4.27E+01	**100.**	**407.**	**1.25**
U235	α, γ, *SF*	7.04E+08 a	1.28E+01	4.63E+00	**100.**	**407.**	**4.28E-02**
U236	α, γ, *SF*	2.342E+07 a	3.33E-01	9.68E-02	100.	407.	1.06E-03
U237	β⁻, γ	6.75 d	5.66E+01	3.48E+00			
U238	α, γ, *SF*	4.47E+09 a	3.96E+01	1.05E+01	**100.**	**407.**	**1.23E-01**
U240	β⁻, γ	14.1 h	1.50E-06	2.21E-11			
Y90	β⁻, γ	2.67 d	6.85E+03	2.09E+05			
Zn65†	β⁺, γ, ε	243.8 d	NR	NR			
Zr93	β⁻, γ	1.5E+06 a	5.63E-03	1.32E-03	1000.	4070.	1.71E-06
Zr95	β⁻, γ	64.02 d	1.15E-09	3.02E-01			
		Sum =	6.42E+06 (h)	1.02E+06 (i)			(1.012E+04) **1.012E+04 (j)**
		Sum =	7.44E+06				

Top 10 Radionuclides (k)

ID (b)	Total Inventory			EPA Unit			
	CH	RH	Total	CH	RH	Total	CUMULATIVE (%)
Pu238	**2.61E+06 (f)**	1.45E+03	2.61E+06	6413.	3.56	6416.	0.63418
Pu239	7.85E+05	1.03E+04	7.95E+05	1929.	25.3	1954.	0.82732
Am241	4.42E+05	5.96E+03	4.48E+05	1086.	14.6	1101.	0.93611
Pu240	2.10E+05	5.07E+03	2.15E+05	516.	12.5	528.	0.98834
Cs137	8.06E+03	**2.16E+05 (g)**	2.24E+05	1.98	53.1	55.1	0.99378
Sr90	6.85E+03	2.09E+05	2.16E+05	1.68	51.4	53.0	0.99902
U233	1.79E+03	1.58E+02	1.95E+03	4.40	0.39	4.79	0.99950
Pu242	1.17E+03	1.50E-01	1.17E+03	2.87	3.69E-04	2.88	0.99978
U234	4.65E+02	4.27E+01	5.08E+02	1.14	0.10	1.25	0.99990
Cm245	1.15E+02	1.46E-06	1.15E+02	0.283	3.59E-09	0.283	0.99993

LGS
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NR Not Reported by sites (see Ref. CCA-2).

‡ Data values for radionuclides were previously reported in Rev. 1 of WTWBIR (BIR-1).

† Data values for radionuclides were previously reported in Rev. 2 of WTWBIR (BIR-2).

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-1.

(c) Decay mode and half-life information taken from the Chart of the Nuclides, 14th Ed. Ref. GE-1. [It is better for technical calculations, to use halflives that are extracted from the databases of ORIGEN2 [Ref. OR-1] because the ORIGEN2 data are of a later version than that of Ref. GE-1 (see Ref. SNL-2 for ORIGEN2 values).]

(d) Total inventory (curie) data taken from Ref. CCA-2. Values correspond to a "WIPP-Scale" design basis.

(e) Release limits are determined in accordance with 40CFR191 (Appendix A, Table 1) [Ref. EPA-1]. Left column corresponds to specific release limits (cumulative releases to the accessible environment for 10,000 years after disposal per "unit of waste" identified in Note 1(e) of Table 1, Appendix A, 40CFR191). Right column corresponds to release limit obtained for 4.07 Units of Waste (see Table 2 for calculation of the Unit of Waste) determined from data in the Transuranic Waste Baseline Inventory Report (BIR) [Ref. BIR-2].

(f) Isotope with dominate curie load for CH-TRU wastes.

(g) Isotope with dominate curie load for RH-TRU wastes.

(h) Note, the total CH-TRU curie load is 6.42 MCi (also, 86.3 % of the total curie load in WIPP). The average CH-TRU volumetric total curie load is 6.42E+06/5.95E+06 = 1.08 (Ci/cu. ft.) = **38.1 (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume. The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values are applicable to expected waste at WIPP (see Ref. BIR-2d).]

(i) Note, the total RH-TRU curie load is only 1.02 MCi (also, only 13.7 % of the total curie load in WIPP). This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1]. The average RH-TRU volumetric total curie load is 1.02E+06/0.25E+06 = 4.08 (Ci/cu. ft.) = **144. (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft.]

(j) Note, there are 42 radionuclides that comprise the "EPA Unit" (see footnote e above). 25 of these radionuclides are included in the WIPP PA data base and correspond to 99.99903% of the total CH- and RH-TRU "EPA Unit" inventory. The average CH-TRU volumetric "EPA Unit" load is 9.956E+03/5.95E+06 = **1.67E-03 (EPA Unit/cu. ft.)** = **5.91E-02 (EPA Unit/cu. m.)**. The average RH-TRU volumetric "EPA Unit" load is 1.611E+02/0.25E+06 = **6.44E-04 (EPA Unit/cu. ft.)** = **2.28E-02 (EPA Unit/cu. m.)**. [The RH contribution to the WIPP-scale inventory of transuranic curie load is 1.611E+02*100%/(1.611E+02 + 9.956E+03)=**1.592% (very small)**.] Note, this value is about two orders of magnitude less than that presented for the CH-TRU wastes -- since the majority of the curie content of the RH-TRU waste is due to shorter-lived non-transuranic radionuclides, this means that as the shorter-lived components decay away the remaining RH-TRU waste will have a lesser curie content than CH-TRU waste (i.e., as the RH-TRU waste decays, it becomes "wimpier" than CH-TRU waste). This is evident from the RH Study (Ref. DOE-1) which showed that after about 150 → 250 years that CH-TRU waste has a higher specific activity than that of RH-TRU waste.

(k) Note, the EPA Unit (calculated to four significant figures) is the same whether the EPA Unit is calculated using all available information in the TWBID (Ref. CCA-2) or using the limited data within the WIPP PA database. [Also, only 4 radionuclides (Pu238, Pu239, Am241, and Pu240) make up 98.83% of the EPA Unit (see Ref. EPA-1b) -- using 6 radionuclides (adding Cs137 & Sr90) makes up 99.9023% -- using the top 10 radionuclides makes up 99.9932% of the EPA Unit].

Table 5.
Unit of Waste and EPA Units for WIPP TRU Waste (a)

Nuclide	WIPP TRU Waste					
ID (b)	Total Ci Inventory [Curies] (c)		Total TRU Inventory [α-Curies] (d)		EPA Unit (e)	
	1995	2033	1995	2030	1995	2033
Ac225	3.00E+00	9.97E+00				
Ac227	6.09E-01	5.05E-01			1.50E-03	1.47E-03
Ac228	8.24E-01	1.00E+00				
Ag109m	1.57E+01	1.55E-08				
Ag110	8.81E-09	1.68E-25				
Ag110m	6.62E-07	1.26E-23				
Am241	**4.48E+05**	**4.88E+05**	**4.48E+05**	**4.88E+05**	**1101.**	**1419.**
Am242	1.75E+00	1.47E+00				
Am242m	1.75E+00	1.47E+00				
Am243	**3.26E+01**	**3.25E+01**	**3.26E+01**	**3.25E+01**	**8.01E-02**	**9.45E-02**
Am245	1.33E-09	1.17E-22				
At217	3.00E+00	9.97E+00				
Ba137m	2.12E+05	8.81E+04				
Bi210	2.55E+00	8.75E+00				
Bi211	6.10E-01	5.06E-01				
Bi212	2.72E+01	1.94E+01				
Bi213	3.00E+00	9.97E+00				
Bi214	1.16E+01	1.14E+01				
Bk249	9.17E-05	8.06E-18				
Bk250	4.37E-11	2.97E-26				
C14	1.29E+01	1.28E+01			3.17E-02	3.72E-02
Cd109	1.57E+01	1.55E-08				
Cd113m	2.39E-06	3.92E-07				
Ce144	5.19E+00	1.04E-14				
Cf249	6.87E-02	6.38E-02	6.87E-02	6.38E-02	1.69E-04	1.86E-04
Cf250	3.30E-01	4.41E-02				
Cf251	3.78E-03	3.67E-03	3.78E-03	3.67E-03	9.29E-06	1.07E-05
Cf252	**2.41E+02**	**1.11E-02**				
Cm242	1.14E+00	1.21E+00				
Cm243	**5.23E+01**	**2.07E+01**	**5.23E+01**	**2.07E+01**	**0.128**	**0.060**
Cm244	**3.18E+04**	**7.44E+03**				
Cm245	**1.15E+02**	**1.15E+02**	**1.15E+02**	**1.15E+02**	**0.283**	**0.334**
Cm246	1.02E-01	1.02E-01	1.02E-01	1.02E-01	2.51E-04	2.97E-04
Cm247	3.21E-09	9.51E-09	3.21E-09	9.51E-09	7.89E-12	2.77E-11
Cm248	**8.98E-02**	**9.16E-02**	**8.98E-02**	**9.16E-02**	**2.21E-04**	**2.66E-04**
Co58	1.27E-11	0.00E+00				
Co60	1.05E+04	7.06E+01				
Cr51	3.04E-06	0.00E+00				
Cs134	1.84E+01	5.22E-05				
Cs135	6.19E-04	6.19E-04			1.52E-07	1.80E-07

Table 5 Continued.
Unit of Waste and EPA Units for WIPP TRU Waste (a)

Nuclide	WIPP TRU Waste					
ID (b)	Total Ci Inventory [Curies] (c)		Total TRU Inventory [α-Curies] (d)		EPA Unit (e)	
	1995	2033	1995	2030	1995	2033
Cs137	**2.24E+05**	**9.31E+04**			**55.0**	**27.1**
Es254	4.24E-11	2.97E-26				
Eu150	3.51E-05	1.69E-05				
Eu152	1.22E+03	1.76E+02				
Eu154	5.92E+02	2.77E+01				
Eu155	1.19E+02	5.87E-01				
Fe55	1.69E-01	6.73E-06				
Fe59	2.64E-07	0.00E+00				
Fr221	3.00E+00	9.97E+00				
Fr223	8.41E-03	6.98E-03				
Gd152	0.00E+00	3.67E-11				
H3	9.40E-01	1.11E-01				
I129	7.05E-07	7.05E-07			1.73E-09	2.05E-09
Kr85	1.88E+00	1.61E-01				
Mn54	2.43E-02	1.04E-15				
Nb93m	0.00E+00	5.65E-03				
Nb95	6.69E-01	0.00E+00				
Nb95m	2.24E-03	0.00E+00				
Nd144	0.00E+00	1.90E-15				
Ni59	7.52E-03	7.51E-03			1.85E-06	2.18E-06
Ni63	1.91E+00	1.43E+00			4.69E-04	4.16E-04
Np237	**5.90E+01**	**6.49E+01**	**5.90E+01**	**6.49E+01**	**1.45E-01**	**1.89E-01**
Np238	8.78E-03	7.36E-03				
Np239	3.26E+01	3.25E+01				
Np240m	1.50E-06	1.53E-06				
Pa231	**4.53E-01**	**4.67E-01**			**1.11E-03**	**1.36E-03**
Pa233	5.90E+01	6.49E+01				
Pa234	6.50E-02	6.52E-02				
Pa234m	5.01E+01	5.01E+01				
Pb209	3.00E+00	9.97E+00				
Pb210	**2.55E+00**	**8.75E+00**			**6.26E-03**	**2.54E-02**
Pb211	0.00E+00	5.06E-01				
Pb212	2.72E+01	1.94E+01				
Pb214	1.16E+01	1.14E+01				
Pd107	9.14E-05	9.14E-05			2.25E-08	2.66E-08
Pm147	**1.86E+01**	**8.10E-04**				
Po210	2.55E+00	8.75E+00				
Po211	1.71E-03	1.42E-03				
Po212	1.74E+01	1.24E+01				
Po213	2.94E+00	9.76E+00				

Table 5 Continued.
Unit of Waste and EPA Units for WIPP TRU Waste (a)

Nuclide	WIPP TRU Waste					
ID (b)	Total Ci Inventory [Curies] (c)		Total TRU Inventory [α-Curies] (d)		EPA Unit (e)	
	1995	2033	1995	2030	1995	2033
Po214	1.16E+01	1.14E+01				
Po215	6.10E-01	5.06E-01				
Po216	2.72E+01	1.94E+01				
Po218	1.16E+01	1.14E+01				
Pr144	5.13E+00	1.03E-14				
Pu236	1.04E-02	1.01E-06				
Pu238	**2.61E+06**	**1.94E+06**	**2.61E+06**	**1.94E+06**	**6412.**	**5642.**
Pu239	**7.96E+05**	**7.95E+05**	**7.96E+05**	**7.95E+05**	**1956.**	**2312.**
Pu240	**2.15E+05**	**2.14E+05**	**2.15E+05**	**2.14E+05**	**528.**	**622.**
Pu241	**2.45E+06**	**3.94E+05**				
Pu242	**1.17E+03**	**1.17E+03**	**1.17E+03**	**1.17E+03**	**2.87**	**3.40**
Pu243	3.21E-09	9.51E-09				
Pu244	**1.50E-06**	**1.53E-06**	**1.50E-06**	**1.53E-06**	**3.69E-09**	**4.45E-09**
Ra223	6.10E-01	5.06E-01				
Ra224	2.72E+01	1.94E+01				
Ra225	3.00E+00	9.97E+00				
Ra226	**1.16E+01**	**1.14E+01**			**2.85E-02**	**3.32E-02**
Ra228	**8.25E-01**	**1.00E+00**				
Rh106	1.09E+01	4.90E-11				
Rn219	6.10E-01	5.06E-01				
Rn220	2.72E+01	1.94E+01				
Rn222	1.16E+01	1.14E+01				
Ru106	1.09E+01	4.90E-11				
Sb125	2.01E+00	1.49E-04				
Sb126	1.67E-04	1.67E-04				
Sb126m	1.19E-03	1.19E-03				
Se79	5.37E-04	5.37E-04			1.32E-07	1.56E-07
Sm147	0.00E+00	4.55E-10			0.00E+00	1.32E-12
Sm148	0.00E+00	7.87E-26			0.00E+00	2.29E-28
Sm151	1.83E+00	1.36E+00			4.50E-04	3.96E-04
Sn119m	5.10E-06	4.52E-23				
Sn121m	3.33E-02	1.96E-02			8.18E-06	5.70E-06
Sn126	1.19E-03	1.19E-03			2.92E-07	3.46E-07
Sr90	**2.16E+05**	**8.73E+04**			**53.1**	**25.4**
Ta182	4.21E-08	0.00E+00				
Tc99	2.52E+01	2.52E+01			6.19E-04	7.33E-04
Te125m	4.94E-01	3.64E-05				
Te127	1.32E-07	0.00E+00				
Te127m	1.35E-07	0.00E+00				
Th227	6.02E-01	4.99E-01				
Th228	2.72E+01	1.94E+01				

Table 5 Continued.
Unit of Waste and EPA Units for WIPP TRU Waste (a)

Nuclide	WIPP TRU Waste					
ID (b)	Total Ci Inventory [Curies] (c)		Total TRU Inventory [α-Curies] (d)		EPA Unit (e)	
	1995	2033	1995	2030	1995	2033
Th229	**3.00E+00**	**9.97E+00**			**7.37E-03**	**2.90E-02**
Th230	**8.82E-02**	**3.06E-01**			**2.17E-03**	**8.90E-03**
Th231	1.74E+01	1.75E+01				
Th232	**1.01E+00**	**1.01E+00**			**2.48E-02**	**2.94E-02**
Th234	5.01E+01	5.01E+01				
Tl207	6.08E-01	5.04E-01				
Tl208	9.76E+00	6.97E+00				
Tl209	6.48E-02	2.15E-01				
U232	2.58E+01	1.79E+01			6.34E-02	5.21E-02
U233	**1.95E+03**	**1.95E+03**			**4.79**	**5.67**
U234	**5.08E+02**	**7.51E+02**			**1.25**	**2.18**
U235	**1.74E+01**	**1.75E+01**			**4.27E-02**	**5.09E-02**
U236	**4.30E-01**	**6.72E-01**			**1.06E-03**	**1.95E-02**
U237	6.01E+01	9.67E+00				
U238	**5.01E+01**	**5.01E+01**			**1.23E-01**	**1.46E-01**
U240	1.50E-06	1.53E-06				
Y90	2.16E+05	8.73E+04				
Zr93	6.95E-03	6.95E-03			1.71E-06	2.02E-06
Zr95	3.02E-01	0.00E+00				
Sum	7.44E+06	4.20E+06	4.07E+06	3.44E+06	1.011E+04	1.006E+04
Top 4 Radionuclides						
Pu238	**2.61E+06**	**1.94E+06**	**2.61E+06**	**1.94E+06**	**6412.**	**5642.**
Pu239	**7.96E+05**	**7.95E+05**	**7.96E+05**	**7.95E+05**	**1956.**	**2312.**
Am241	**4.48E+05**	**4.88E+05**	**4.48E+05**	**4.88E+05**	**1101.**	**1419.**
Pu240	**2.15E+05**	**2.14E+05**	**2.15E+05**	**2.14E+05**	**528.**	**622.**

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-1.

(c) Total inventory (curie) data taken from Ref. CCA-2. Values correspond to a "WIPP-Scale" design basis.

(d) Transuranic inventory data corresponds to the activity (curie) data only for radionuclides that are "transuranic waste" per definitions in 40CFR191 Inventory data in bold corresponds to those data incorporated into the WIPP PA database (see Ref. SNL-1).

(e) EPA Units are determined using Unit of Waste values from columns 4 and 5.

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.2

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PREFACE TO ATTACHMENT WCA.8.2

Title 40 of the Code of Federal Regulations (CFR) § 194.31 states that

The release limits shall be calculated according to part 191, appendix A of this chapter, using the total activity, in curies, that will exist in the disposal system at the time of disposal.

Making an exact assessment of the total activity (the radionuclide inventory) at the time of disposal (2033) requires assessing the total activity, in 2033, of three categories of contact-handled transuranic (CH-TRU) waste.

Category 1: the stored, "legacy" waste; CH-TRU waste that currently exists, is packaged, and has been inventoried and decayed to the year 1995.

Category 2: future waste that has already been generated; CH-TRU waste that currently exists and has been identified, is not packaged, and has not been inventoried for shipment to the Waste Isolation Pilot Plant (WIPP).

Category 3: future to-be-generated waste; CH-TRU waste that has not been identified.

Categories 2 and 3, the projected waste, comprise 66% of the WIPP waste by volume (Transuranic Waste Baseline Inventory Report [TWBIR], DOE 1995, p. 3-1).

Category 1 waste has already been inventoried and the inventory data can be readily decayed to any common base year (that is, to 1995, as is done in the TWBIR). Category 2 waste is expected to be similar to Category 1 waste, and could thus also be assessed at any common base year (for example, 1995). The Category 1 and 2 inventories can also be decayed to any other common year such as the year of closure, 2033. However, Category 3 waste is not necessarily similar to the other two categories and therefore should be estimated separately on a year-by-year basis as it is generated. Then each yearly contribution should be decayed separately to the closure year (2033).

TWBIR data collection methods estimated Category 3 data in the same manner as Category 2 data, and prorated Category 3 data accordingly. Thus, Category 3 data are estimated at 1995 instead of the later years during which the waste would be generated. Additional decay calculations of Category 3 data would result in over-decay of the inventory. For example, waste assayed in 2030 should be decayed for only three years to 2033; decaying such waste for the 38 years from 1995 to 2033 would result in an underestimate, particularly since the fraction of projected waste that is Category 3 cannot be determined. 40 CFR § 194.31 requires assessing the radionuclide inventory at the time of closure, that is, the year 2033. This can be done readily for Category 1 and Category 2 data. Because the Category 3 data were not separated from the Category 2 data, decaying from 1995 to 2033 underestimates portions of the Category 3 inventory by between one and 37 years of decay.

Because Category 3 wastes cannot currently be assessed separately from Category 2 wastes, there are two alternatives for calculating the waste unit factor: (1) calculation on the basis of the entire inventory decayed to 1995 or (2) calculation on the basis of the entire inventory decayed to 2033. The first yields a waste unit factor of 4.07×10^6, and the second, a waste unit factor of 3.44×10^6. The waste unit factor determines the normalization factor used in calculating the release limit, according to Table 1 of 40 CFR Part 191 Appendix A. The curies of radionuclides are divided by the release limit to determine the EPA units. All else being equal, a smaller release limit (and thus a smaller waste unit factor) is the more conservative of the two possibilities. Therefore, the entire inventory is decayed to 2033 for the performance assessment calculations as specified in 40 CFR § 194.31 above.

Attachment WCA.8.1 states that the inventory decayed to 1995 is used. However, as described above, in keeping with the specification of 40 CFR § 194.31 the inventory decayed to 2033 is used instead.

Reference:

DOE (U. S. Department of Energy). 1995. *Transuranic Waste Baseline Inventory Report, Rev. 2,* DOE/CAO 95-1121, Carlsbad, NM.

WPO 37431

INFORMATION ONLY

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date : April 25, 1996

to : Distribution

Lawrence C. Sanchez

from : L. C. Sanchez, Org 6741, MS-1328, PH-(505)848-0685, Fax-848-0705

subject : **Identification of Important Radionuclides Used in 1996 CCA WIPP Performance Assessment**

Recently the data in the Transuranic Waste Baseline Inventory Database (TWBID) has been updated to reflect reassessments of key radionuclides at some of the major transuranic (TRU) waste generation sites. These new TWBID values (Ref. CCA-2) are termed the "CCA data" and they supersede the data currently published in Revision 2 of the Transuranic Waste Baseline Inventory Report (TWBIR, Ref. BIR-2). This memo identifies which of these radionuclides are of most concern to the Performance Assessment (PA) of WIPP. Of the CCA radionuclides, those that are of the most concern to PA and will be studied in the 1996 CCA calculations are shown in Table 1. The basis for their importance is based upon several factors: 1) the subsurface transportability of the radionuclides (solubility in brine, chemical sorption, etc.,), 2) transuranic inventory, and 3) allowable release limits. There are other serious concerns such as the fissile material (e.g., fissile gram equivalent (FGE) of Pu239), Pu239 equivalent activities, etc. But, these would be more applicable to transportation and WIPP operations limits than to WIPP PA and are not addressed in this memo.

In order to understand why the radionuclides in Table 1 are considered the most important, with respect to WIPP PA, one must become familiar with Table 2, which identifies the the release limits per 40CFR191 (Ref. EPA-1). These release limits are normalized to a "Unit of Waste". For the TRU waste to be disposed of in the WIPP, the unit of waste is "An amount of transuranic (TRU) wastes containing one million curies of alpha-emitting transuranic radionuclides with half lives greater than 20 years" (Ref. EPA-1b). The unit of waste is determined in Table 3. From this table it can be seen that of the 135 radionuclides in the current TWBIR, there are reported data for 15 transuranic waste radionuclides that contribute to the unit of waste. In total there are only 17 possible radionuclides that fall into the "transuranic waste" category. The two that are not identified in the TWBIR are: 1) Am242m and 2) Bk247. Since these radionuclides are very proton rich, it is expected that they are very difficult to generate and should not exist in appreciable quantities. The overall quantity of transuranic waste radionuclides from Table 3 that apply to the unit of waste is 4.07E+06 curies, thus the value for the unit of waste is 4.07. From this table it easily identified that the plutonium and americium radionuclides dominate the unit of waste. For releases to the accessible environment that involve a mix of radionuclides, the limits in Table 2 are used to define normalized releases for comparison with the release limits. Now the unit of waste and the specific release limits are used to determine release limits and cumulative normalized release limits. (To help describe the 40CFR191 containment requirements, the following two paragraphs were taken as is from Ref RE-1 -- This reference gives a very through introduction to the mechanics of the WIPP PA process and is considered a must for reading if a person wants to be able to understand the results presented in Ref. SNL-1 or any comparable PA reports.) Containments Requirements (40CFR191.13, Ref. EPA-1) specify general limits on the release of transuranic (TRU) waste, high-level waste, or spent nuclear fuel (SNF) from a geologic repository. Environmental Protection Agency (EPA) release limits are defined as the normalizing factors for various radionuclides listed in Table 1 of Appendix A of EPA regulation 40 CFR 191 (see Table 2). According to the Containment Requirements, there must be a reasonable expectation, based on a performance assessment that includes all significant process and events, that the cumulative release of any one radionuclide over 10,000 yr to the accessible environment shall have (these two points alone determine the EPA limits drawn on all WIPP CCDFs):

- less than 1 chance in 10 of exceeding the promulgated EPA radionuclide limits (L_i), and
- less than 1 chance in 1000 of exceeding 10 times those quantities.

For a mix of radionuclides, the sum of all releases, where each radionuclide is normalized with respect to its L_i, shall have:

- less than 1 chance in 10 of exceeding 1, and
- less than 1 chance in 1000 of exceeding 10.

Where the sum of all releases is expressed by:

$$R_j = \frac{1}{f_w}\left[\frac{Q_{1j}}{L_1}+\frac{Q_{2j}}{L_2}+\cdots+\frac{Q_{nRj}}{L_{nR}}\right] = \sum_{i=1}^{nR}\frac{Q_{ij}}{f_w L_i} \leq 1\ (or\ \ 10) \qquad (1)$$

where

f_w = waste unit factor = $\frac{\sum W_i}{10^6\,Ci}$, see Table 2 for units
W_i = activity in curies (Ci) for α-emitting TRU repository wastes having half-lives ($\tau_{1/2}$) ≥ 20 years
L_i = the EPA release limit for radionuclide i (see Table 2 for examples and units)
nR = number of radionuclides contributing to the release
R_j = total normalized release (EPA sum) for the jth scenario
Q_{ij} = cumulative release for radionuclide u beyond a specified boundary, $\int_{o}^{10{,}000yr} q_{ij}\,dt$
q_{ij} = release rate into accessible environment at time t for radionuclide i and scenario j calculated from consequence model(s) (see Chapter 5.0 Ref. RE-1)

The EPA release limits (L_i), for radionuclides $i=1$, ..., nR are based on generic analyses of hypothetical repositories containing SNF, not TRU waste. The models the contractors for the EPA used to establish the limits considered releases to a river, an ocean, and the land surface. The analysis assumed radionuclides released from the disposal-system boundary were instantaneously deposited into a river, an ocean, or into the land surface. The total cancers per curie were then calculated for each of the three pathways to humans. The most stringent of the three pathways, river water ingestion, was used in calculating the release limits. That is, the release limits are

addition to limiting the RH-TRU canister surface dose equivalent rate to 1,000 rem/hr also limits the design capacity of (all) transuranics to 6.2 million cubic feet of volume of which no more than 5.1 million curies (Ci) may be RH-TRU. The volume limit for the RH-TRU is identified in the WIPP ROD (Record of Decision) to be 0.25 million cubic feet of volume [Ref. DOE-2]. Also, prior to the WIPP LWA 6.2 million cubic feet volume was assign to CH-TRU waste only (for instance, Ref. DOE-3 identifies that the total volume of WIPP was to be 6.45 million cubic feet -- 6.2 for CH-TRU and 0.25 for RH-TRU) and not CH-TRU plus RH-TRU. The WIPP LWA seems to be patterned after the WIPP C&C agreement [DOE-4]. It is in the WIPP C&C that a misquote was made to the WIPP ROD. The WIPP C&C quotes the WIPP ROD as applying the 6.2 million cubic meters to (all) transuranic waste. Even though the WIPP LWA is technically incorrect, the volumes identified there are to be used for WIPP calculations. More thorough discussion can be found in Ref. SA-1.]

[OR-1]Croff, A.G.; "ORIGEN2: A Users Manual for ORIGEN2 Computer Code," Oak Ridge National Laboratory, July 1980. (Further generalized discussion on ORIGEN2 can be found in Ref. OR-2.) (Detailed information on the validation (as applied to analysis of PWR spent fuel) and functional requirements (related to long-term storage of LWR spent fuel) of ORIGEN2 can be found in Refs. OR-3 and OR-4.)

[OR-2]Croff, A.G.; "ORIGEN2: A Versatile Computer Code for Calculating the Nuclide Compositions and Characteristics of Nuclear Materials," **Nuclear Technology**, Vol. 62, September 1983.

[OR-3]Hermann, O.W., S.M. Bowman, M.C. Brady and C.V. Parks; "Validation of the Scale System for PWR Spent Fuel Isotropic Composition Analyses," ORNL/TM-12667, Oak Ridge National Laboratory, March 1995.

[OR-4]Broadhead, B.L., M.D. DeHart, J.C. Ryman, J.S. Tang and C.V. Parks; "Investigation of Nuclide Importance to Functional Requirements Related to Transport and Long-Term Storage of LWR Spent Fuel," Oak Ridge National Laboratory, June 1995. ORNL/TM-12742,

[RE-1]Rechard, R.P.; "An Introduction to the Mechanics of Performance Assessment Using Examples of Calculations Done for the Waste Isolation Pilot Plant Between 1990 and 1992", SAND93-1378, UC-721, Sandia National Laboratories, Albuquerque, New Mexico, Printed October 1995.

[SA-1]L.C. Sanchez (SNL Org 6741) and S.G. Bertram (SNL Org 6747); Memo to L.E. Shephard (SNL Org 6800), subject: "WIPP Capacity", dated October 6, 1995.

[SNL-1]

Sandia WIPP Project. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992.* (SAND92-0700), Albuquerque, NM; Sandia National Laboratories.

[SNL-2]

L.C. Sanchez (SNL Org 6741); Memo to M. Marietta (SNL Org 6821), dated February 26, 1995.

[SNL-3]

Helton,J.C., J.W. Garner, R.P. Rechard, D.K. Rudeen, and P.N. Swift. 1992; *Preliminary Comparison with 40CFR191, Subpart B for the Waste Isolation Pilot Plant, December 1991. Volume 4: Uncertainty and Sensitivity Analysis Results,* SAND91-0893/4. Albuquerque, NM; Sandia National Laboratories.

[SNL-4]

J.W. Garner (SNL Org 6749); Memo to: C.T. Stockman (SNL Org 6749), Subject: "Radioisotopes to be used in the 1996 CCA Calculations", dated: 3/15/96

determined such that releases from the disposal system, the land withdrawal boundary for the WIPP [less than the maximum 5 km (~ 3 mi) from the boundary of the disposal region] into a river providing a large population with drinking water, would result in fewer than 1000 cancer deaths over 10,000 yr, a health hazard from the amount of unmined uranium ore needed to produce 100,000 metric tons of reactor fuel (Ref. EPA-2).

Further information can be found in Table 4. This table identifies the 42 radionuclides within the TWBIR that contribute to the release limits. From this table it easily identified that the plutonium and americium radionuclides dominate the EPA units. Also, the total number of EPA units is 10,120 Ci for a unit of waste value of 4.07. This indicates that over the regulatory time frame, on an average, the allowable release of radionuclides is 1/10,120 or ~ 100 ppm (parts per million). In Table 5, there is a list of the radionuclides that are not reported in the TWBIR but are applicable to 40CFR191 (these radionuclides tend to be difficult to produce and are not expected in appreciable amounts). (Should significant quantities of any of these radionuclides be identified in the future, they will be factored into the normalized release calculations.) Also presented in this memo are Tables 6 and 7. These tables, only of minor concern with respect to EPA limits, are shown to give additional information.

From the tables presented in this memo, especially Tables 2, 3 and 4, it should be apparent that the most important radionuclide are the americiums, plutoniums, and uraniums. This was verified by Helton et al. (Ref. SNL-3), and the eight isotopes that dominate the radioactive material that could cross the WIPP regulatory boundary under breach scenarios are: Pu-239, Am-241, Pu-238, Pu-240, Np-237, U-234, U-233, and Th-230. U-234, U-233, and Th-230 are not strictly speaking "transuranic", but are included because they are long-lived daughters of the transuranic radionuclides, and are expected to be present in the TRU waste in non-negligible amounts (either as initial inventory or as ingrowth during the 10,000 year regulatory time frame). This is also demonstrated in Figure 1 which shows the temporal changes in radionuclide activity in a panel of the WIPP repository that occurs as a result of radioactivity decay for the eight most important radionuclides [the plots in Figure are taken from RE-1]. At 10,000 yr, the total normalization activity in a panel for all omitted radionuclides is less than 2 percent of the EPA limit (inclusion of radium-226 drops the total normalized activity to one percent).

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[BIR-1]

DOE (U.S. Department of Energy); Waste Isolation Pilot Plant Transuranic Waste Baseline Inventory Report; CAO-94-1005; Revision 1; February 1995, Volume 1, Table 4-2, pg. 4-6.

[BIR-2]

DOE (U.S. Department of Energy); Transuranic Waste Baseline Inventory Report; DOE/CAO-95-1121; Revision 2; printed December 1995.

[BIR-2b]

Ibid., Table 3-4, pp. 3-30 → 3-36 (Volume 1).

[BIR-2c]

Ibid., Table 3-4, pg. 3-31 (Volume 1).

[BIR-2d]

Ibid., Table 3-4, pp. 3-27 → 29 (Volume 1).

[BIR-2e]
Ibid., pg. 1-20 (Volume 1).

[CCA-1]
S. Chakraborti (SAIC/CTAC); Letter to: J. Harvill (ASI/CTAC), Subject: "Revised Radionuclide Data In Support Of The CCA", Dated: April 12, 1996.

[CCA-2]
S. Chakraborti (SAIC/CTAC); Letter to: J. Harvill (ASI/CTAC), Subject: "Final Radionuclide Data In Support Of The CCA", Dated: April 19, 1996. [This letter gives radionuclide data that supersedes Rev. 2 of the TWBIR and should be used in the 1996 CCA calculations for the WIPP facility. This letter also supersedes Ref. CCA-1, which had preliminary values. The reason that that this reference was generated was that after publication of Ref. BIR-2 it was identified that inventory data for several key radionuclides needed to be modified in accordance to new information obtained from the waste generation sites (this information was deemed important enough that the updated information was needed for the 1996 CCA calculations).]

[DOE-1]
DOE (U.S. Department of Energy); Remote-Handled Transuranic Waste Study; DOE/CAO-1095, DOE Carlsbad Area Office; Carlsbad, NM, October 1995.

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DOE (U.S. Department of Energy), Waste Isolation Pilot Plant (WIPP); Record of Decision, **Federal Register** , Vol. 46, No. 18, pg. 9163, January 28, 1981 (46 FR 9162), Office of Environmental Restoration and Waste Management, Washington, D.C.

[DOE-3]
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[DOE-4]
DOE (U.S. Department of Energy) and State of New Mexico (1981 originally); Agreement for Consulation and Cooperation Between Department of Energy and the State of New Mexico on the Waste Isolation Pilot Plant, Updated April 18, 1988; Article VI (WIPP Mission), pg. 7.

[EPA-1]
EPA (Environmental Protection Agency). 1985a. :40 CFR Part 191: Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radionactive Waste: Final Rule," *Federal Register,* **Vol. 50,** No, 182, 38066-38089 (1985).

[EPA-1b]
Ibid., Appendix A to Part 191, Subpart B, Table 1, Note 1 (e).

[EPA-2]
EPA (Environmental Protection Agency). 1985b. *Background Information Document - Final Rule for High-Level and Transuranic Radioactive Wastes,* EPA 520/1-85-023. Washington, DC; U.S. Environmental Protection Agency, Office of Radiation Programs.

[GE-1]General Electric Company (Nuclear Energy Operations), **Nuclides and Isotopes** , Fourteenth Edition, 1989.

[GE-1b]
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Public Law 102-579, 102d Congress, October 30, 1992; *Waste Isolation Pilot Plant Land Withdrawal Act.;* 1992. Section 7, subparts (a)(1)(A) and (a)(3). [Note, the WIPP LWA in

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L.C. Sanchez (SNL Org 6741); Memo to: M. Martell (SNL Org 6747), Subject: "Radionuclide Half-lives and Specific Activities Obtained From ORIGEN2 Data", dated: March 28, 1996.

[YMP-1]
Sandia YMP Project. 1994. *Total-System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993), Volume 1.* (SAND93-2675), Albuquerque, NM; Sandia National Laboratories.

[YMP-1b]
Ibid., Table 5-1, pg. 5-1 (Volume 1).

[YMP-1c]
Ibid., Table 5-2, pp. 5-2 → 5-3 (Volume 1).

[YMP-1d]
Ibid., Table 5-7, pg. 5-6 (Volume 1).

LCS:6741:lcs/(96-~~2099~~ 2109) LCS 7-11-96

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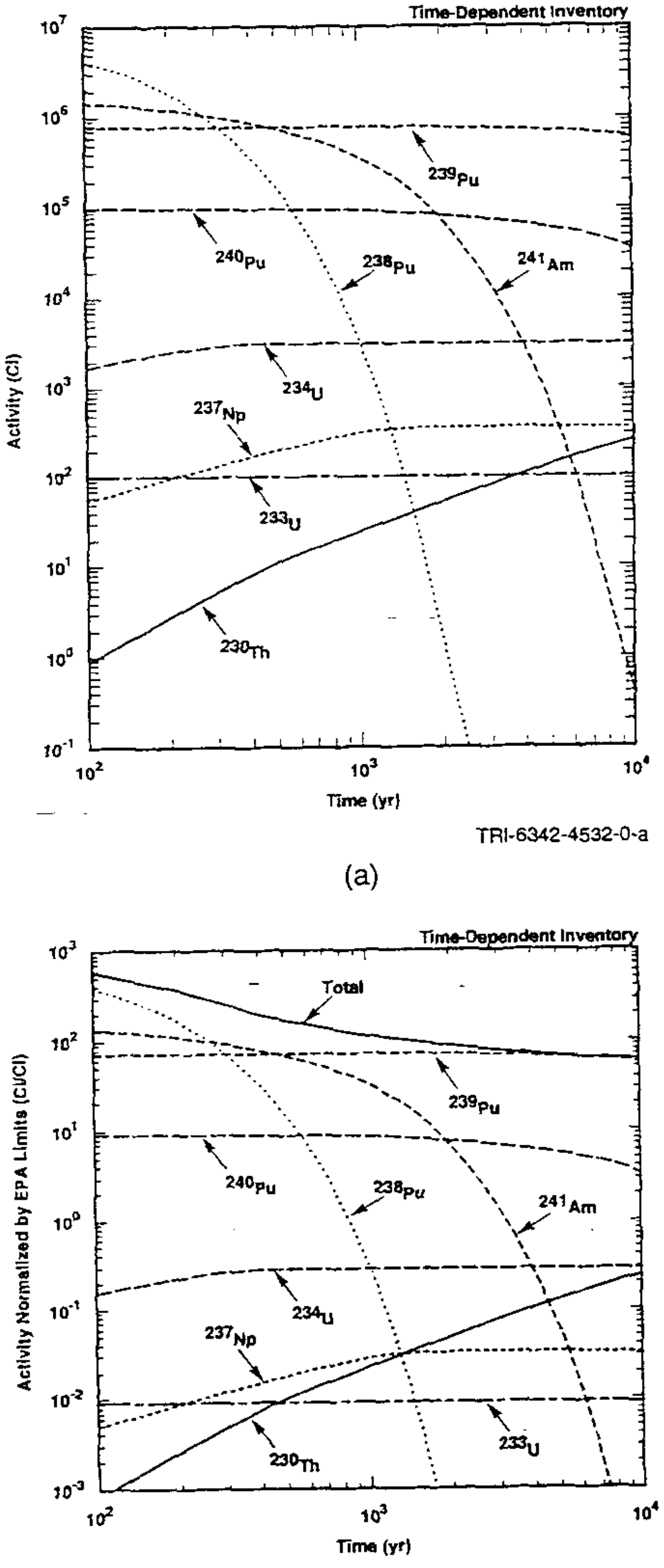
File - SWCF-A WBS 1.1.6.2;PA;PBWAC - WIPP ACTIVITY



TRI-6342-4532-0-a

(a)

TRI-6342-4532-0-b

(b)

Figure 1. Changes in radionuclide activity of waste in (based on the inventory used in the 1991 performance assessment calculations) a) activity unnormalized, b) and the one WIPP panel normalized by number of panels in the WIPP (9.49), waste factor 4.225 (million curies in 1992), and the EPA release limits (usually 1000) [Taken from Ref. RE-1].

LCS 7-11-96

Table 1.
Key Radionuclides of Concern to 199~~7~~6 WIPP PA (a)

Am-241	Cm-248	Pu-238	Ra-226	U-233
Am-243	Cs-137	Pu-239	Ra-228	U-234
Cf-252	Np-237	Pu-240	Sr-90	U-235
Cm-243	Pa-231	Pu-241	Th-229	U-236
Cm-244	Pb-210	Pu-242	Th-230	U-238
Cm-245	Pm-147	Pu-244	Th-232	

(a) Not shown are decay daughters that are be calculated within the PA codes for the 1996 CCA calculations. (See Ref. SNL-4)

Table 2.
Release Limits for the Containment Requirements (a)

Radionuclide	Release Limit per 1000 MTHM (b) or Other Unit of Waste (c) (Ci)
Americium (Am)-241 or -243	100
Carbon (C)-14	100
Cesium (Cs)-135 or -137	1,000
Iodine (I)-129	100
Neptunium (Np)-237	100
Plutonium (Pu)-238, -239, -240, or -242	100
Radium (Ra)-226	100
Strontium (Sr)-90	1,000
Technetium (Tc)-99	10,000
Thorium (Th)-230 or -232	10
Tin (Sn)-126	1,000
Uranium (U)-233, -234, -235, -236, or -238	100
Any other alpha-emitting radionuclide with a half-life greater than 20 years	100
Any other radionuclide with a half-life greater than 20 years that does not emit alpha particles	1,000

(a) Based on Table I of Appendix A of Ref. EPA-1
(b) Metric tons of heavy metal exposed to a burnup between 25,000 and 40,000 MWd/tonne heavy metal.
(c) For TRU waste the unit of waste is "An amount of Transuranic (TRU) wastes containing one million curies of alpha-emitting transuranic radionuclides with half lives greater than 20 years" (Ref. EPA-1b).

Table 3.
40CFR191 Unit of Waste for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID **(b)**	Decay Mode **(c)**	Half-Life **(c)**	Total Inventory [Curies] **(d)**		Transuranic Inventory [α-Curies] **(e)**		% of Unit of Waste
			CH	RH	CH	RH	(%)
Ac225	α,γ	10.0 d	2.88E+00	1.17E-01			
Ac227	α,β^-,γ	21.77 a	6.08E-01	7.57E-04			
Ac228	α,β^-,γ	6.15 h	7.46E-01	7.77E-02			
Ag109m	$\mathit{IT}e^-$	39.8 s	1.57E+01	NR			
Ag110	$\beta^-,\gamma,\varepsilon$	24.6 s	7.07E-09	1.74E-09			
Ag110m	$\beta^-,\gamma,\mathit{IT}e^-$	249.8 d	5.31E-07	1.31E-07			
Am241	$\alpha,\gamma,\mathit{SF}$	432.7 a	4.42E+05	5.96E+03	**4.42E+05**	**5.96E+03**	**11.0**
Am242	$\beta,\gamma,\varepsilon e^-$	16.02 h	1.75E+00	NR			
Am242m	$\alpha,\mathit{IT}e^-$	141. h	1.75E+00	NR			
Am243	α,β^-,γ	7.37E+03 a	3.26E+01	2.28E-04	**3.26E+01**	**2.28E-04**	**8.01E-04**
Am245	β^-,γ	2.05 h	1.33E-09	2.87E-16			
At217	α,β^-,γ	32 ms	2.88E+00	1.17E-01			
Ba137m	IT	2.552 m	7.63E+03	2.04E+05			
Bi210	α,β^-,γ	5.01 d	2.55E+00	7.16E-06			
Bi211	α,β^-,γ	2.14 m	6.09E-01	7.58E-04			
Bi212	α,β^-,γ	1.009 h	2.71E+01	7.36E-02			
Bi213	α,β^-,γ	45.6 m	2.88E+00	1.17E-01			
Bi214	α,β^-,γ	19.9 m	1.16E+01	3.58E-05			
Bk249	α,β^-,γ	3.2E+02 d	9.16E-05	1.98E-11			
Bk250	β^-,γ	3.217 h	4.37E-11	NR			
C14	β^-	5730 a	1.08E+01	2.05E+00			
Cd109	γ,ε	462.0 d	1.57E+01	NR			
Cd113m	β^-,IT	14.1 a	1.82E-06	5.46E-07			
Ce144	β^-,γ	284.6 d	6.26E-02	5.13E+00			
Cf249	$\alpha,\gamma,\mathit{SF}$	351 a	6.42E-02	4.47E-03	6.42E-02	4.47E-03	1.69E-06
Cf250	$\alpha,\gamma,\mathit{SF}$	13.1 a	3.30E-01	NR			
Cf251	α,γ	9.0E+02 a	3.78E-03	NR	3.78E-03	NR	9.28E-08
Cf252	$\alpha,\gamma,\mathit{SF}$	2.638 a	2.39E+02	1.29E+00			
Cm242	$\alpha,\gamma,\mathit{SF}$	162.8 d	1.14E+00	NR			
Cm243	$\alpha,\gamma,\mathit{SF},\varepsilon$	29.1 a	2.72E+00	4.95E+01	**2.72E+00**	**4.95E+01**	**1.28E-03**
Cm244	$\alpha,\gamma,\mathit{SF}$	18.1 a	3.15E+04	3.15E+02			
Cm245	$\alpha,\gamma,\mathit{SF}$	8.5E+03 a	1.15E+02	1.46E-06	**1.15E+02**	**1.46E-06**	**2.82E-03**
Cm246	$\alpha,\gamma,\mathit{SF}$	4.76E+03 a	1.02E-01	NR	1.02E-01	NR	2.51E-06
Cm247	α,γ	1.56E+07 a	3.21E-09	NR	3.21E-09	NR	7.88E-14
Cm248	α,SF	3.48E+05 a	8.95E-02	2.05E-04	**8.95E-02**	**2.05E-04**	**2.20E-06**
Co58	$\beta^+,\gamma,\varepsilon$	70.88 d	3.05E-13	1.24E-11			
Co60	β^-,γ	5.271 a	6.46E+01	1.04E+04			
Cr51	$\varepsilon\gamma$	27.70 d	NR	3.04E-06			
Cs134	$\beta^-,\gamma,\varepsilon$	2.065 a	1.34E-02	1.84E+01			
Cs135	β^-	2.3E+06 a	5.02E-04	1.17E-04			
Cs137	β^-,γ	30.17 a	8.06E+03	**2.16E+05 (g)**			
Es254	α,γ	276 d	4.24E-11	NR			

Table 3 Continued.
40CFR191 Unit of Waste for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (**d**)		Transuranic Inventory [α-Curies] (**e**)		% of Unit of Waste
			CH	RH	CH	RH	(%)
Eu150	γ,ε	36 a	3.51E-05	NR			
Eu152	$\beta^-,\gamma,\varepsilon\beta^+$	13.48 a	1.26E+00	1.22E+03			
Eu154	$\beta^-,\gamma,\varepsilon\gamma$	8.59 a	1.15E+00	5.91E+02			
Eu155	β^-,γ	4.71 a	9.46E-01	1.18E+02			
Fe55	ε	2.73 a	1.91E-05	1.69E-01			
Fe59	β^-,γ	44.51 d	2.64E-07	NR			
Fr221	α,γ	4.8 m	2.88E+00	1.17E-01			
Fr223	α,β^-,γ	21.8 m	8.39E-03	1.04E-05			
H3	β^-	12.3 a	8.69E-01	6.60E-02			
I129	β^-,γ	1.57E+07 a	7.05E-07	NR			
Kr85	β^-,γ	10.73 a	2.02E-01	1.68E+00			
Mn54	$\varepsilon\gamma$	312.2 d	8.51E-04	2.35E-02			
Nb95	β^-,γ	34.97 d	2.54E-09	6.69E-01			
Nb95m	β^-,γ,IT	3.61 d	8.50E-12	2.24E-03			
Ni59	ε	7.6E+04 a	7.52E-03	NR			
Ni63	β^-	100. a	9.19E-01	9.88E-01			
Np237	α,γ	2.14E+06 a	5.61E+01	2.85E+00	**5.61E+01**	**2.85E+00**	**1.45E-03**
Np238	β,γ	2.117 d	8.77E-03	NR			
Np239	β^-,γ	2.355 d	3.26E+01	2.28E-04			
Np240‡	β,γ	1.032 h	NR	NR			
Np240m	β^-,γ,IT	7.22 m	1.50E-06	2.21E-11			
Pa231	α,γ	3.28E+04 a	4.51E-01	1.91E-03			
Pa233	β^-,γ	27.0 d	5.61E+01	2.85E+00			
Pa234	β^-,γ	6.69 h	5.14E-02	1.36E-02			
Pa234m	β^-,γ,IT	1.17 m	3.96E+01	1.05E+01			
Pb209	β^-	3.25 h	2.88E+00	1.17E-01			
Pb210	α,β^-,γ	22.3 a	2.55E+00	7.16E-06			
Pb211	β^-,γ	36.1 m	6.09E-01	7.58E-04			
Pb212	β^-,γ	10.64 hr	2.71E+01	7.36E-02			
Pb214	β^-,γ	27 m	1.16E+01	3.58E-05			
Pd107	β^-,γ	6.5E+06 a	7.41E-05	1.73E-05			
Pm147	β^-,γ	2.6234 a	7.87E+00	1.07E+01			
Po210	α,γ	138.38 d	2.55E+00	7.16E-06			
Po211	α,γ	0.516 s	1.71E-03	2.12E-06			
Po212	α	0.298 μs	1.73E+01	4.72E-02			
Po213	α	4 μs	2.82E+00	1.15E-01			
Po214	α,γ	163.7 μs	1.16E+01	3.57E-05			
Po215	α,β^-,γ	1.780 ms	6.09E-01	7.58E-04			
Po216	α,γ	0.145 s	2.71E+01	7.36E-02			
Po218	α,β^-,γ	3.10 m	1.16E+01	3.58E-05			
Pr144	β^-,γ	17.28 m	6.18E-02	5.07E+00			
Pu236	α,γ,SF	2.87 a	1.04E-02	NR			

Table 3 Continued.
40CFR191 Unit of Waste for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] **(d)**		Transuranic Inventory [α-Curies] **(e)**		% of Unit of Waste
			CH	RH	CH	RH	(%)
Pu238	α,γ,SF	87.7 a	**2.61E+06 (f)**	1.45E+03	**2.61E+06**	**1.45E+03**	**64.1**
Pu239	α,γ,SF	2.410E+04 a	7.85E+05	1.03E+04	**7.85E+05**	**1.03E+04**	**19.5**
Pu240	α,γ,SF	6.56E+03 a	2.10E+05	5.07E+03	**2.10E+05**	**5.07E+03**	**5.28**
Pu241	α,β^-,γ	14.4 a	2.31E+06	1.42E+05			
Pu242	α,γ,SF	3.75E+05 a	1.17E+03	1.50E-01	**1.17E+03**	**1.50E-01**	**2.87E-02**
Pu243	β^-,γ	4.956 h	3.21E-09	NR			
Pu244	α,SF	8.0E+07 a	1.50E-06	2.21E-11	**1.50E-06**	**2.21E-11**	**3.68E-11**
Ra223	α,γ	11.435 d	6.09E-01	7.58E-04			
Ra224	α,γ	3.66 d	2.71E+01	7.36E-02			
Ra225	β^-,γ	14.9 d	2.88E+00	1.17E-01			
Ra226	α,γ	1.60E+03 a	1.16E+01	3.58E-05			
Ra228	β^-,γ	5.76 a	7.47E-01	7.77E-02			
Rh106	β^-,γ	29.9 s	2.90E-02	1.09E+01			
Rn219	α,γ	3.96 s	6.09E-01	7.58E-04			
Rn220	α,γ	55.6 s	2.71E+01	7.36E-02			
Rn222	α,γ	3.8235 d	1.16E+01	3.58E-05			
Ru106	β^-	1.02 a	2.90E-02	1.09E+01			
Sb125	β^-,γ	2.758 a	1.21E-01	1.89E+00			
Sb126	β^-,γ	12.4 d	1.35E-04	3.16E-05			
Sb126m	$\gamma,\varepsilon e^-$	19.0 m	9.65E-04	2.25E-04			
Se79	β^-	6.5E+04 a	4.35E-04	1.02E-04			
Sm151	β^-,γ	90 a	1.47E+00	3.57E-01			
Sn119m	γ,ITe^-	293 d	4.14E-06	9.59E-07			
Sn121m	β^-,γ,ITe^-	55 a	2.66E-02	6.69E-03			
Sn126	β^-,γ	1.0E+05 a	9.65E-04	2.25E-04			
Sr89†	β^-,γ	50.52 d	NR	NR			
Sr90	β^-	29.1 a	6.85E+03	2.09E+05			
Ta182	β^-,γ	114.43 d	NR	4.21E-08			
Tc99	β^-,γ	2.13E+05 a	2.52E+01	5.85E-03			
Te125m	γ,ITe^-	58 d	2.95E-02	4.65E-01			
Te127	β^-,γ	9.4 h	1.30E-07	1.71E-09			
Te127m	β^-,γ,ITe^-	109 d	1.33E-07	1.75E-09			
Th227	α,γ	18.72 d	6.01E-01	7.47E-04			
Th228	α,γ	1.913 a	2.71E+01	7.36E-02			
Th229	α,γ	7.3E+03 a	2.88E+00	1.17E-01			
Th230	α,γ	7.54E+04 a	8.06E-02	7.56E-03			
Th231	β^-,γ	1.063 d	1.28E+01	4.63E+00			
Th232	α,γ	1.4E+10 a	9.13E-01	9.25E-02			
Th234	β^-,γ	24.10 m	3.96E+01	1.05E+01			
Tl207	β^-,γ	4.77 m	6.07E-01	7.56E-04			
Tl208	β^-,γ	3.053 m	9.73E+00	2.65E-02			

Table 3 Continued.
40CFR191 Unit of Waste for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (d)		Transuranic Inventory [α-Curies] (e)		% of Unit of Waste
			CH	RH	CH	RH	(%)
Tl209	β^-,γ	2.2 m	6.22E-02	2.53E-03			
Tl210‡	β,γ	1.30 m	NR	NR			
U232	α,γ,SF	70 a	2.58E+01	NR			
U233	α,γ,SF	1.592E+05 a	1.79E+03	1.58E+02			
U234	α,γ,SF	2.46E+05 a	4.65E+02	4.27E+01			
U235	α,γ,SF	7.04E+08 a	1.28E+01	4.63E+00			
U236	α,γ,SF	2.342E+07 a	3.33E-01	9.68E-02			
U237	β^-,γ	6.75 d	5.66E+01	3.48E+00			
U238	α,γ,SF	4.47E+09 a	3.96E+01	1.05E+01			
U240	β^-,γ	14.1 h	1.50E-06	2.21E-11			
Y90	β^-,γ	2.67 d	6.85E+03	2.09E+05			
Zn65†	$\beta^+,\gamma,\varepsilon$	243.8 d	NR	NR			
Zr93	β^-,γ	1.5E+06 a	5.63E-03	1.32E-03			
Zr95	β^-,γ	64.02 d	1.15E-09	3.02E-01			
		Sum =	6.42E+06 (h)	1.02E+06 (i)	(4.048E+06) **4.048E+06 (j)**	(2.283E+04) **2.283E+04 (k)**	100.00 %
		Sum =	7.44E+06 (l)		(4.07E+06) **4.07E+06** **(Unit of Waste = 4.07) (m)**		
Top 5 Radionuclides							
Pu238	α,γ,SF	87.7 a	**2.61E+06 (f)**	1.45E+03	**2.61E+06**	**1.45E+03**	**64.1**
Pu239	α,γ,SF	2.410E+04 a	7.85E+05	1.03E+04	**7.85E+05**	**1.03E+04**	**19.5**
Am241	α,γ,SF	432.7 a	4.42E+05	5.96E+03	**4.42E+05**	**5.96E+03**	**11.0**
Pu240	α,γ,SF	6.56E+03 a	2.10E+05	5.07E+03	**2.10E+05**	**5.07E+03**	**5.28**
Pu242	α,γ,SF	3.75E+05 a	1.17E+03	1.50E-01	**1.17E+03**	**1.50E-01**	**2.87E-02**

NR Not Reported by sites (see Ref. CCA-2).

‡ Data values for radionuclides were previously reported in Rev. 1 of WTWBIR (Ref. BIR-1).

† Data values for radionuclides were previously reported in Rev. 2 of TWBIR (Ref. BIR-2).

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-4.

(c) Decay mode and half-life information taken from the Chart of the Nuclides, 14th Ed. Ref. GE-1. [It is better for technical calculations, to use halflives that are extracted from the databases of ORIGEN2 [Ref. OR-1] because the ORIGEN2 data are of a later version than that of Ref. GE-1 (see Ref. SNL-5 for ORIGEN2 values).].

(d) Total inventory (curie) data taken from Ref. CCA-2. Values correspond to a "WIPP-Scale" design basis.

(e) Transuranic inventory data corresponds to the activity (curie) data only for radionuclides that are "transuranic waste" per definitions in 40CFR191 Inventory data in bold corresponds to those data incorporated into the WIPP PA database (see Ref. SNL-4).

(f) Isotope with dominate curie load for CH-TRU wastes.

(g) Isotope with dominate curie load for RH-TRU wastes.

(h) Note, the total CH-TRU curie load is 6.42 MCi (also, 86.3 % of the total curie load in WIPP). The average CH-TRU volumetric total curie load is 6.42E+06/5.95E+06 = 1.08 (Ci/cu. ft.) = **38.1 (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume. The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values are applicable to expected waste at WIPP (see Ref. BIR-2d).]

(i) Note, the total RH-TRU curie load is only 1.02 MCi (also, only 13.7 % of the total curie load in WIPP). This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1]. The average RH-TRU volumetric total curie load is 1.02E+06/0.25E+06 = 4.08 (Ci/cu. ft.) = **144. (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft.]

(j) Note, there are only 15 radionuclides that comprise the "transuranic waste" (see footnote e above). Eleven of these radionuclides are included in the WIPP PA data base and correspond to 99.99999% of the total CH "transuranic" inventory. The average CH-TRU volumetric "transuranic" curie load is 4.048E+06/5.95E+06 = **0.680 (TRU-Ci/cu. ft.)** = **24.0 (TRU-Ci/cu. m.)**.

(k) Note, there are only 15 radionuclides that comprise the "transuranic waste" (see footnote e above). Eleven of these radionuclides are included in the WIPP PA data base and correspond to 99.99998% of the total RH "transuranic" inventory. The average RH-TRU volumetric "transuranic" curie load is 2.283E+04/0.25E+06 = **0.0913 (TRU-Ci/cu. ft.)** = **3.22 (TRU-Ci/cu. m.)**. [The RH contribution to the WIPP-scale inventory of transuranic curie load is 2.283E+04*100%/(2.283E+04 + 4.048E+06)**=0.561% (very small)**.] Note, this value is an order of magnitude less than that presented for the CH-TRU wastes -- since the majority of the curie content of the RH-TRU waste is due to shorter-lived non-transuranic radionuclides, this means that as the shorter-lived components decay away the remaining RH-TRU waste will have a lesser curie content than CH-TRU waste (i.e., as the RH-TRU waste decays, it becomes "wimpier" than CH-TRU waste). This is evident from the RH Study (Ref. DOE-1) which showed that after about 150 → 250 years that CH-TRU waste has a higher specific activity than that of RH-TRU waste.

(l) It is interesting to know that the Yucca Mountain Project (YMP) has approximately 12.4 billion curies of inventory (spent fuel -- 63,000 MTU [YMP-1b] × 1.57E+05 Ci/MTU [YMP-1c] + vitrified high-level waste -- 2.47E+09 Ci [YMP-1d]). Thus YMP is equivalent to 1660 WIPPs as far as curie load is concerned. Even though WIPP is less than one part in a thousand in comparison to YMP it still requires the same amount of work (with the exception of thermal effects) to demonstrate compliance for WIPP as it does for YMP because the EPA compliance requirements are based on a normalized basis (i.e., whether a repository has a radionuclide inventory on the order of millicuries, curies, millions of curies (like WIPP), or billions of curies (like YMP), the amount of work (with the exception of thermal effects) to show compliance is the same).

(m) Note, the unit of waste (UW, calculated to three significant figures) is the same whether the UW is calculated using all available information in the TWBID (Ref. CCA-2) or using the limited data within the WIPP PA database. [Also, only 4 radionuclides (Am241, Pu238, Pu239, and Pu240) make up 99.96% of the Unit of Waste value [see Ref. EPA-1b] -- using 5 radionuclides (adding Pu242) makes up 99.9936% of the Unit of Waste value].

Table 4.
40CFR191 Release Limits for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID **(b)**	Decay Mode **(c)**	Half-Life **(c)**	Total Inventory [Curies] **(d)**		Release Limits Inventory [α-Curies] **(e)**		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Ac225	α, γ	10.0 d	2.88E+00	1.17E-01			
Ac227	α, β^-, γ	21.77 a	6.08E-01	7.57E-04	100.	407.	1.50E-03
Ac228	α, β^-, γ	6.15 h	7.46E-01	7.77E-02			
Ag109m	ITe^-	39.8 s	1.57E+01	NR			
Ag110	$\beta^-, \gamma, \varepsilon$	24.6 s	7.07E-09	1.74E-09			
Ag110m	β^-, γ, ITe^-	249.8 d	5.31E-07	1.31E-07			
Am241	α, γ, SF	432.7 a	4.42E+05	5.96E+03	**100.**	**407.**	**1101.**
Am242	$\beta, \gamma, \varepsilon e^-$	16.02 h	1.75E+00	NR			
Am242m	α, ITe^-	141. h	1.75E+00	NR			
Am243	α, β^-, γ	7.37E+03 a	3.26E+01	2.28E-04	**100.**	**407.**	**8.01E-02**
Am245	β^-, γ	2.05 h	1.33E-09	2.87E-16			
At217	α, β^-, γ	32 ms	2.88E+00	1.17E-01			
Ba137m	IT	2.552 m	7.63E+03	2.04E+05			
Bi210	α, β^-, γ	5.01 d	2.55E+00	7.16E-06			
Bi211	α, β^-, γ	2.14 m	6.09E-01	7.58E-04			
Bi212	α, β^-, γ	1.009 h	2.71E+01	7.36E-02			
Bi213	α, β^-, γ	45.6 m	2.88E+00	1.17E-01			
Bi214	α, β^-, γ	19.9 m	1.16E+01	3.58E-05			
Bk249	α, β^-, γ	3.2E+02 d	9.16E-05	1.98E-11			
Bk250	β^-, γ	3.217 h	4.37E-11	NR			
C14	β^-	5730 a	1.08E+01	2.05E+00	100.	407.	3.16E-02
Cd109	γ, ε	462.0 d	1.57E+01	NR			
Cd113m	β^-, IT	14.1 a	1.82E-06	5.46E-07			
Ce144	β^-, γ	284.6 d	6.26E-02	5.13E+00			
Cf249	α, γ, SF	351 a	6.42E-02	4.47E-03	100.	407.	1.69E-04
Cf250	α, γ, SF	13.1 a	3.30E-01	NR			
Cf251	α, γ	9.0E+02 a	3.78E-03	NR	100.	407.	9.29E-06
Cf252	α, γ, SF	2.638 a	2.39E+02	1.29E+00			
Cm242	α, γ, SF	162.8 d	1.14E+00	NR			
Cm243	$\alpha, \gamma, SF, \varepsilon$	29.1 a	2.72E+00	4.95E+01	**100.**	**407.**	**0.128**
Cm244	α, γ, SF	18.1 a	3.15E+04	3.15E+02			
Cm245	α, γ, SF	8.5E+03 a	1.15E+02	1.46E-06	**100.**	**407.**	**0.283**
Cm246	α, γ, SF	4.76E+03 a	1.02E-01	NR	100.	407.	2.51E-04
Cm247	α, γ	1.56E+07 a	3.21E-09	NR	100.	407.	7.89E-12
Cm248	α, SF	3.48E+05 a	8.95E-02	2.05E-04	**100.**	**407.**	**2.20E-04**
Co58	$\beta^+, \gamma, \varepsilon$	70.88 d	3.05E-13	1.24E-11			
Co60	β^-, γ	5.271 a	6.46E+01	1.04E+04			
Cr51	$\varepsilon\gamma$	27.70 d	NR	3.04E-06			
Cs134	$\beta^-, \gamma, \varepsilon$	2.065 a	1.34E-02	1.84E+01			
Cs135	β^-	2.3E+06 a	5.02E-04	1.17E-04	1000.	4070.	1.52E-07
Cs137	β^-, γ	30.17 a	8.06E+03	**2.16E+05 (g)**	**1000.**	**4070.**	**55.1**
Es254	α, γ	276 d	4.24E-11	NR			

Table 4 Continued.
40CFR191 Release Limits for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] (d)		Release Limits Inventory [α-Curies] (e)		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Eu150	γ,ε	36 a	3.51E-05	NR			
Eu152	$\beta^-,\gamma,\varepsilon\beta^+$	13.48 a	1.26E+00	1.22E+03			
Eu154	$\beta^-,\gamma,\varepsilon\gamma$	8.59 a	1.15E+00	5.91E+02			
Eu155	β^-,γ	4.71 a	9.46E-01	1.18E+02			
Fe55	ε	2.73 a	1.91E-05	1.69E-01			
Fe59	β^-,γ	44.51 d	2.64E-07	NR			
Fr221	α,γ	4.8 m	2.88E+00	1.17E-01			
Fr223	α,β^-,γ	21.8 m	8.39E-03	1.04E-05			
H3	β^-	12.3 a	8.69E-01	6.60E-02			
I129	β^-,γ	1.57E+07 a	7.05E-07	NR	100.	407.	1.73E-09
Kr85	β^-,γ	10.73 a	2.02E-01	1.68E+00			
Mn54	εγ	312.2 d	8.51E-04	2.35E-02			
Nb95	β^-,γ	34.97 d	2.54E-09	6.69E-01			
Nb95m	$\beta^-,\gamma,\mathit{IT}$	3.61 d	8.50E-12	2.24E-03			
Ni59	ε	7.6E+04 a	7.52E-03	NR	1000.	4070.	1.85E-06
Ni63	β^-	100. a	9.19E-01	9.88E-01	1000.	4070.	4.69E-04
Np237	α,γ	2.14E+06 a	5.61E+01	2.85E+00	**100.**	**407.**	**1.45E-01**
Np238	β,γ	2.117 d	8.77E-03	NR			
Np239	β^-,γ	2.355 d	3.26E+01	2.28E-04			
Np240‡	β,γ	1.032 h	NR	NR			
Np240m	$\beta^-,\gamma,\mathit{IT}$	7.22 m	1.50E-06	2.21E-11			
Pa231	α,γ	3.28E+04 a	4.51E-01	1.91E-03	**100.**	**407.**	**1.11E-03**
Pa233	β^-,γ	27.0 d	5.61E+01	2.85E+00			
Pa234	β^-,γ	6.69 h	5.14E-02	1.36E-02			
Pa234m	$\beta^-,\gamma,\mathit{IT}$	1.17 m	3.96E+01	1.05E+01			
Pb209	β^-	3.25 h	2.88E+00	1.17E-01			
Pb210	α,β^-,γ	22.3 a	2.55E+00	7.16E-06	**100.**	**407.**	**6.27E-03**
Pb211	β^-,γ	36.1 m	6.09E-01	7.58E-04			
Pb212	β^-,γ	10.64 hr	2.71E+01	7.36E-02			
Pb214	β^-,γ	27 m	1.16E+01	3.58E-05			
Pd107	β^-,γ	6.5E+06 a	7.41E-05	1.73E-05	1000.	4070.	2.25E-08
Pm147	β^-,γ	2.6234 a	7.87E+00	1.07E+01			
Po210	α,γ	138.38 d	2.55E+00	7.16E-06			
Po211	α,γ	0.516 s	1.71E-03	2.12E-06			
Po212	α	0.298 μs	1.73E+01	4.72E-02			
Po213	α	4 μs	2.82E+00	1.15E-01			
Po214	α,γ	163.7 μs	1.16E+01	3.57E-05			
Po215	α,β^-,γ	1.780 ms	6.09E-01	7.58E-04			
Po216	α,γ	0.145 s	2.71E+01	7.36E-02			
Po218	α,β^-,γ	3.10 m	1.16E+01	3.58E-05			
Pr144	β^-,γ	17.28 m	6.18E-02	5.07E+00			
Pu236	α,γ,*SF*	2.87 a	1.04E-02	NR			

Table 4 Continued.
40CFR191 Release Limits for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID **(b)**	Decay Mode **(c)**	Half-Life **(c)**	Total Inventory [Curies] **(d)**		Release Limits Inventory [α-Curies] **(e)**		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Pu238	α,γ,SF	87.7 a	**2.61E+06 (f)**	1.45E+03	**100.**	**407.**	**6416.**
Pu239	α,γ,SF	2.410E+04 a	7.85E+05	1.03E+04	**100.**	**407.**	**1954.**
Pu240	α,γ,SF	6.56E+03 a	2.10E+05	5.07E+03	**100.**	**407.**	**528.**
Pu241	α,β^-,γ	14.4 a	2.31E+06	1.42E+05			
Pu242	α,γ,SF	3.75E+05 a	1.17E+03	1.50E-01	**100.**	**407.**	**2.88**
Pu243	β^-,γ	4.956 h	3.21E-09	NR			
Pu244	α,SF	8.0E+07 a	1.50E-06	2.21E-11	**100.**	**407.**	**3.69E-09**
Ra223	α,γ	11.435 d	6.09E-01	7.58E-04			
Ra224	α,γ	3.66 d	2.71E+01	7.36E-02			
Ra225	β^-,γ	14.9 d	2.88E+00	1.17E-01			
Ra226	α,γ	1.60E+03 a	1.16E+01	3.58E-05	**100.**	**407.**	**2.85E-02**
Ra228	β^-,γ	5.76 a	7.47E-01	7.77E-02			
Rh106	β^-,γ	29.9 s	2.90E-02	1.09E+01			
Rn219	α,γ	3.96 s	6.09E-01	7.58E-04			
Rn220	α,γ	55.6 s	2.71E+01	7.36E-02			
Rn222	α,γ	3.8235 d	1.16E+01	3.58E-05			
Ru106	β^-	1.02 a	2.90E-02	1.09E+01			
Sb125	β^-,γ	2.758 a	1.21E-01	1.89E+00			
Sb126	β^-,γ	12.4 d	1.35E-04	3.16E-05			
Sb126m	$\gamma,\varepsilon e^-$	19.0 m	9.65E-04	2.25E-04			
Se79	β^-	6.5E+04 a	4.35E-04	1.02E-04	1000.	4070.	1.32E-07
Sm151	β^-,γ	90 a	1.47E+00	3.57E-01	1000.	4070.	4.49E-04
Sn119m	γ,ITe^-	293 d	4.14E-06	9.59E-07			
Sn121m	β^-,γ,ITe^-	55 a	2.66E-02	6.69E-03	1000.	4070.	8.18E-06
Sn126	β^-,γ	1.0E+05 a	9.65E-04	2.25E-04	1000.	4070.	2.92E-07
Sr89†	β^-,γ	50.52 d	NR	NR			
Sr90	β^-	29.1 a	6.85E+03	2.09E+05	**1000.**	**4070.**	**53.0**
Ta182	β^-,γ	114.43 d	NR	4.21E-08			
Tc99	β^-,γ	2.13E+05 a	2.52E+01	5.85E-03	10000.	40700.	6.19E-04
Te125m	γ,ITe^-	58 d	2.95E-02	4.65E-01			
Te127	β^-,γ	9.4 h	1.30E-07	1.71E-09			
Te127m	β^-,γ,ITe^-	109 d	1.33E-07	1.75E-09			
Th227	α,γ	18.72 d	6.01E-01	7.47E-04			
Th228	α,γ	1.913 a	2.71E+01	7.36E-02			
Th229	α,γ	7.3E+03 a	2.88E+00	1.17E-01	**100.**	**407.**	**7.36E-03**
Th230	α,γ	7.54E+04 a	8.06E-02	7.56E-03	**10.**	**40.7**	**2.17E-03**
Th231	β^-,γ	1.063 d	1.28E+01	4.63E+00			
Th232	α,γ	1.4E+10 a	9.13E-01	9.25E-02	**10.**	**40.7**	**2.48E-02**
Th234	β^-,γ	24.10 m	3.96E+01	1.05E+01			
Tl207	β^-,γ	4.77 m	6.07E-01	7.56E-04			
Tl208	β^-,γ	3.053 m	9.73E+00	2.65E-02			

Table 4 Continued.
40CFR191 Release Limits for WIPP TRU Waste (a)

Nuclide			WIPP TRU Waste				
ID (b)	Decay Mode (c)	Half-Life (c)	Total Inventory [Curies] **(d)**		Release Limits Inventory [α-Curies] **(e)**		EPA Unit
			CH	RH	(Ci./UW)	(Ci)	
Tl209	β^-,γ	2.2 m	6.22E-02	2.53E-03			
Tl210‡	β,γ	1.30 m	NR	NR			
U232	α,γ,SF	70 a	2.58E+01	NR	100.	407.	6.34E-02
U233	α,γ,SF	1.592E+05 a	1.79E+03	1.58E+02	**100.**	**407.**	**4.79**
U234	α,γ,SF	2.46E+05 a	4.65E+02	4.27E+01	**100.**	**407.**	**1.25**
U235	α,γ,SF	7.04E+08 a	1.28E+01	4.63E+00	**100.**	**407.**	**4.28E-02**
U236	α,γ,SF	2.342E+07 a	3.33E-01	9.68E-02	100.	407.	1.06E-03
U237	β^-,γ	6.75 d	5.66E+01	3.48E+00			
U238	α,γ,SF	4.47E+09 a	3.96E+01	1.05E+01	**100.**	**407.**	**1.23E-01**
U240	β^-,γ	14.1 h	1.50E-06	2.21E-11			
Y90	β^-,γ	2.67 d	6.85E+03	2.09E+05			
Zn65†	$\beta^+,\gamma,\varepsilon$	243.8 d	NR	NR			
Zr93	β^-,γ	1.5E+06 a	5.63E-03	1.32E-03	1000.	4070.	1.71E-06
Zr95	β^-,γ	64.02 d	1.15E-09	3.02E-01			
		Sum =	6.42E+06 (h)	1.02E+06 (i)			(1.012E+04) **1.012E+04 (j)**
		Sum =	7.44E+06				

Top 10 Radionuclides (k)

ID (b)	Total Inventory			EPA Unit			
	CH	RH	Total	CH	RH	Total	Cumulative
Pu238	**2.61E+06 (f)**	1.45E+03	2.61E+06	6413.	3.56	6416.	0.63418
Pu239	7.85E+05	1.03E+04	7.95E+05	1929.	25.3	1954.	0.82732
Am241	4.42E+05	5.96E+03	4.48E+05	1086.	14.6	1101.	0.93611
Pu240	2.10E+05	5.07E+03	2.15E+05	516.	12.5	528.	0.98834
Cs137	8.06E+03	**2.16E+05 (g)**	2.24E+05	1.98	53.1	55.1	0.99378
Sr90	6.85E+03	2.09E+05	2.16E+05	1.68	51.4	53.0	0.99902
U233	1.79E+03	1.58E+02	1.95E+03	4.40	0.39	4.79	0.99950
Pu242	1.17E+03	1.50E-01	1.17E+03	2.87	3.69E-04	2.88	0.99978
U234	4.65E+02	4.27E+01	5.08E+02	1.14	0.10	1.25	0.99990
Cm245	1.15E+02	1.46E-06	1.15E+02	0.283	3.59E-09	0.283	0.99993

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NR Not Reported by sites (see Ref. CCA-2).

‡ Data values for radionuclides were previously reported in Rev. 1 of WTWBIR (Ref. BIR-1).

† Data values for radionuclides were previously reported in Rev. 2 of TWBIR (Ref. BIR-2).

(a) Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID)

(b) Radionuclides in bold are those 29 incorporated into the WIPP PA database, Ref. SNL-4.

(c) Decay mode and half-life information taken from the Chart of the Nuclides, 14th Ed. Ref. GE-1. [It is better for technical calculations, to use halflives that are extracted from the databases of ORIGEN2 [Ref. OR-1] because the ORIGEN2 data are of a later version than that of Ref. GE-1 (see Ref. SNL-5 for ORIGEN2 values).]

(d) Total inventory (curie) data taken from Ref. CCA-2. Values correspond to a "WIPP-Scale" design basis.

(e) Release limits are determined in accordance with 40CFR191 (Appendix A, Table 1) [Ref. EPA-1]. Left column corresponds to specific release limits (cumulative releases to the accessible environment for 10,000 years after disposal per "unit of waste" identified in Note 1(e) of Table 1, Appendix A, 40CFR191). Right column corresponds to release limit obtained for 4.07 Units of Waste (see Table 2 for calculation of the Unit of Waste) determined from data in the Transuranic Waste Baseline Inventory Database (BID) [Ref. CCA-2].

(f) Isotope with dominate curie load for CH-TRU wastes.

(g) Isotope with dominate curie load for RH-TRU wastes.

(h) Note, the total CH-TRU curie load is 6.42 MCi (also, 86.3 % of the total curie load in WIPP). The average CH-TRU volumetric total curie load is 6.42E+06/5.95E+06 = 1.08 (Ci/cu. ft.) = **38.1 (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume. The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values are applicable to expected waste at WIPP (see Ref. BIR-2d).]

(i) Note, the total RH-TRU curie load is only 1.02 MCi (also, only 13.7 % of the total curie load in WIPP). This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1]. The average RH-TRU volumetric total curie load is 1.02E+06/0.25E+06 = 4.08 (Ci/cu. ft.) = **144. (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft.]

(j) Note, there are 42 radionuclides that comprise the "EPA Unit" (see footnote e above). 25 of these radionuclides are included in the WIPP PA data base and correspond to 99.99903% of the total CH- and RH-TRU "EPA Unit" inventory. The average CH-TRU volumetric "EPA Unit" load is 9.956E+03/5.95E+06 = **1.67E-03 (EPA Unit/cu. ft.)** = **5.91E-02 (EPA Unit/cu. m.)**. The average RH-TRU volumetric "EPA Unit" load is 1.611E+02/0.25E+06 = **6.44E-04 (EPA Unit/cu. ft.)** = **2.28E-02 (EPA Unit/cu. m.)**. [The RH contribution to the WIPP-scale inventory of transuranic curie load is 1.611E+02*100%/(1.611E+02 + 9.956E+03)=**1.592% (very small)**.] Note, this value is about two orders of magnitude less than that presented for the CH-TRU wastes -- since the majority of the curie content of the RH-TRU waste is due to shorter-lived non-transuranic radionuclides, this means that as the shorter-lived components decay away the remaining RH-TRU waste will have a lesser curie content than CH-TRU waste (i.e., as the RH-TRU waste decays, it becomes "wimpier" than CH-TRU waste). This is evident from the RH Study (Ref. DOE-1) which showed that after about 150 → 250 years that CH-TRU waste has a higher specific activity than that of RH-TRU waste.

(k) Note, the EPA Unit (calculated to four significant figures) is the same whether the EPA Unit is calculated using all available information in the TWBID (Ref. CCA-2) or using the limited data within the WIPP PA database. [Also, only 4 radionuclides (Pu238, Pu239, Am241, and Pu240) make up 98.83% of the EPA Unit (see Ref. EPA-1b) -- using 6 radionuclides (adding Cs137 & Sr90) makes up 99.9023% -- using the top 10 radionuclides makes up 99.9932% of the EPA Unit].

Table 5.
Radionuclides Applicable to 40CFR191 But Not Reported in TWBIR (a)

Any other alpha-emitting radionuclide with a half-life > 20 yr

Ac-227
Am-242m
Bi-210m
Bk-247
Dy-154
Gd-148
Gd-150
Gd-152
Hf-174
Nd-144
Np-235
Os-186
Po-209
Pt-190
Sm-146
Sm-147
Sm-148

Any other radionuclide with a half-life > 20 yr that does not emit alpha particles

Ag-108m
Al-26
Ar-39
Ar-42
Be-10
Bi-207
Bi-208
Ca-41
Cd-113
Cl-36
Cm-250 **(b)**
Fe-60
Hf-178m
Hf-182
Hg-194
Ho-163
Ho-166m
In-115
Ir-192m
K-40
Kr-81
La-137
La-138
Lu-176
Mn-53
Mo-93
Nb-91
Nb-92
Nb-94
Np-236
Pb-202
Pb-205
Pt-193
Rb-87
Re-186m
Re-187
Se-82
Si-32
Ta-180m
Tb-157
Tb-158
Tc-97
Tc-98
Te-123
Te-130
Ti-44
V-50

(a) See Refs. BIR-2b & EPA-1.

(b) It has not yet been proven that Cm-250 decays by anything other than spontaneous fission (since Cm-250 is very neutron rich, it is very difficult to generate it [GE-1b]).

Table 6. Disposal Radionuclide Inventory

Nuclide	WIPP TRU Waste							
ID	Total Inventory [Curies] (a)		Mass Load [Kg] (b)			Moles Load [Moles] (c)		
	CH	RH	CH	RH	Total	CH	RH	Total
Ac225	2.88E+00	1.17E-01	4.96E-08	2.02E-09	5.16E-08	2.21E-07	8.96E-09	2.30E-07
Ac227	6.08E-01	7.57E-04	8.41E-06	1.05E-08	8.42E-06	3.70E-05	4.61E-08	3.71E-05
Ac228	7.46E-01	7.77E-02	3.33E-10	3.47E-11	3.67E-10	1.46E-09	1.52E-10	1.61E-09
Ag109m	1.57E+01	NR	6.00E-12	--	6.00E-12	5.51E-11	--	5.51E-11
Ag110	7.07E-09	1.74E-09	1.69E-21	4.17E-22	2.11E-21	1.54E-20	3.79E-21	1.92E-20
Ag110m	5.31E-07	1.31E-07	1.12E-13	2.76E-14	1.39E-13	1.02E-12	2.51E-13	1.27E-12
Am241	4.42E+05	5.96E+03	1.29E+02	1.74E+00	1.31E+02	5.34E+02	7.21E+00	5.42E+02
Am242	1.75E+00	NR	2.17E-09	--	2.17E-09	8.95E-09	--	8.95E-09
Am242m	1.75E+00	NR	1.80E-04	--	1.80E-04	7.44E-04	--	7.44E-04
Am243	3.26E+01	2.28E-04	1.64E-01	1.14E-06	1.64E-01	6.73E-01	4.71E-06	6.73E-01
Am245	1.33E-09	2.87E-16	2.15E-19	4.65E-26	2.15E-19	8.79E-19	1.90E-25	8.79E-19
At217	2.88E+00	1.17E-01	1.79E-15	7.27E-17	1.86E-15	8.25E-15	3.35E-16	8.58E-15
Ba137m	7.63E+03	2.04E+05	1.42E-08	3.79E-07	3.93E-07	1.04E-07	2.77E-06	2.87E-06
Bi210	2.55E+00	7.16E-06	2.06E-08	5.77E-14	2.06E-08	9.79E-08	2.75E-13	9.79E-08
Bi211	6.09E-01	7.58E-04	1.46E-12	1.81E-15	1.46E-12	6.90E-12	8.59E-15	6.91E-12
Bi212	2.71E+01	7.36E-02	1.85E-09	5.02E-12	1.86E-09	8.73E-09	2.37E-11	8.75E-09
Bi213	2.88E+00	1.17E-01	1.49E-10	6.05E-12	1.55E-10	6.99E-10	2.84E-11	7.28E-10
Bi214	1.16E+01	3.58E-05	2.63E-10	8.11E-16	2.63E-10	1.23E-09	3.79E-15	1.23E-09
Bk249	9.16E-05	1.98E-11	5.59E-11	1.21E-17	5.59E-11	2.25E-10	4.85E-17	2.25E-10
BK250	4.37E-11	NR	1.12E-20	--	1.12E-20	4.49E-20	--	4.49E-20
C14		1.08E+01	2.05E+00	2.42E-03	4.60E-04	2.88E-03	1.73E-01	3.29E-02
Cd109	1.57E+01	NR	6.08E-06	--	6.08E-06	5.58E-05	--	5.58E-05
Cd113m	1.84E-06	5.46E-07	8.48E-12	2.52E-12	1.10E-11	7.51E-11	2.23E-11	9.74E-11
Ce144	6.26E-02	5.13E+00	1.96E-08	1.61E-06	1.63E-06	1.36E-07	1.12E-05	1.13E-05
Cf249	6.42E-02	4.47E-03	1.57E-05	1.09E-06	1.68E-05	6.29E-05	4.38E-06	6.73E-05
Cf250	3.30E-01	NR	3.02E-06	--	3.02E-06	1.21E-05	--	1.21E-05
Cf251	3.78E-03	NR	2.38E-06	--	2.38E-06	9.50E-06	--	9.50E-06
Cf252	2.39E+02	1.29E+00	4.45E-04	2.40E-06	4.47E-04	1.76E-03	9.52E-06	1.77E-03
Cm242	1.14E+00	NR	3.45E-07	--	3.45E-07	1.42E-06	--	1.42E-06
Cm243	2.72E+00	4.95E+01	5.27E-05	9.59E-04	1.01E-03	2.17E-04	3.95E-03	4.16E-03
Cm244	3.15E+04	3.15E+02	3.89E-01	3.89E-03	3.93E-01	1.60E+00	1.60E-02	1.61E+00
Cm245	1.15E+02	1.46E-06	6.70E-01	8.51E-09	6.70E-01	2.73E+00	3.47E-08	2.73E+00
Cm246	1.02E-01	NR	3.32E-04	--	3.32E-04	1.35E-03	--	1.35E-03
Cm247	3.21E-09	NR	3.46E-08	--	3.46E-08	1.40E-07	--	1.40E-07
Cm248	8.95E-02	2.05E-04	2.11E-02	4.82E-05	2.11E-02	8.49E-02	1.94E-04	8.51E-02
Co58	3.05E-13	1.24E-11	9.58E-21	3.89E-19	3.99E-19	1.65E-19	6.72E-18	6.89E-18
Co60	6.46E+01	1.04E+04	5.71E-05	9.19E-03	9.25E-03	9.52E-04	1.53E-01	1.54E-01
Cr51	NR	3.04E-06	--	3.29E-14	3.29E-14	--	6.45E-13	6.45E-13
Cs134	1.34E-02	1.84E+01	1.03E-08	1.42E-05	1.42E-05	7.73E-08	1.06E-04	1.06E-04
Cs135	5.02E-04	1.17E-04	4.36E-04	1.02E-04	5.37E-04	3.23E-03	7.53E-04	3.98E-03
Cs137	8.06E+03	**2.16E+05** (f)	9.26E-02	2.48E+00	2.57E+00	6.76E-01	1.81E+01	1.88E+01

2.06 E-01

LCS
7-11-96

Table 6 Continued. Disposal Radionuclide Inventory

Nuclide	WIPP TRU Waste							
ID	Total Inventory [Curies] (a)		Mass Load [Kg] (b)			Moles Load [Moles] (c)		
	CH	RH	CH	RH	Total	CH	RH	Total
Es254	4.24E-11	NR	2.27E-17	--	2.27E-17	8.95E-17	--	8.95E-17
Eu150	3.51E-05	NR	5.30E-10	--	5.30E-10	3.53E-09	--	3.53E-09
Eu152	1.26E+00	1.22E+03	7.28E-06	7.05E-03	7.06E-03	4.79E-05	4.64E-02	4.65E-02
Eu154	1.15E+00	5.91E+02	4.26E-06	2.19E-03	2.19E-03	2.77E-05	1.42E-02	1.42E-02
Eu155	9.46E-01	1.18E+02	2.03E-06	2.54E-04	2.56E-04	1.31E-05	1.64E-03	1.65E-03
Fe55	1.91E-05	1.69E-01	7.63E-12	6.75E-08	6.75E-08	1.39E-10	1.23E-06	1.23E-06
Fe59	2.64E-07	NR	5.36E-15	--	5.36E-15	9.10E-14	--	9.10E-14
Fr221	2.88E+00	1.17E-01	1.62E-11	6.60E-13	1.69E-11	7.35E-11	2.99E-12	7.65E-11
Fr223	8.39E-03	1.04E-05	2.17E-13	2.69E-16	2.17E-13	9.73E-13	1.21E-15	9.74E-13
H3	8.69E-01	6.60E-02	9.05E-08	6.88E-09	9.74E-08	3.00E-05	2.28E-06	3.23E-05
I129	7.05E-07	NR	3.99E-06	--	3.99E-06	3.10E-05	--	3.10E-05
Kr85	2.02E-01	1.68E+00	5.14E-07	4.28E-06	4.79E-06	6.06E-06	5.04E-05	5.64E-05
Mn54	8.51E-04	2.35E-02	1.10E-10	3.03E-09	3.14E-09	2.04E-09	5.62E-08	5.83E-08
Nb95	2.54E-09	6.69E-01	6.49E-17	1.71E-08	1.71E-08	6.84E-16	1.80E-07	1.80E-07
Nb95m	8.50E-12	2.24E-03	2.23E-20	5.88E-12	5.88E-12	2.35E-19	6.19E-11	6.19E-11
Ni59	7.52E-03	NR	9.92E-05	--	9.92E-05	1.68E-03	--	1.68E-03
Ni63	9.19E-01	9.88E-01	1.49E-05	1.60E-05	3.09E-05	2.36E-04	2.54E-04	4.91E-04
Np237	5.61E+01	2.85E+00	7.96E+01	4.04E+00	8.36E+01	3.36E+02	1.71E+01	3.53E+02
Np238	8.77E-03	NR	3.38E-11	--	3.38E-11	1.42E-10	--	1.42E-10
Np239	3.26E+01	2.28E-04	1.41E-07	9.83E-13	1.41E-07	5.88E-07	4.11E-12	5.88E-07
Np240m	1.50E-06	2.21E-11	1.42E-17	2.09E-22	1.42E-17	5.90E-17	8.70E-22	5.90E-17
Pa231	4.51E-01	1.91E-03	9.55E-03	4.04E-05	9.59E-03	4.13E-02	1.75E-04	4.15E-02
Pa233	5.61E+01	2.85E+00	2.70E-06	1.37E-07	2.84E-06	1.16E-05	5.89E-07	1.22E-05
Pa234	5.14E-02	1.36E-02	2.57E-11	6.81E-12	3.25E-11	1.10E-10	2.91E-11	1.39E-10
Pa234m	3.96E+01	1.05E+01	5.77E-11	1.53E-11	7.30E-11	2.46E-10	6.53E-11	3.12E-10
Pb209	2.88E+00	1.17E-01	6.34E-10	2.57E-11	6.60E-10	3.03E-09	1.23E-10	3.16E-09
Pb210	2.55E+00	7.16E-06	3.34E-05	9.38E-11	3.34E-05	1.59E-04	4.47E-10	1.59E-04
Pb211	6.09E-01	7.58E-04	2.47E-11	3.07E-14	2.47E-11	1.17E-10	1.46E-13	1.17E-10
Pb212	2.71E+01	7.36E-02	1.95E-08	5.30E-11	1.96E-08	9.20E-08	2.50E-10	9.23E-08
Pb214	1.16E+01	3.58E-05	3.54E-10	1.09E-15	3.54E-10	1.65E-09	5.10E-15	1.65E-09
Pd107	7.41E-05	1.73E-05	1.44E-04	3.36E-05	1.78E-04	1.35E-03	3.14E-04	1.66E-03
Pm147	7.87E+00	1.07E+01	8.48E-06	1.15E-05	2.00E-05	5.78E-05	7.85E-05	1.36E-04
Po210	2.55E+00	7.16E-06	5.68E-07	1.59E-12	5.68E-07	2.70E-06	7.59E-12	2.70E-06
Po211	1.71E-03	2.12E-06	1.79E-17	2.22E-20	1.79E-17	8.49E-17	1.05E-19	8.50E-17
Po212	1.73E+01	4.72E-02	9.75E-20	2.66E-22	9.78E-20	4.60E-19	1.26E-21	4.61E-19
Po213	2.82E+00	1.15E-01	2.24E-19	9.12E-21	2.33E-19	1.05E-18	4.28E-20	1.09E-18
Po214	1.16E+01	3.57E-05	3.62E-17	1.11E-22	3.62E-17	1.69E-16	5.20E-22	1.69E-16
Po215	6.09E-01	7.58E-04	2.07E-17	2.57E-20	2.07E-17	9.61E-17	1.20E-19	9.62E-17
Po216	2.71E+01	7.36E-02	7.78E-14	2.11E-16	7.80E-14	3.60E-13	9.79E-16	3.61E-13
Po218	1.16E+01	3.58E-05	4.10E-11	1.27E-16	4.10E-11	1.88E-10	5.81E-16	1.88E-10
Pr144	6.18E-02	5.07E+00	8.18E-13	6.71E-11	6.79E-11	5.68E-12	4.66E-10	4.72E-10
Pu236	1.04E-02	NR	1.96E-08	--	1.96E-08	8.29E-08	--	8.29E-08

Table 6 Continued. Disposal Radionuclide Inventory

Nuclide	WIPP TRU Waste							
ID	Total Inventory [Curies] (a)		Mass Load [Kg] (b)			Moles Load [Moles] (c)		
	CH	RH	CH	RH	Total	CH	RH	Total
Pu238	**2.61E+06** (e)	1.45E+03	1.52E+02	8.47E-02	1.53E+02	6.41E+02	3.56E-01	6.41E+02
Pu239	7.85E+05	1.03E+04	1.26E+04	1.66E+02	1.28E+04	5.28E+04	6.93E+02	5.35E+04
Pu240	2.10E+05	5.07E+03	9.22E+02	2.23E+01	9.44E+02	3.84E+03	9.27E+01	3.93E+03
Pu241	2.31E+06	1.42E+05	2.24E+01	1.38E+00	2.38E+01	9.30E+01	5.72E+00	9.88E+01
Pu242	1.17E+03	1.50E-01	3.07E+02	3.93E-02	3.07E+02	1.27E+03	1.62E-01	1.27E+03
Pu243	3.21E-09	NR	1.23E-18	--	1.23E-18	5.08E-18	--	5.08E-18
Pu244	1.50E-06	2.21E-11	8.46E-05	1.25E-09	8.46E-05	3.47E-04	5.11E-09	3.47E-04
Ra223	6.09E-01	7.58E-04	1.19E-08	1.48E-11	1.19E-08	5.33E-08	6.64E-11	5.34E-08
Ra224	2.71E+01	7.36E-02	1.70E-07	4.62E-10	1.71E-07	7.60E-07	2.06E-09	7.62E-07
Ra225	2.88E+00	1.17E-01	7.35E-08	2.98E-09	7.65E-08	3.27E-07	1.33E-08	3.40E-07
Ra226	1.16E+01	3.58E-05	1.17E-02	3.62E-08	1.17E-02	5.19E-02	1.60E-07	5.19E-02
Ra228	7.47E-01	7.77E-02	3.19E-06	3.32E-07	3.52E-06	1.40E-05	1.46E-06	1.55E-05
Rh106	2.90E-02	1.09E+01	8.14E-15	3.06E-12	3.07E-12	7.69E-14	2.89E-11	2.90E-11
Rn219	6.09E-01	7.58E-04	4.68E-14	5.83E-17	4.69E-14	2.14E-13	2.66E-16	2.14E-13
Rn220	2.71E+01	7.36E-02	2.94E-11	7.98E-14	2.95E-11	1.34E-10	3.63E-13	1.34E-10
Rn222	1.16E+01	3.58E-05	7.54E-08	2.33E-13	7.54E-08	3.40E-07	1.05E-12	3.40E-07
Ru106	2.90E-02	1.09E+01	8.66E-09	3.25E-06	3.26E-06	8.18E-08	3.07E-05	3.08E-05
Sb125	1.21E-01	1.89E+00	1.17E-07	1.83E-06	1.95E-06	9.38E-07	1.46E-05	1.56E-05
Sb126	1.35E-04	3.16E-05	1.61E-12	3.78E-13	1.99E-12	1.28E-11	3.00E-12	1.58E-11
Sb126m	9.65E-04	2.25E-04	1.23E-14	2.86E-15	1.51E-14	9.75E-14	2.27E-14	1.20E-13
Se79	4.35E-04	1.02E-04	6.24E-06	1.46E-06	7.70E-06	7.90E-05	1.85E-05	9.76E-05
Sm151	1.47E+00	3.57E-01	5.58E-05	1.36E-05	6.94E-05	3.70E-04	8.99E-05	4.60E-04
Sn119m	4.14E-06	9.59E-07	9.24E-13	2.14E-13	1.14E-12	7.77E-12	1.80E-12	9.57E-12
Sn121m	2.66E-02	6.69E-03	4.50E-07	1.13E-07	5.63E-07	3.72E-06	9.35E-07	4.65E-06
Sn126	9.65E-04	2.25E-04	3.40E-05	7.93E-06	4.19E-05	2.70E-04	6.29E-05	3.33E-04
Sr89†	NR	NR	--	--	--	–	–	–
Sr90	6.85E+03	2.09E+05	5.02E-02	1.53E+00	1.58E+00	5.58E-01	1.70E+01	1.76E+01
Ta182	NR	4.21E-08	–	6.75E-15	6.75E-15	–	3.71E-14	3.71E-14
Tc99	2.52E+01	5.85E-03	1.49E+00	3.45E-04	1.49E+00	1.50E+01	3.49E-03	1.50E+01
Te125m	2.95E-02	4.65E-01	1.64E-09	2.58E-08	2.74E-08	1.31E-08	2.07E-07	2.20E-07
Te127	1.30E-07	1.71E-09	4.92E-17	6.47E-19	4.99E-17	3.88E-16	5.10E-18	3.93E-16
Te127m	1.33E-07	1.75E-09	1.41E-14	1.85E-16	1.43E-14	1.11E-13	1.46E-15	1.12E-13
Th227	6.01E-01	7.47E-04	1.96E-08	2.43E-11	1.96E-08	8.61E-08	1.07E-10	8.62E-08
Th228	2.71E+01	7.36E-02	3.31E-05	8.98E-08	3.32E-05	1.45E-04	3.94E-07	1.45E-04
Th229	2.88E+00	1.17E-01	1.35E-02	5.50E-04	1.41E-02	5.91E-02	2.40E-03	6.15E-02
Th230	8.06E-02	7.56E-03	3.99E-03	3.75E-04	4.37E-03	1.74E-02	1.63E-03	1.90E-02
Th231	1.28E+01	4.63E+00	2.41E-08	8.71E-09	3.28E-08	1.04E-07	3.77E-08	1.42E-07
Th232	9.13E-01	9.25E-02	8.33E+03	8.44E+02	9.17E+03	3.59E+04	3.64E+03	3.95E+04
Th234	3.96E+01	1.05E+01	1.71E-06	4.54E-07	2.16E-06	7.31E-06	1.94E-06	9.25E-06
Tl207	6.07E-01	7.56E-04	3.19E-12	3.97E-15	3.19E-12	1.54E-11	1.92E-14	1.54E-11
Tl208	9.73E+00	2.65E-02	3.30E-11	9.00E-14	3.31E-11	1.59E-10	4.33E-13	1.59E-10

Table 6 Continued. Disposal Radionuclide Inventory

Nuclide	WIPP TRU Waste							
ID	Total Inventory [Curies] (a)		Mass Load [Kg] (b)			Moles Load [Moles] (c)		
	CH	RH	CH	RH	Total	CH	RH	Total
Tl209	6.22E-02	2.53E-03	1.52E-13	6.19E-15	1.58E-13	7.28E-13	2.96E-14	7.57E-13
U232	2.58E+01	NR	1.21E-03	--	1.21E-03	5.20E-03	--	5.20E-03
U233	1.79E+03	1.58E+02	1.85E+02	1.63E+01	2.01E+02	7.94E+02	7.01E+01	8.64E+02
U234	4.65E+02	4.27E+01	7.44E+01	6.83E+00	8.13E+01	3.18E+02	2.92E+01	3.47E+02
U235	1.28E+01	4.63E+00	5.92E+03	2.14E+03	8.07E+03	2.52E+04	9.12E+03	3.43E+04
U236	3.33E-01	9.68E-02	5.15E+00	1.50E+00	6.64E+00	2.18E+01	6.34E+00	2.82E+01
U237	5.66E+01	3.48E+00	6.94E-07	4.26E-08	7.36E-07	2.93E-06	1.80E-07	3.11E-06
U238	3.96E+01	1.05E+01	**1.18E+05**	**3.12E+04**	**1.49E+05**	**4.95E+05**	**1.31E+05**	**6.26E+05**
			(g)	**(h)**	**(i)**	**(j)**	**(k)**	**(l)**
U240	1.50E-06	2.21E-11	1.62E-15	2.39E-20	1.62E-15	6.75E-15	9.94E-20	6.75E-15
Y90	6.85E+03	2.09E+05	1.26E-05	3.84E-04	3.96E-04	1.40E-04	4.27E-03	4.41E-03
Zn65†	NR	NR	--	--	--	--	--	--
Zr93	5.63E-03	1.32E-03	2.24E-03	5.25E-04	2.76E-03	2.41E-02	5.65E-03	2.97E-02
Zr95	1.15E-09	3.02E-01	5.35E-17	1.40E-08	1.40E-08	5.64E-16	1.48E-07	1.48E-07
Total	6.42E+06	1.02E+06	1.47E+05	3.44E+04	1.81E+05	6.17E+05	1.45E+05	7.62E+05

--	Not calculated.
NR	Not Reported by sites (see Ref. CCA-2).
†	Data values for radionuclides were previously reported in Rev. 2 of TWBIR (Ref. BIR-2).
(a)	Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID) Values correspond to a "WIPP-Scale" design basis.
(b)	Data calculated from the equation; $\text{Mass Load} = TOTAL\ ACTIVITY(Ci)\frac{3.7E+10(dis/sec)}{Ci}\frac{\tau_{1/2}}{ln(2)}\frac{AtWt}{Na}\frac{kg}{1000\,gm}$
(c)	Data calculated from the equation; $\text{Mole Load} = MassLoad\ \frac{1}{AtWt}\frac{1000\,gm}{kg}$
(e)	Isotope with dominate curie load for CH-TRU wastes.
(f)	Isotope with dominate curie load for RH-TRU wastes.
(g)	Isotope with dominate mass load for CH-TRU wastes.
(h)	Isotope with dominate mass load for RH-TRU wastes.
(i)	Isotope with dominate mass load for CH- & RH-TRU wastes.
(j)	Isotope with dominate mole load for CH-TRU wastes.
(k)	Isotope with dominate mole load for RH-TRU wastes.
(l)	Isotope with dominate mole load for CH- & RH-TRU wastes.

Table 7. Disposal Radionuclide Inventory

Nuclide			WIPP TRU Waste					
ID	Energy		Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
	$\frac{MeV}{dis}$(a)	$\frac{W}{Ci}$	CH	RH	CH	RH	CH	RH
Ac225	5.893	3.49E-02	2.88E+00	1.17E-01	1.01E-01	4.09E-03	7.56E-05	1.22E-04
Ac227	0.082	4.84E-04	6.08E-01	7.57E-04	2.94E-04	3.67E-07	2.21E-07	1.09E-08
Ac228	1.458	8.64E-03	7.46E-01	7.77E-02	6.45E-03	6.72E-04	4.85E-06	2.00E-05
Ag109m	0.087	5.15E-04	1.57E+01	NR	8.09E-03	--	6.08E-06	--
Ag110	1.212	7.18E-03	7.07E-09	1.74E-09	5.08E-11	1.25E-11	3.82E-14	3.72E-13
Ag110m	2.817	1.67E-02	5.31E-07	1.31E-07	8.87E-09	2.19E-09	6.67E-12	6.51E-11
Am241	5.604	3.32E-02	4.42E+05	5.96E+03	1.47E+04	1.98E+02	1.10E+01	5.89E+00
Am242	0.192	1.14E-03	1.75E+00	NR	1.99E-03	--	1.49E-06	--
Am242m	0.067	3.95E-04	1.75E+00	NR	6.91E-04	--	5.20E-07	--
Am243	5.423	3.21E-02	3.26E+01	2.28E-04	1.05E+00	7.33E-06	7.88E-04	2.18E-07
Am245	0.313	1.86E-03	1.33E-09	2.87E-16	2.47E-12	5.32E-19	1.86E-15	1.58E-20
At217	7.199	4.27E-02	2.88E+00	1.17E-01	1.23E-01	4.99E-03	9.24E-05	1.49E-04
Ba137m	0.662	3.93E-03	7.63E+03	2.04E+05	3.00E+01	8.01E+02	2.25E-02	2.38E+01
Bi210	0.389	2.31E-03	2.55E+00	7.16E-06	5.88E-03	1.65E-08	4.42E-06	4.91E-10
Bi211	6.729	3.99E-02	6.09E-01	7.58E-04	2.43E-02	3.02E-05	1.83E-05	9.00E-07
Bi212	2.869	1.70E-02	2.71E+01	7.36E-02	4.61E-01	1.25E-03	3.47E-04	3.73E-05
Bi213	0.709	4.20E-03	2.88E+00	1.17E-01	1.21E-02	4.92E-04	9.10E-06	1.46E-05
Bi214	2.162	1.28E-02	1.16E+01	3.58E-05	1.49E-01	4.59E-07	1.12E-04	1.37E-08
Bk249	0.125	7.41E-04	9.16E-05	1.98E-11	6.79E-08	1.47E-14	5.10E-11	4.37E-16
Bk250	1.172	6.95E-03	4.37E-11	NR	3.04E-13	--	2.28E-16	–
C14	0.049	2.93E-04	1.08E+01	2.05E+00	3.17E-03	6.01E-04	2.38E-06	1.79E-05
Cd109	0.020	1.16E-04	1.57E+01	NR	1.82E-03	--	1.37E-06	--
Cd113m	0.284	1.68E-03	1.84E-06	5.46E-07	3.10E-09	9.19E-10	2.33E-12	2.74E-11
Ce144	0.112	6.63E-04	6.26E-02	5.13E+00	4.15E-05	3.40E-03	3.12E-08	1.01E-04
Cf249	7.806	4.63E-02	6.42E-02	4.47E-03	2.97E-03	2.07E-04	2.23E-06	6.16E-06
Cf250	6.267	3.71E-02	3.30E-01	NR	1.23E-02	--	9.22E-06	--
Cf251	6.027	3.57E-02	3.78E-03	NR	1.35E-04	–	1.02E-07	–
Cf252	12.04	7.14E-02	2.39E+02	1.29E+00	1.71E+01	9.21E-02	1.28E-02	2.74E-03
Cm242	6.216	3.68E-02	1.14E+00	NR	4.20E-02	--	3.16E-05	--
Cm243	6.189	3.67E-02	2.72E+00	4.95E+01	9.98E-02	1.82E+00	7.50E-05	5.40E-02
Cm244	5.901	3.50E-02	3.15E+04	3.15E+02	1.10E+03	1.10E+01	8.28E-01	3.28E-01
Cm245	5.598	3.32E-02	1.15E+02	1.46E-06	3.82E+00	4.84E-08	2.87E-03	1.44E-09
Cm246	5.523	3.27E-02	1.02E-01	NR	3.34E-03	--	2.51E-06	--
Cm247	5.390	3.20E-02	3.21E-09	NR	1.03E-10	--	7.71E-14	--
Cm248	21.00	1.24E-01	8.95E-02	2.05E-04	1.11E-02	2.55E-05	8.38E-06	7.59E-07
Co58	1.009	5.98E-03	3.05E-13	1.24E-11	1.82E-15	7.42E-14	1.37E-18	2.21E-15
Co60	2.601	1.54E-02	6.46E+01	1.04E+04	9.96E-01	1.60E+02	7.49E-04	4.77E+00
Cr51	0.036	2.15E-04	NR	3.04E-06	--	6.52E-10	--	1.94E-11
Cs134	1.717	1.02E-02	1.34E-02	1.84E+01	1.36E-04	1.87E-01	1.03E-07	5.57E-03
Cs135	0.056	3.34E-04	5.02E-04	1.17E-04	1.68E-07	3.90E-08	1.26E-10	1.16E-09
Cs137	0.187	1.11E-03	8.06E+03	**2.16E+05** **(f)**	8.92E+00	2.39E+02	6.70E-03	7.11E+00
Es254	6.623	3.93E-02	4.24E-11	NR	1.66E-12	--	1.25E-15	–

Table 7 Continue. Disposal Radionuclide Inventory

Nuclide			WIPP TRU Waste					
ID	Energy		Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
	$\frac{MeV}{dis}$(a)	$\frac{W}{Ci}$	CH	RH	CH	RH	CH	RH
Eu150	1.540	9.13E-03	3.51E-05	NR	3.20E-07	--	2.41E-10	--
Eu152	1.276	7.56E-03	1.26E+00	1.22E+03	9.53E-03	9.23E+00	7.17E-06	2.75E-01
Eu154	1.509	8.95E-03	1.15E+00	5.91E+02	1.03E-02	5.29E+00	7.73E-06	1.57E-01
Eu155	0.123	7.27E-04	9.46E-01	1.18E+02	6.88E-04	8.58E-02	5.17E-07	2.55E-03
Fe55	0.006	3.38E-05	1.91E-05	1.69E-01	6.45E-10	5.71E-06	4.85E-13	1.70E-07
Fe59	1.306	7.74E-03	2.64E-07	NR	2.04E-09	--	1.54E-12	--
Fr221	6.511	3.86E-02	2.88E+00	1.17E-01	1.11E-01	4.52E-03	8.36E-05	1.34E-04
Fr223	0.438	2.60E-03	8.39E-03	1.04E-05	2.18E-05	2.70E-08	1.64E-08	8.04E-10
H3	0.006	3.37E-05	8.69E-01	6.60E-02	2.93E-05	2.22E-06	2.20E-08	6.61E-08
I129	0.078	4.63E-04	7.05E-07	NR	3.26E-10	--	2.45E-13	--
Kr85	0.253	1.50E-03	2.02E-01	1.68E+00	3.03E-04	2.52E-03	2.28E-07	7.49E-05
Mn54	0.840	4.98E-03	8.51E-04	2.35E-02	4.24E-06	1.17E-04	3.19E-09	3.48E-06
Nb95	0.809	4.80E-03	2.54E-09	6.69E-01	1.22E-11	3.21E-03	9.16E-15	9.55E-05
Nb95m	0.234	1.39E-03	8.50E-12	2.24E-03	1.18E-14	3.11E-06	8.88E-18	9.26E-08
Ni59	0.007	3.97E-05	7.52E-03	NR	2.99E-07	--	2.25E-10	--
Ni63	0.017	1.01E-04	9.19E-01	9.88E-01	9.26E-05	9.96E-05	6.96E-08	2.96E-06
Np237	5.156	3.06E-02	5.61E+01	2.85E+00	1.71E+00	8.71E-02	1.29E-03	2.59E-03
Np238	0.408	4.79E-03	8.77E-03	NR	4.20E-05	--	3.16E-08	--
Np239	1.788	2.42E-03	3.26E+01	2.28E-04	7.88E-02	5.51E-07	5.93E-05	1.64E-08
Np240m	0.978	5.80E-03	1.50E-06	2.21E-11	8.69E-09	1.28E-13	6.54E-12	3.81E-15
Pa231	5.083	3.01E-02	4.51E-01	1.91E-03	1.36E-02	5.76E-05	1.02E-05	1.71E-06
Pa233	0.383	2.27E-03	5.61E+01	2.85E+00	1.27E-01	6.47E-03	9.57E-05	1.93E-04
Pa234	2.423	1.44E-02	5.14E-02	1.36E-02	7.38E-04	1.95E-04	5.55E-07	5.81E-06
Pa234m	0.834	4.94E-03	3.96E+01	1.05E+01	1.96E-01	5.19E-02	1.47E-04	1.54E-03
Pb209	0.194	1.15E-03	2.88E+00	1.17E-01	3.31E-03	1.35E-04	2.49E-06	4.00E-06
Pb210	0.039	2.32E-04	2.55E+00	7.16E-06	5.91E-04	1.66E-09	4.44E-07	4.94E-11
Pb211	0.505	3.00E-03	6.09E-01	7.58E-04	1.82E-03	2.27E-06	1.37E-06	6.76E-08
Pb212	0.321	1.90E-03	2.71E+01	7.36E-02	5.16E-02	1.40E-04	3.88E-05	4.17E-06
Pb214	0.538	3.19E-03	1.16E+01	3.58E-05	3.70E-02	1.14E-07	2.78E-05	3.40E-09
Pd107	0.010	5.93E-05	7.41E-05	1.73E-05	4.39E-09	1.03E-09	3.30E-12	3.05E-11
Pm147	0.061	3.59E-04	7.87E+00	1.07E+01	2.82E-03	3.84E-03	2.12E-06	1.14E-04
Po210	5.408	3.21E-02	2.55E+00	7.16E-06	8.17E-02	2.30E-07	6.15E-05	6.83E-09
Po211	7.592	4.50E-02	1.71E-03	2.12E-06	7.70E-05	9.54E-08	5.79E-08	2.84E-09
Po212	8.940	5.30E-02	1.73E+01	4.72E-02	9.17E-01	2.50E-03	6.89E-04	7.44E-05
Po213	8.537	5.06E-02	2.82E+00	1.15E-01	1.43E-01	5.82E-03	1.07E-04	1.73E-04
Po214	7.833	4.64E-02	1.16E+01	3.57E-05	5.39E-01	1.66E-06	4.05E-04	4.93E-08
Po215	7.531	4.46E-02	6.09E-01	7.58E-04	2.72E-02	3.38E-05	2.04E-05	1.01E-06
Po216	6.906	4.09E-02	2.71E+01	7.36E-02	1.11E+00	3.01E-03	8.34E-04	8.97E-05
Po218	6.113	3.62E-02	1.16E+01	3.58E-05	4.20E-01	1.30E-06	3.16E-04	3.86E-08
Pr144	1.240	7.35E-03	6.18E-02	5.07E+00	4.54E-04	3.73E-02	3.42E-07	1.11E-03
Pu236	5.871	3.48E-02	1.04E-02	NR	3.62E-04	--	2.72E-07	--

Table 7 Continue. Disposal Radionuclide Inventory

Nuclide			WIPP TRU Waste					
ID	Energy		Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
	$\frac{MeV}{dis}$ (a)	$\frac{W}{Ci}$	CH	RH	CH	RH	CH	RH
Pu238	5.591	3.31E-02	**2.61E+06** (e)	1.45E+03	**8.65E+04** (g)	4.81E+01	**6.50E+01** (g)	1.43E+00
Pu239	5.199	3.08E-02	7.85E+05	1.03E+04	2.42E+04	3.17E+02	1.82E+01	9.45E+00
Pu240	5.253	3.11E-02	2.10E+05	5.07E+03	6.54E+03	1.58E+02	4.92E+00	4.70E+00
Pu241	0.005	3.10E-05	2.31E+06	1.42E+05	7.16E+01	4.40E+00	5.38E-02	1.31E-01
Pu242	4.982	2.95E-02	1.17E+03	1.50E-01	3.46E+01	4.43E-03	2.60E-02	1.32E-04
Pu243	0.195	1.15E-03	3.21E-09	NR	3.70E-12	--	2.79E-15	--
Pu244	4.892	2.90E-02	1.50E-06	2.21E-11	4.35E-08	6.41E-13	3.27E-11	1.91E-14
Ra223	6.007	3.56E-02	6.09E-01	7.58E-04	2.17E-02	2.70E-05	1.63E-05	8.03E-07
Ra224	5.790	3.43E-02	2.71E+01	7.36E-02	9.30E-01	2.53E-03	6.99E-04	7.52E-05
Ra225	0.118	7.01E-04	2.88E+00	1.17E-01	2.02E-03	8.20E-05	1.52E-06	2.44E-06
Ra226	4.871	2.89E-02	1.16E+01	3.58E-05	3.35E-01	1.03E-06	2.52E-04	3.08E-08
Ra228	0.013	7.71E-05	7.47E-01	7.77E-02	5.76E-05	5.99E-06	4.33E-08	1.78E-07
Rh106	1.618	9.59E-03	2.90E-02	1.09E+01	2.78E-04	1.05E-01	2.09E-07	3.11E-03
Rn219	7.000	4.15E-02	6.09E-01	7.58E-04	2.53E-02	3.15E-05	1.90E-05	9.36E-07
Rn220	6.405	3.80E-02	2.71E+01	7.36E-02	1.03E+00	2.79E-03	7.74E-04	8.32E-05
Rn222	5.590	3.31E-02	1.16E+01	3.58E-05	3.84E-01	1.19E-06	2.89E-04	3.53E-08
Ru106	0.010	5.95E-05	2.90E-02	1.09E+01	1.72E-06	6.48E-04	1.30E-09	1.93E-05
Sb125	0.527	3.13E-03	1.21E-01	1.89E+00	3.78E-04	5.91E-03	2.84E-07	1.76E-04
Sb126	3.117	1.85E-02	1.35E-04	3.16E-05	2.49E-06	5.84E-07	1.88E-09	1.74E-08
Sb126m	2.148	1.27E-02	9.65E-04	2.25E-04	1.23E-05	2.86E-06	9.24E-09	8.53E-08
Se79	0.042	2.49E-04	4.35E-04	1.02E-04	1.08E-07	2.54E-08	8.14E-11	7.56E-10
Sm151	0.020	1.17E-04	1.47E+00	3.57E-01	1.72E-04	4.19E-05	1.30E-07	1.25E-06
Sn119m	0.087	5.17E-04	4.14E-06	9.59E-07	2.14E-09	4.96E-10	1.61E-12	1.48E-11
Sn121m	0.338	2.00E-03	2.66E-02	6.69E-03	5.33E-05	1.34E-05	4.01E-08	3.99E-07
Sn126	0.210	1.25E-03	9.65E-04	2.25E-04	1.20E-06	2.81E-07	9.05E-10	8.35E-09
Sr89†	0.583	3.46E-03	NR	NR	--	--	--	--
Sr90	0.196	1.16E-03	6.85E+03	2.09E+05	7.95E+00	2.43E+02	5.98E-03	7.22E+00
Ta182	1.502	8.90E-03	NR	4.21E-08	--	3.75E-10	--	1.12E-11
Tc99	0.085	5.01E-04	2.52E+01	5.85E-03	1.26E-02	2.93E-06	9.50E-06	8.73E-08
Te125m	0.142	8.41E-04	2.95E-02	4.65E-01	2.48E-05	3.91E-04	1.86E-08	1.16E-05
Te127	0.228	1.35E-03	1.30E-07	1.71E-09	1.76E-10	2.31E-12	1.32E-13	6.87E-14
Te127m	0.091	5.38E-04	1.33E-07	1.75E-09	7.15E-11	9.41E-13	5.38E-14	2.80E-14
Th227	6.157	3.65E-02	6.01E-01	7.47E-04	2.19E-02	2.73E-05	1.65E-05	8.11E-07
Th228	5.517	3.27E-02	2.71E+01	7.36E-02	8.86E-01	2.41E-03	6.66E-04	7.16E-05
Th229	5.161	3.06E-02	2.88E+00	1.17E-01	8.81E-02	3.58E-03	6.62E-05	1.07E-04
Th230	4.774	2.83E-02	8.06E-02	7.56E-03	2.28E-03	2.14E-04	1.71E-06	6.37E-06
Th231	0.095	5.61E-04	1.28E+01	4.63E+00	7.18E-03	2.60E-03	5.40E-06	7.73E-05
Th232	4.084	2.42E-02	9.13E-01	9.25E-02	2.21E-02	2.24E-03	1.66E-05	6.66E-05
Th234	0.068	4.05E-04	3.96E+01	1.05E+01	1.61E-02	4.26E-03	1.21E-05	1.27E-04
Tl207	0.495	2.94E-03	6.07E-01	7.56E-04	1.78E-03	2.22E-06	1.34E-06	6.61E-08
Tl208	3.970	2.35E-02	9.73E+00	2.65E-02	2.29E-01	6.24E-04	1.72E-04	1.86E-05

Table 7 Continue. Disposal Radionuclide Inventory

Nuclide			WIPP TRU Waste					
ID	Energy		Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
	$\frac{MeV}{dis}$ (a)	$\frac{W}{Ci}$	CH	RH	CH	RH	CH	RH
Tl209	2.803	1.66E-02	6.22E-02	2.53E-03	1.03E-03	4.20E-05	7.77E-07	1.25E-06
U232	5.416	3.21E-02	2.58E+01	NR	8.28E-01	--	6.23E-04	--
U233	4.904	2.91E-02	1.79E+03	1.58E+02	5.20E+01	4.59E+00	3.91E-02	1.37E-01
U234	4.859	2.88E-02	4.65E+02	4.27E+01	1.34E+01	1.23E+00	1.01E-02	3.66E-02
U235	4.418	2.62E-02	1.28E+01	4.63E+00	3.35E-01	1.21E-01	2.52E-04	3.61E-03
U236	4.570	2.71E-02	3.33E-01	9.68E-02	9.02E-03	2.62E-03	6.78E-06	7.80E-05
U237	0.319	1.89E-03	5.66E+01	3.48E+00	1.07E-01	6.58E-03	8.05E-05	1.96E-04
U238	4.279	2.54E-02	3.96E+01	1.05E+01	1.00E+00	2.66E-01	7.55E-04	7.93E-03
U240	0.138	8.20E-04	1.50E-06	2.21E-11	1.23E-09	1.81E-14	9.25E-13	5.40E-16
Y90	0.935	5.54E-03	6.85E+03	2.09E+05	3.80E+01	**1.16E+03** **(h)**	2.85E-02	**3.45E+01** **(h)**
Zn65†	0.590	3.50E-03	NR	NR	--	--	--	--
Zr93	0.020	1.16E-04	5.63E-03	1.32E-03	6.54E-07	1.53E-07	4.92E-10	4.56E-09
Zr95	0.855	5.07E-03	1.15E-09	3.02E-01	5.83E-12	1.53E-03	4.38E-15	4.55E-05
Sum=			**6.42E+06** **(i)**	**1.02E+06** **(j)**	**1.33E+05** **(k)**	**3.36E+03** **(l)**	1.00E+02	1.00E+02

--	Not calculated.
NR	Not Reported by sites (see Ref. CCA-2).
†	Data values for radionuclides were previously reported in Rev. 2 of TWBIR (Ref. BIR-2).
(a)	Data from Ref OR-1.
(b)	Radionuclide inventory information taken from Transuranic Waste Baseline Inventory Database (TWBID), Ref. CCA-2. (in total, 135 radionuclides are inventoried in the TWBID) Values correspond to a "WIPP-Scale" design basis.
(c)	Data calculated from the equation;

$$\text{Heat Load} = TOTAL\ ACTIVITY(Ci)\frac{3.7E+10(dis/sec)}{Ci}\ ENERGY(MeV/dis)\ \frac{E+06\,eV}{MeV}\ \frac{1.60219E-19\,J}{eV}\ \frac{watt-sec}{J}$$

$$\text{Heat Load (watts)} = 0.005928103 \times TOTAL\ ACTIVITY(Ci) \times ENERGY(MeV/dis)$$

(e)	Isotope with dominate curie load for CH-TRU wastes.
(f)	Isotope with dominate curie load for RH-TRU wastes.
(g)	Isotope with dominate heat load for CH-TRU wastes.
(h)	Isotope with dominate heat load for RH-TRU wastes.
(i)	Note, the total CH-TRU curie load is 6.42 MCi (also, 86.3 % of the total curie load in WIPP). The average CH-TRU volumetric total curie load is 6.42E+06/5.95E+06 = 1.079 (Ci/cu. ft.) = **38.10 (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume. The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values applicable to expected waste at WIPP (See Ref. BIR-2d).]
(j)	Note, the total RH-TRU curie load is only 1.02 MCi (also, 13.7 % of the total curie load in WIPP). This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1]. The average RH-TRU volumetric total curie load is 1.02E+06/0.25E+06 = 4.08 (Ci/cu. ft.) = **144.1 (Ci/cu. m.)**. [See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft.]

(k) Note, the total CH-TRU heat load is only **133. kW** (also, 97.5 % of the total heat load in WIPP). The ratio for CH-TRU of total heat load to total curie load is 133.E+03/6.42E+06 = **0.0207 W/Ci**. The average CH-TRU volumetric heat load is 133.E+03/5.95E+06 = 0.0224 (W/cu. ft.) = 0.7894 (W/cu. m.). The average CH-TRU drum heat load is 0.7894 (W/cu. m.)x 0.2082 (cu. m.) = **0.1644 W**. [The volume of a CH-TRU drum was set equal to the nominal volume of a 55-gal drum.]

(l) Note, the total RH-TRU heat load is only **3.36 kW** (also, 2.5 % of the total heat load in WIPP). The ratio for RH-TRU of total heat load to total curie load is 3.36E+03/1.02E+06 = **0.003294 W/Ci**. The average RH-TRU volumetric heat load is 3.36E+03/0.25E+06 = 0.0134 (W/cu. ft.) = 0.47 (W/cu. m.). The average RH-TRU canister heat load is 0.47 (W/cu. m.)x 0.6246 (cu. m.) = **0.2964 W** (this is about two times that of an average CH-TRU drum). [The volume of a RH-TRU canister was set equal to three times the nominal volume of a 55-gal drum. Even though the reported volume of a RH-TRU canister is 0.89 cu. m. (Ref. BIR-2e), these canisters are loaded with three 55-gal drums internally. Ref. DOE-1.]

Title 40 CFR Part 191
Compliance Certification Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.3

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WPO 35202

NFORMATION ONL

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 3/15/96

to: Christine T. Stockman, MS-1328

J W Garner

from: James W. Garner, MS-1328

subject: Radioisotopes to be used in the 1996 CCA Calculations

The following 29 isotopes are the ones of interest from the BIR Report. They are as follows:

^{241}Am, ^{243}Am, ^{252}Cf, ^{243}Cm, ^{244}Cm, ^{245}Cm, ^{248}Cm, ^{137}Cs, ^{237}Np, ^{231}Pa, ^{210}Pb, ^{147}Pm, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{244}Pu, ^{226}Ra, ^{228}Ra, ^{90}Sr, ^{229}Th, ^{230}Th, ^{232}Th, ^{233}U, ^{234}U, ^{235}U, ^{236}U, and ^{238}U. ^{14}C is not included because of its small inventory and a large inventory of other forms of carbon.

There were chosen for their inventory content and CFR191 importance values.
All of these isotopes can be used in the codes that evaluate the direct releases from Cuttings, Spalling, and Blowout.

For the codes that compute the indirect releases (i.e., NUTS, CCDFGF and SECOTP), we need a shorter list in order to maintain a reasonable calculation burden.

^{241}Am, ^{243}Am, ^{245}Cm, ^{137}Cs, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{242}Pu, ^{226}Ra, ^{90}Sr, ^{229}Th, ^{230}Th, ^{232}Th, ^{233}U, ^{234}U, ^{235}U, ^{236}U, and ^{238}U are selected because they all have an EPA normalized release greater than .01. This is still a large (19) number of isotopes to transport.

To further reduce the number of isotopes to transport, let us look at uranium. From a EPA normalized perspective, ^{233}U and ^{234}U are a factor of $10^{1.5}$ to 10^{2} higher than the other uranium isotopes. We could drop ^{235}U, ^{236}U, and ^{238}U without any impact on the final EPA normalized release. Since the inventory in moles of ^{233}U and ^{234}U is less than one percent of the uranium inventory, we can reduce the solubility of uranium by a factor of 100. Furthermore, we can combine ^{233}U and ^{234}U into ^{234}U, since their half-lives are similar. Likewise, with thorium we can combine ^{229}Th and ^{230}Th into ^{230}Th and reduce the solubility by a factor of 1000 and drop ^{232}Th. With plutonium, we can combine ^{239}Pu, ^{240}Pu, and ^{242}Pu into ^{239}Pu and we can also combine ^{90}Sr and ^{137}Cs into ^{90}Sr because of similar half-lives and transport properties.

This will leave us with the following ten isotopes:
^{241}Am, ^{243}Am, ^{245}Cm, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{226}Ra, ^{90}Sr, ^{230}Th, ^{234}U.
At late times, we can drop ^{90}Sr and ^{238}Pu because of their short half-lives.

To define late times for ^{90}Sr, we can look at the plots and determine when the EPA releases drop below .1. This is about 300 years. For ^{238}Pu, we can define late times as when the ratio of ^{238}Pu to ^{239}Pu is less than .01. This is about 800 years.

We can rank these isotopes in order of EPA normalized release.

all times:

1) ^{239}Pu releases from 2000 to 1000
2) ^{241}Am releases from 1000 to .1
3) ^{234}U releases from 7 to 8
4) ^{230}Th releases from .06 to 5.0
5) ^{237}Np releases from .1 to .3
6) ^{245}Cm releases from .2 to .1
7) ^{226}Ra releases from .02 to .2
8) ^{243}Am releases from .06 to .025

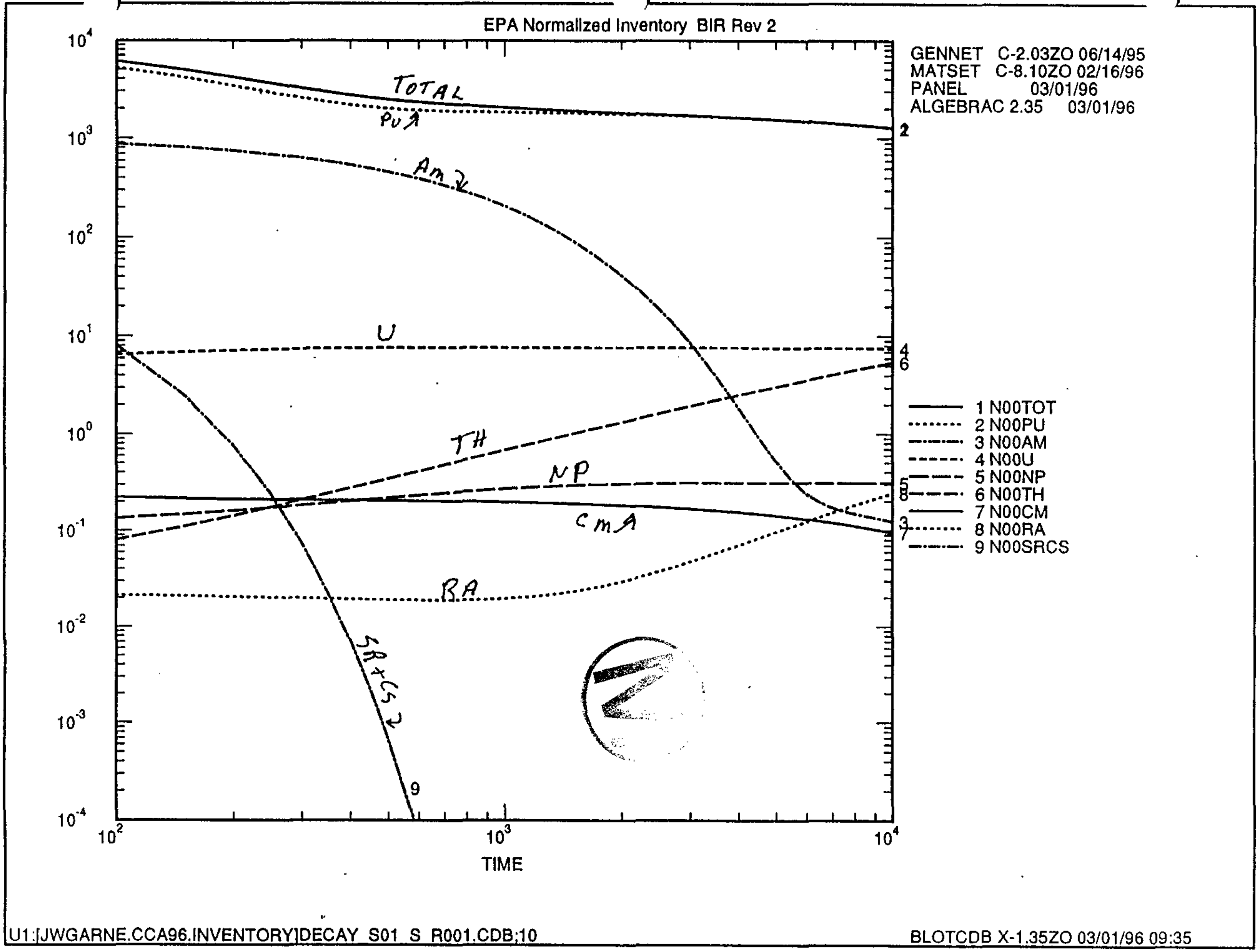
early times only:

1) ^{238}Pu from 3000 to 100@800yr
2) ^{90}Sr from 8 to .07@300 yr

It then appears that we only need to transport ^{239}Pu, ^{241}Am, ^{234}U, and ^{230}Th. Any realizations that are close to the regulatory limit can be re-computed with the ten isotopes listed above. This scheme can be verified by a duplicate run using the 19 isotopes listed above.

If a further reduction in the number of radioisotopes in needed to reduce calculation time, we could also eliminate ^{234}U and ^{230}Th. This elimination should only be done as a last resort.

cc:
MS-1320 Richard V. Bynum
MS-1320 E. James Novak
MS-1328 Mert E. Fewell
MS-1328 Jon C. Helton
MS-1328 James L. Ramsey
MS-1328 Ali A. Shinta
MS-1335 Margaret S. Y. Chu
MS-1341 Larry H. Brush
MS-1343 Ruth F. Weiner
MS-1395 Mel G. Marietta
...
SWCF-A: 1.2.07.4.1: PA: QA: CCA: Radionuclide Source Term (2 copies)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MATSET C-8.10ZO 02/16/96
PANEL 03/01/96
ALGEBRAC 2.35 03/01/96
10^4
10^3
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^2
10^3
10^4
TIME
TOTAL
Pu
Am
U
TH
NP
CmA
RA
SR+CS
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2
4
6
5
8
3
7
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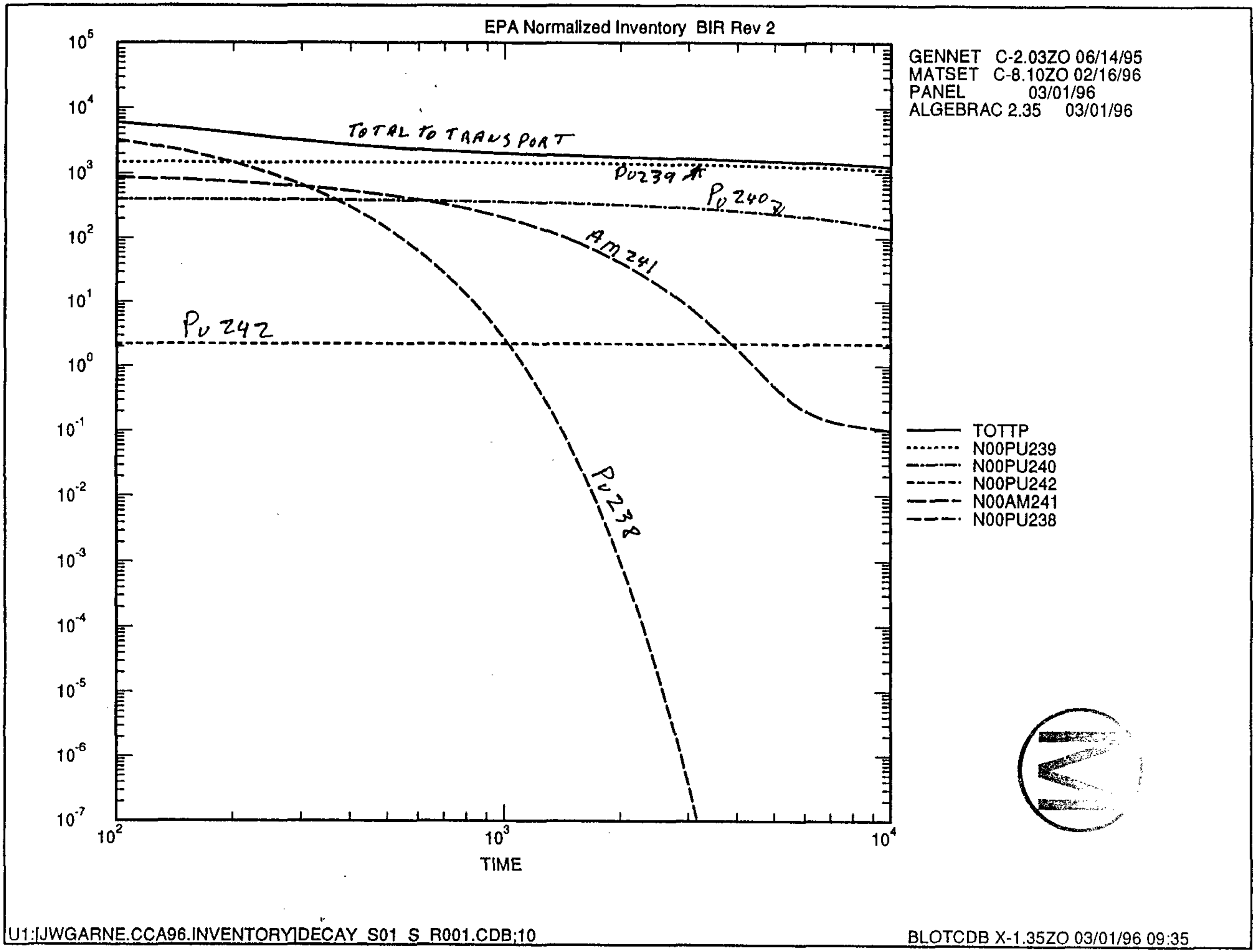
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PANEL 03/01/96
ALGEBRAC 2.35 03/01/96
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Pu 240
Am 241
Pu 242
Pu 238
TOTTP
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N00PU240
N00PU242
N00AM241
N00PU238
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
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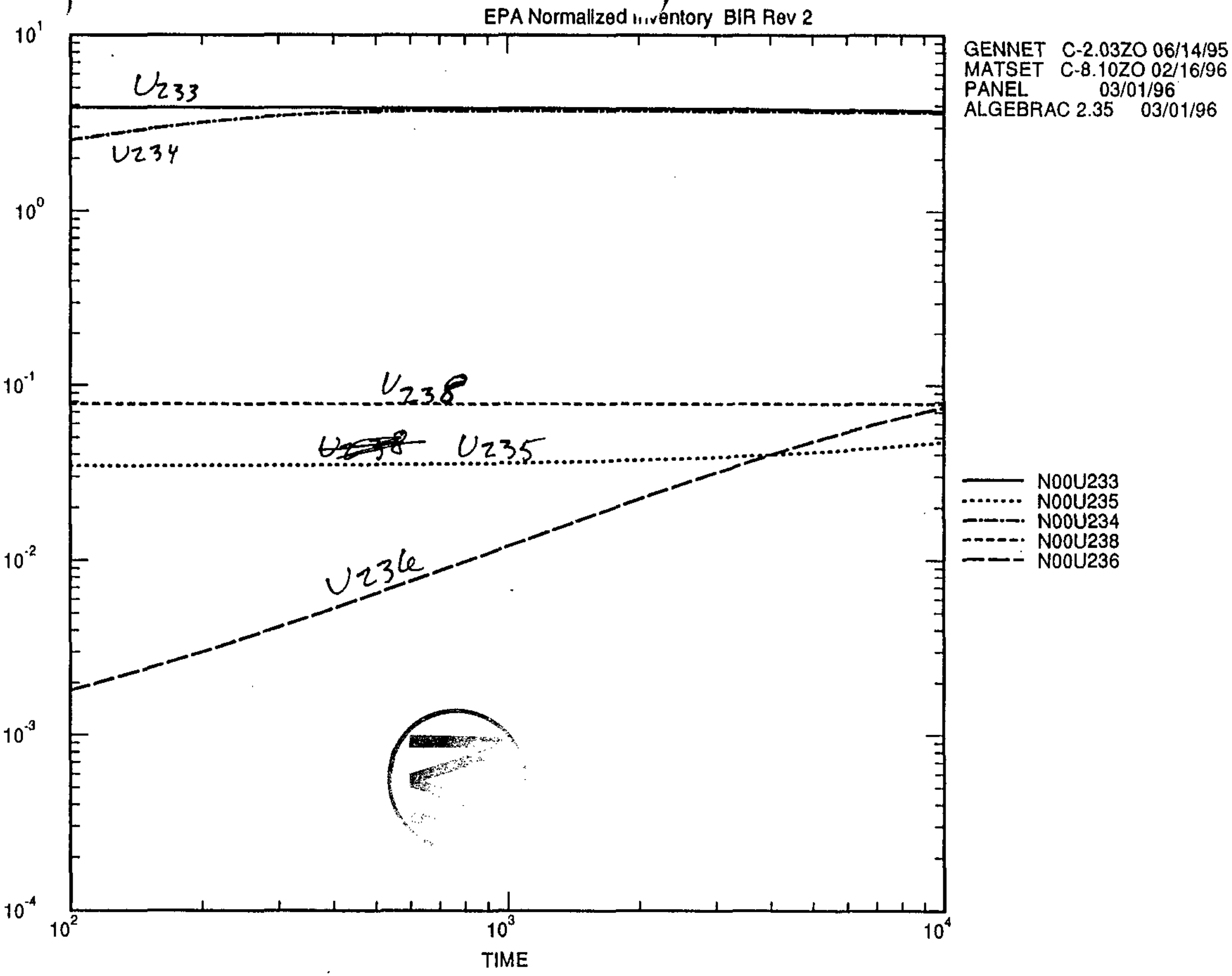

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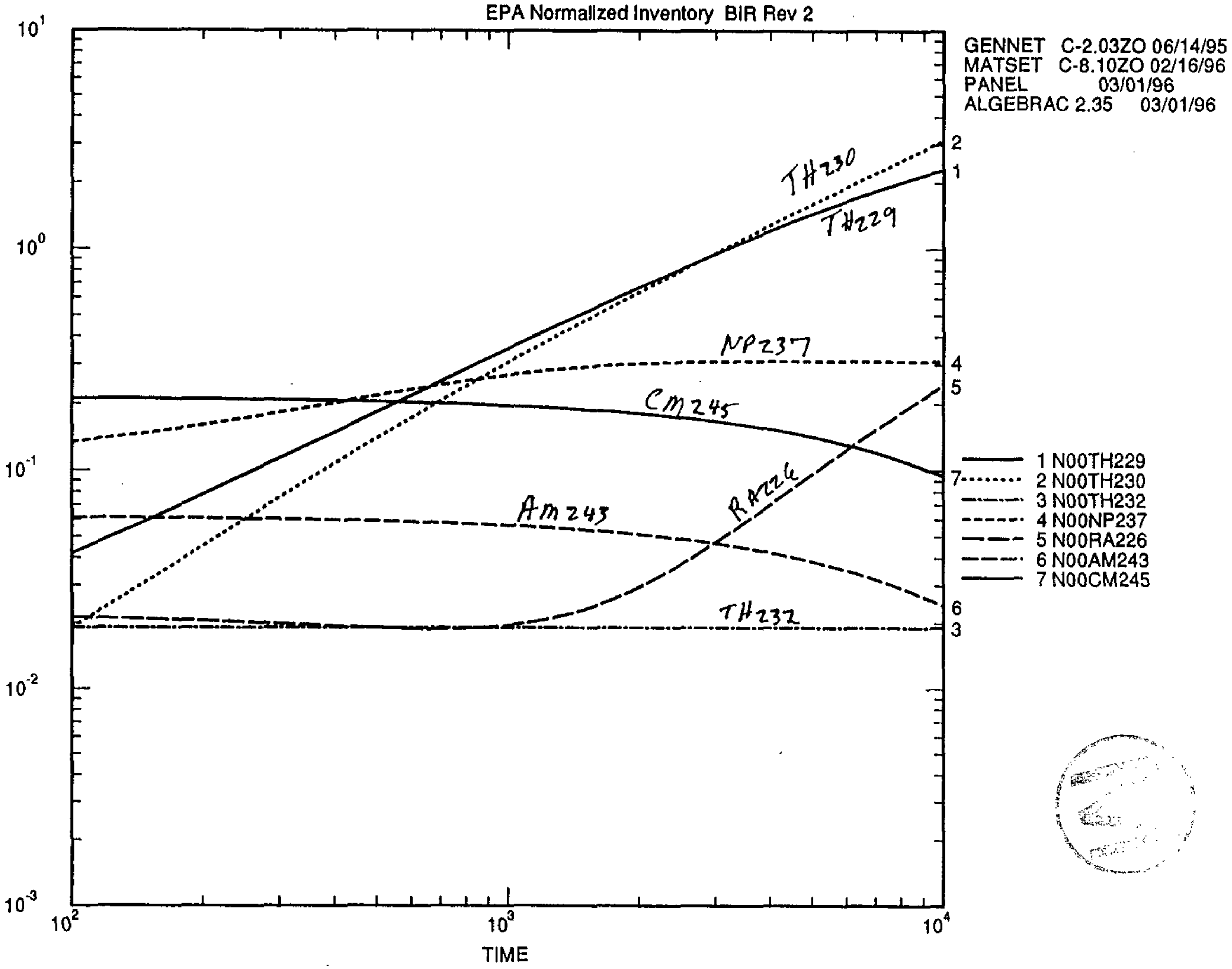

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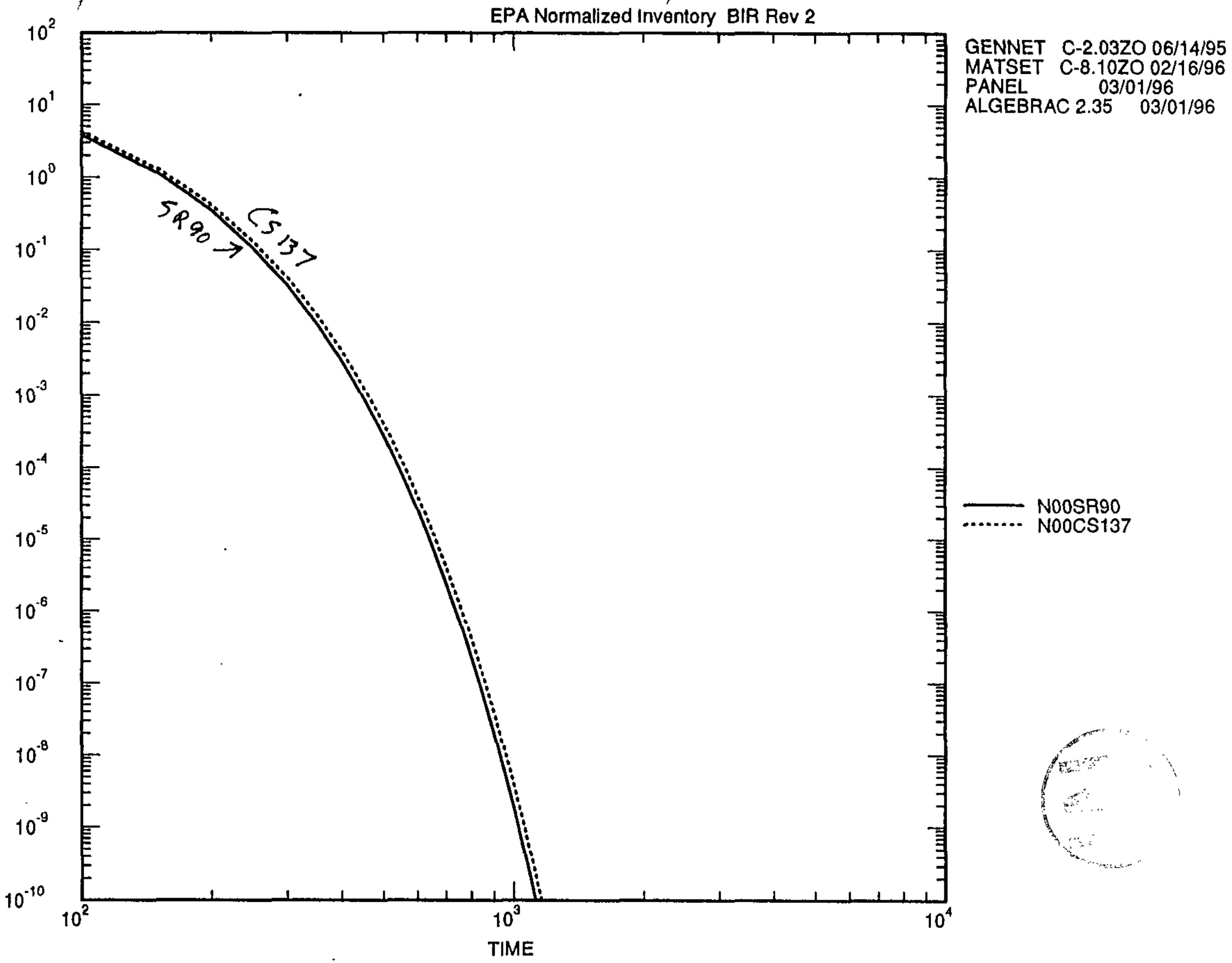

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MATSET C-8.10ZO 02/16/96
PANEL 03/01/96
ALGEBRAC 2.35 03/01/96

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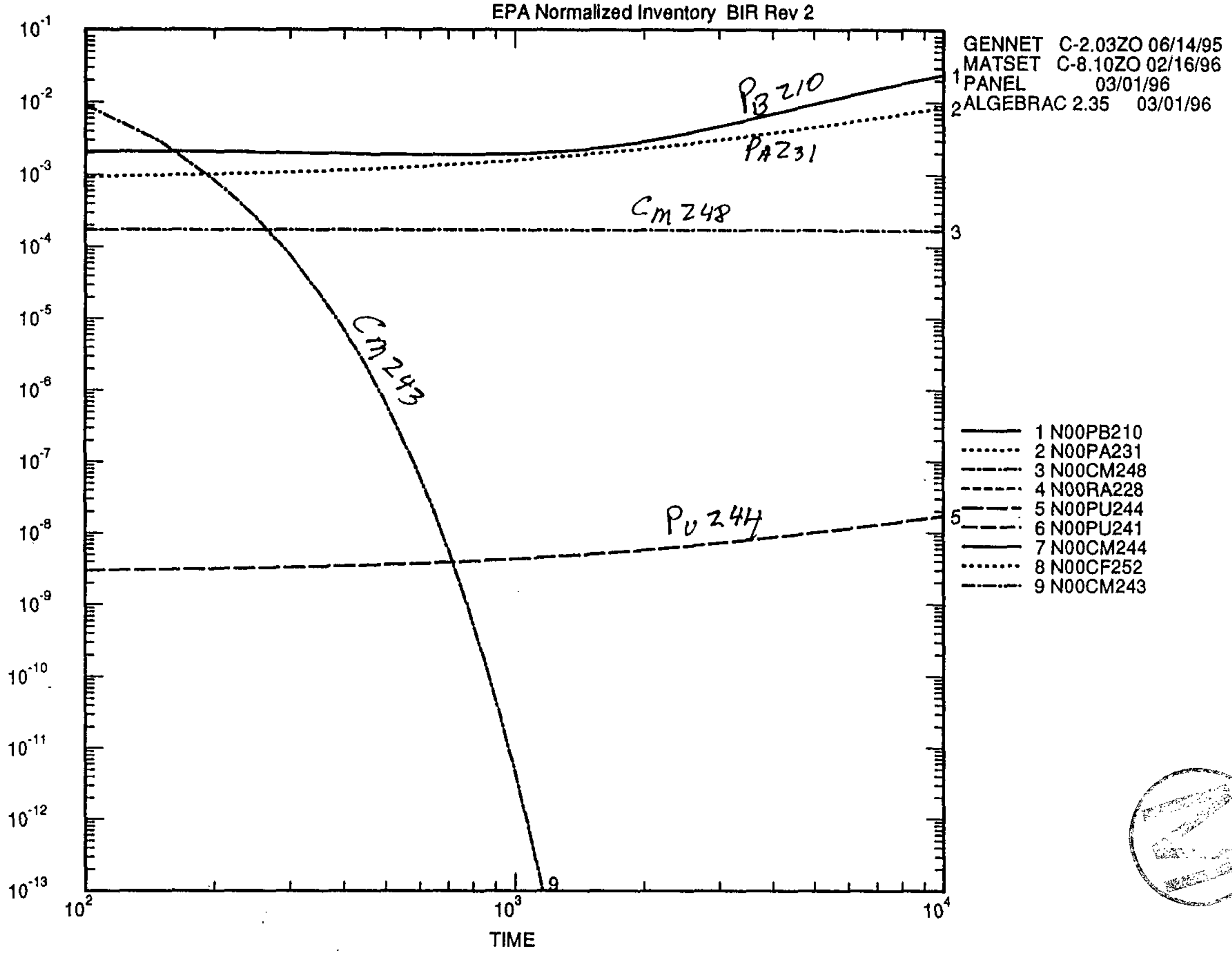

EPA Normalized Inventory BIR Rev 2

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MATSET C-8.10ZO 02/16/96
PANEL 03/01/96
ALGEBRAC 2.35 03/01/96

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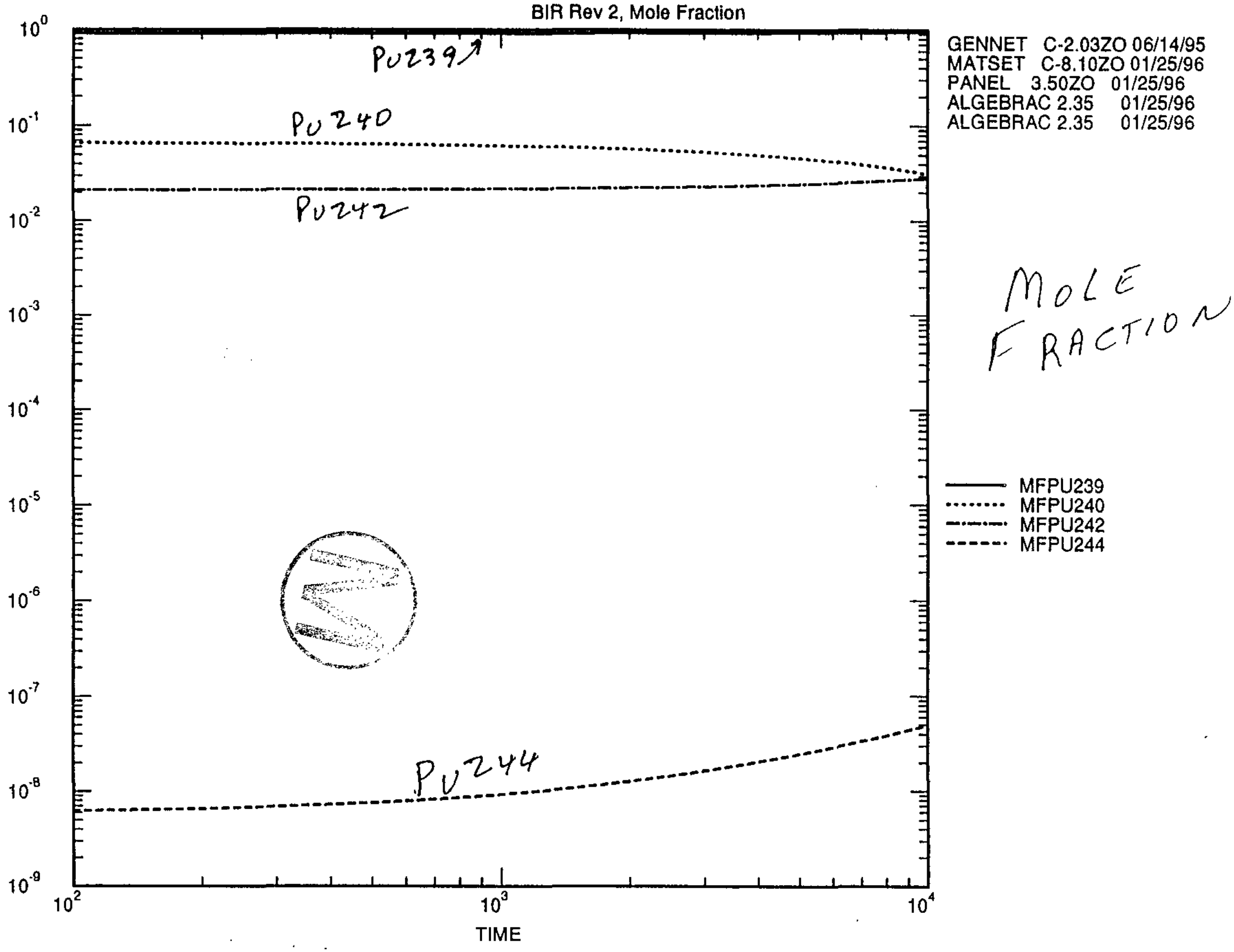

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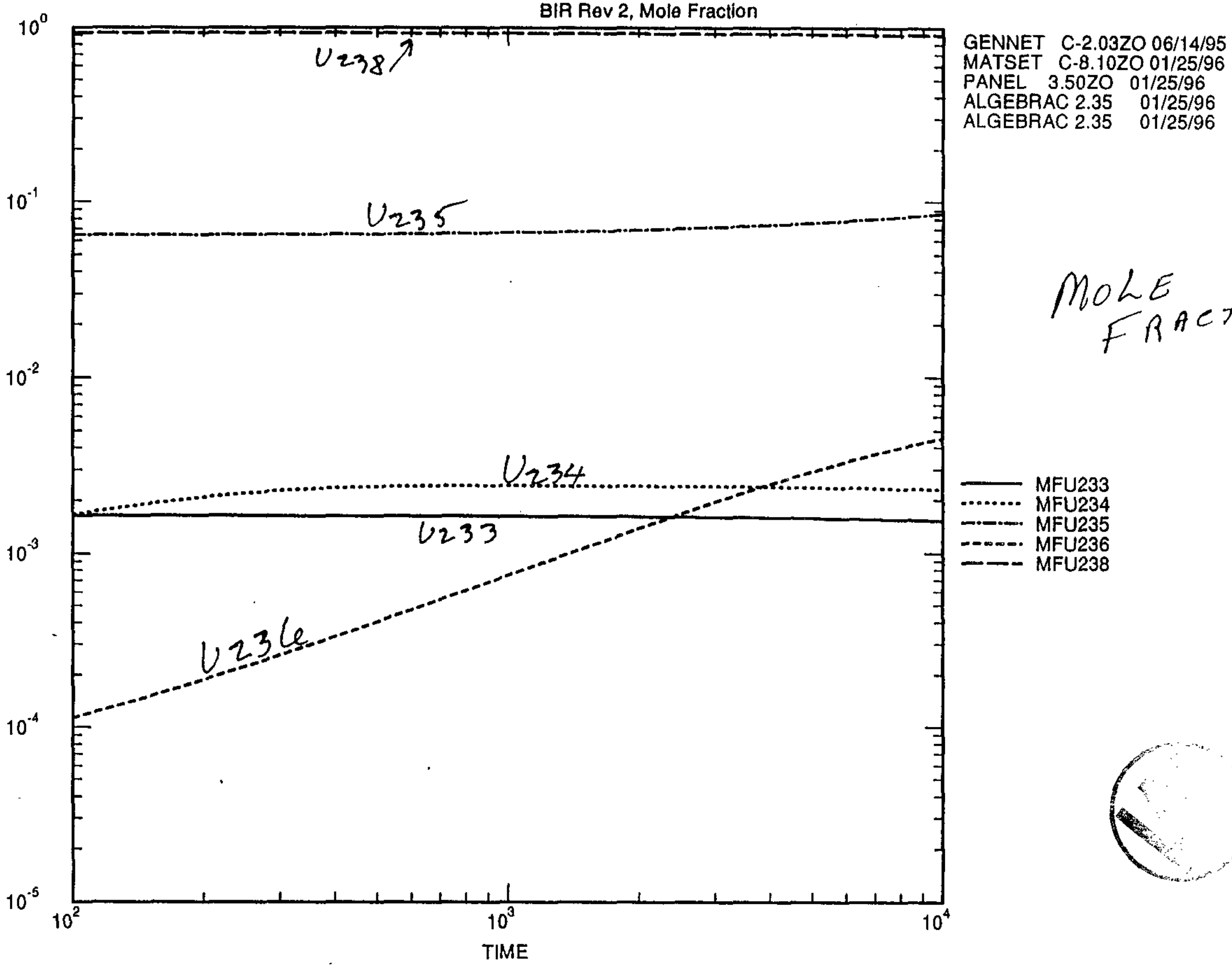

BIR Rev 2, Mole Fraction

MOLE FRACTION

U1:[JWGARNE.CCA96.INVENTORY.TRY]DECAY_S01_S_R001.CDB;4

BLOTCDB X-1.35ZO 01/25/96 14:52

BIR Rev 2, Mole Fraction

GENNET C-2.03ZO 06/14/95
MATSET C-8.10ZO 01/25/96
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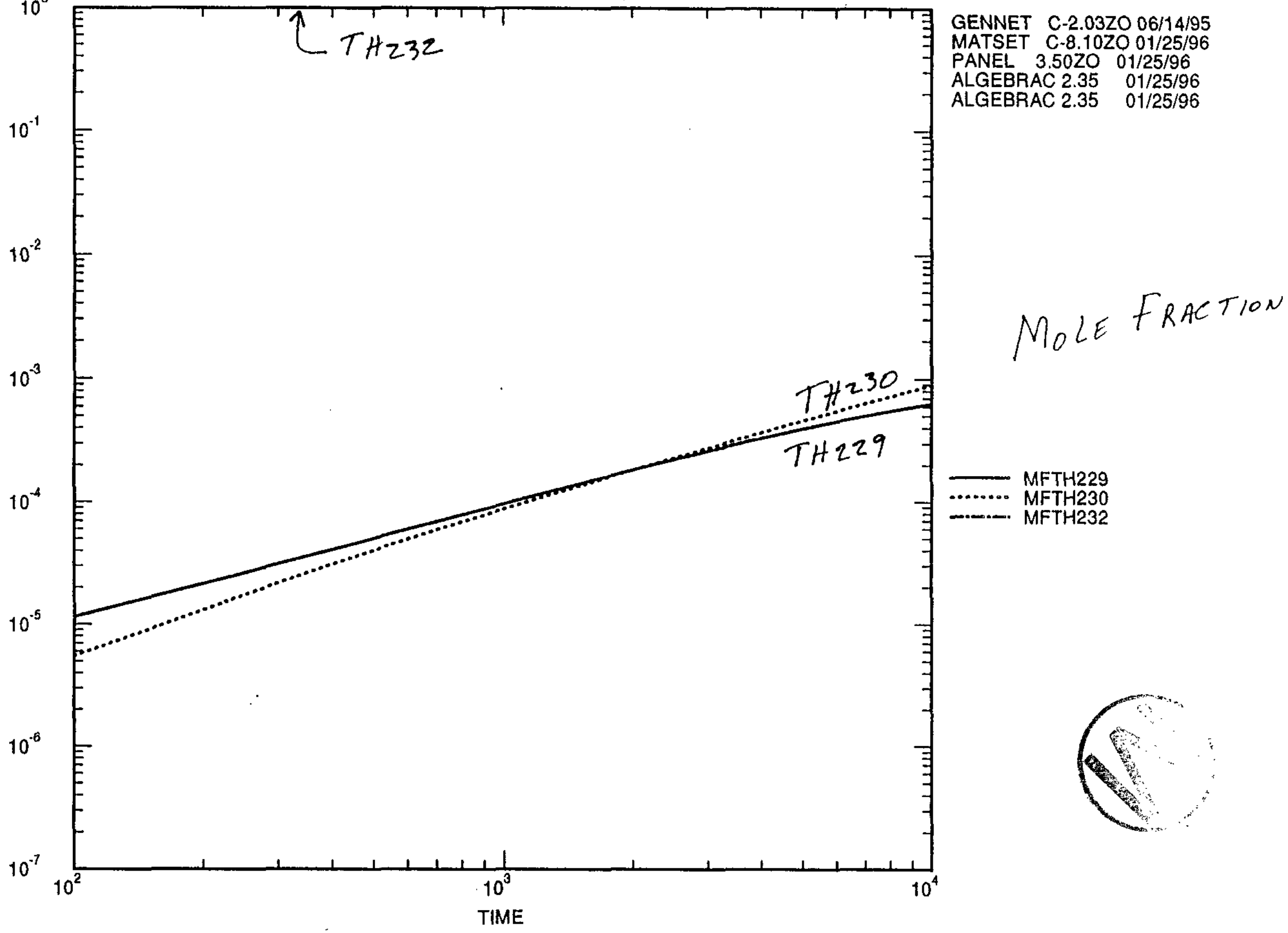
ALGEBRAC 2.35 01/25/96



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Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

WCA Attachment WCA.8.4

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Sandia National Laboratories
Albuquerque, New Mexico 87185

date: 29 March 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters

This memorandum summarizes best estimates for the mobile colloidal actinide source term for input to the WIPP Compliance Certification Application. The use of material and parameter identification codes is consistent with your letter to me dated 29 March 1996 requesting parameter values. In the attached table, I have provided best estimates for the following material-parameter combinations:

IDMTRL: Th, U, Np, Pu, Am

IDPRAM:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids
	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
	CAPHUM	maximum concentration of actinide associated with mobile humic colloids
	CAPMIC	maximum concentration of actinide associated with mobile microbes
	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids
	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes

As a first approximation, the colloidal behavior of curium can be simulated be using parameter values for americium. The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CONCMIN	Th	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
CONCMIN	U	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
CONCMIN	Np	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
CONCMIN	Pu	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
CONCMIN	Am	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	
CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
PROPHUM	Th	6.4e+00	6.4e+00	6.4e+00	moles colloidal humic-bound Th per moles dissolved Th	constant	2,3
PROPHUM	U	1.4e+00	1.6e-01	2.0e+00	moles colloidal humic-bound U per moles dissolved U	triangular	2,3,4
PROPHUM	Np	4.0e+00	4.0e+00	4.0e+00	moles colloidal humic-bound Np per moles dissolved Np	constant	2,3
PROPHUM	Pu	5.9e+00	5.9e+00	5.9e+00	moles colloidal humic-bound Pu per moles dissolved Pu	constant	2,3
PROPHUM	Am	2.5e+00	1.9e-01	3.9e+00	moles colloidal humic-bound Am per moles dissolved Am	triangular	2,3,4

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.5

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WPO # 35852

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 7 May 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Parameter Record Package for Colloidal Actinide Source Term Parameters

Attached is the Parameter Record Package for the WIPP PA parameters describing actinide concentrations associated with mobile **actinide intrinsic colloids**. This Package is one of four describing the concentration of actinides associated with the four colloidal particle types. The complete set of Packages consists of the following:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy with Attachments to:

MS 1320	Hans W. Papenguth, 6748
MS 1320	W. George Perkins, 6748
DOE/CAO	Robert A. Stroud

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.
SWCF-A:WPO#35852: Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids

copy without Attachments to:

MS 1320	E. James Nowak, 6831
MS 1324	Susan A. Howarth, 6115
MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1328	Mary-Alena Martell, 6749
MS 1341	John T. Holmes, 6748

Parameter Record Package for Mobile-Colloidal Actinide Source Term.
Part 2. Actinide Intrinsic Colloids

The parameter values in this package are based on data which were collected under the guidance of the Principal Investigator for the Waste Isolation Pilot Plant (WIPP) Colloid Research Program, Hans W. Papenguth, for input to the WIPP Data Entry Form and for use in WIPP Performance Assessment (PA) calculations.

I. *Parameter No. (id):* Not applicable.

II. *Data/Parameter:* Not applicable.

III. *Parameter id (idpram):* CONCINT.

IV. *Material:* Intrinsic colloids of actinides Th, U, Np, Pu, and Am.

V. *Material Identification (idmtrl):* Th, U, Np, Pu, and Am.

VI. *Units:* Concentrations of actinide intrinsic colloids (CONCINT) are in units of "moles colloidal actinide per liter of dispersion."

VII. *Distribution Information.*

  A. *Category:* The development of parameter values and their distributions is described in Attachment A. Summaries of the parameter values are presented in Attachments C, E, and F. Constant CONCINT values are supplied for all five actinide elements listed above.

  B. *Mean:* See Attachments A, C, E, and F.

  C. *Median:* Not applicable.

  D. *Standard Deviation:* Not applicable.

  E. *Maximum:* See Attachments A, C, E, and F.

  F. *Minimum:* See Attachments A, C, E, and F.

  G. *Number of data points:* Not applicable.

VIII. *Data Collection and Interpretation Information.*

  A. *Data Source Information:* WIPP observational data and literature.

  B. *Data Collection (for WIPP observational data).*

    1. *Data Collection or Test Method:* Experiments were conducted at Lawrence Livermore National Laboratory (LLNL; contract number AG-4965; Cynthia E. A. Palmer, LLNL PI). Descriptions of experiments conducted at LLNL are included in Attachment A.

    2. *Assumptions Made During Testing:* See Attachment A.

3. *Standard Error of Measurement of Tests Performed:* See Attachment A.

4. *Form of Raw Data:* Data on actinide concentration associated with actinide intrinsic colloids is reported in molarity.

5. *References Related to Data Collection:* See Attachment A.

6. *QA Status of Data:*

   a. *Are all of the data qualified?* Yes.

   b. *Were data qualified by QAP 20-3?* No. Data packages will be submitted for work conducted at LLNL (see VIII,B,1 above for contract numbers), under File code WBS 1.1.10.2.1.

   c. *Were the data the subject of audit/surveillance by SNL or DOE?* Yes. LLNL (contract number AG-4965) was audited twice by SNL (94-04; EA95-13). DOE/CAO conducted a surveillance (S-96-08). LLNL is scheduled to be audited by SNL (EA96-22) in May 1996.

   d. *Were the data collected under an SNL approved QA program?* Yes. Data were collected under SNL WIPP QAPD, Rev. P, effective October 1, 1992, and SNL WIPP QAPD, Rev. R, effective July 31, 1995. LLNL conducted work under an approved QAPP prepared especially for their program (WIPP Actinide Source Term Test Program Quality Assurance Program Plan (LLNL WIPP-LLNL-NCD-ETG-CS-QAPP, Rev. 0-CN1). Data were collected under a test plan for the WIPP Colloid Research Program (Papenguth and Behl, 1996). Detailed descriptions of the experiments and interpretation listed herein will be published in a SAND report. Documents related to data collection at LLNL will be archived in the Sandia WIPP Central Files (SWCF; File code WBS 1.1.10.2.1).

C. *Interpretation of Data.*

1. *Was the interpretation made by reference to previous work.* No.

2. *Was the interpretation made by using newly performed calculations?* Yes.

3. *Form of Interpreted Data.* List of interpreted values.

4. *Assumptions Made During Interpretation.* See Attachment A.

5. *Name of Code(s)/Software used to Interpret Data:* Not applicable.

6. *QA Status of Code(s) used to Interpret Data:* Not applicable.

   a. *Was the code qualified under QAP 19-1?* Not applicable.

   b. *Was the code qualified under QAP 9-1?* Not applicable.

7. *References Related to Data Interpretation:* See XI below and Attachment A.

8. *For interpretations made by using a newly performed calculations provide documentation that you followed the requirements of QAP 9-1 Appendix B.* The data analysis is controlled by Analysis Plan for the Colloid Research Program, AP-004 (Behl and Papenguth, 1996).

9. *For routine calculations (not using code) did you follow requirements of QAP 9-5?* Yes.

IX. *Correlation with other Parameters:* None.

X. *Limitations or qualifications for usage of data by Performance Assessment (PA):* None.

XI. *References cited above:*

Behl, Y.K., and Papenguth, H.W., 1996, Analysis Plan for the WIPP Colloid Research Program WBS #1.1.10.2.1, SNL Analysis Plan AP-004.

Papenguth, H.W., and Behl, Y.K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

XII. *Attachments:*

Attachment A:	Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids.
Attachment B:	Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.
Attachment C:	Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.
Attachment D:	Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.
Attachment E:	Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.
Attachment F:	Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

XIII. *Distribution*

SWCF-A:WPO# 35852: Mobile-Colloidal Actinide Source Term. 2. Actinide Intrinsic Colloids.

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.

Attachment A:

Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids.

Attachment A.
Rationale for Definition of Parameter Values for Actinide Intrinsic Colloids

Hans W. Papenguth

Introduction

The actinide source term at the WIPP is defined as the sum of contributions from dissolved actinide species and mobile colloidal actinide species. The dissolved actinide source term has been defined elsewhere (Novak, 1996; Novak and Moore, 1996; Siegel, 1996). It is important to note that colloidal actinides which are not suspended in the aqueous phase (i.e., not mobile) are not included in the colloidal actinide source term. Colloidal actinides may become immobilized by several mechanisms, including precipitation followed by coagulation and gravitational settling (humic substances and actinide intrinsic colloids), adhesion to fixed substrates (microbes), and flocculation or coagulation of colloidal particles followed by gravitational settling (mineral fragments). Sorption of colloidal actinides onto fixed substrates will also reduce the mobile colloidal actinide source term, but no credit is currently being taken for reduction by that means.

To facilitate quantification of the colloidal actinide source term, as well as an efficient experimental approach, the source term has been divided into four components according to colloid types. On the basis of (1) the behavior of colloidal particles in high ionic strength electrolytes, (2) the way in which colloidal particles interact with actinide ions, and (3) the transport behaviors of colloidal particles, four colloidal particle types are recognized (Papenguth and Behl, 1996): mineral fragments, actinide intrinsic colloids, humic substances, and microbes.

In this document, we focus on the quantification of the actinide concentration mobilized by actinide intrinsic colloidal particles. In terms of the WIPP performance assessment (PA) calculations, we discuss the rationale for selecting the values corresponding to the following parameter designators:

idpram:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids.
idmtrl:	Th	thorium [i.e., Th(IV)];
	U	uranium [i.e., U(IV) and U(VI)];
	Np	neptunium [i.e., Np(IV) and Np(V)];
	Pu	plutonium [i.e., Pu(III) and Pu(IV)]; and
	Am	americium [i.e., Am(III)].

Actinide intrinsic colloids (also known as true colloids, real colloids, type I colloids, and Eigenkolloide) form by condensation reactions of hydrolyzed actinide ions and consist solely of actinide cations linked by anions. There are several stages in the development of actinide intrinsic colloids at which they have significantly different behaviors. When immature, actinide intrinsic colloids display physicochemical properties that are similar to ionized humic substances. With age, they become more similar to mineral-fragment type colloidal particles.

The experimental approach used was strongly influenced by reviews of published literature on actinide intrinsic colloids. Pertinent literature is discussed below (see also Papenguth and Behl, 1996).

Intrinsic Colloids of Plutonium

The most well-known and well-studied actinide intrinsic colloid is the Pu(IV) intrinsic colloid, which has been used as a basis of comparison for investigating intrinsic colloids of other actinides. Most of the knowledge about the Pu(IV) intrinsic colloid comes from research at high Pu concentrations in highly acidic solutions, which was conducted to help improve the efficiency of processing techniques. The Pu(IV) intrinsic colloid is notorious in its propensity to polymerize to form a gel-like material, which can even plug process lines.

A conclusive demonstration of the mechanisms of formation of the Pu(IV) intrinsic colloid has not yet been made, but there is a preponderance of evidence that suggests that polymerization is strongly linked to hydrolysis, and that the initial polymerization, or condensation, produces a macromolecule that becomes progressively more crystalline with time. The final mature colloid has a composition between $Pu(OH)_{4\ (amorphous)}$ and $PuO_{2\ (crystalline)}$, although the latter compound may be only partly crystalline and both may include interstitial water molecules.

The most convincing and consistent explanation for the chemistry of the Pu(IV) intrinsic colloid is presented by Johnson and Toth (1978) of Oak Ridge National Laboratory. Those authors developed a conceptual model to explain the solution chemistry of a variety of metal cations and a variety of oxidation states. The conceptual model involves processes referred to as "olation" and "oxolation" in which metal cations become bridged with hydroxyl groups, which in turn undergo irreversible elimination of water and concurrent formation of oxygen bridges. Johnson and Toth demonstrate that the model is consistent with the observed behavior of the Pu(IV) intrinsic colloid.

Hydrolysis reactions for metal cations such as plutonium may be written as follows:

first: $Pu^{4+}_{(aq)} + H_2O \leftrightarrow PuOH^{3+}_{(aq)} + H^+$ (1)

second: $PuOH^{3+}_{(aq)} + H_2O \leftrightarrow Pu(OH)^{2+}_{2\,(aq)} + H^+$ (2)

third: $Pu(OH)^{2+}_{2\,(aq)} + H_2O \leftrightarrow Pu(OH)^{+}_{3\,(aq)} + H^+$ (3)

fourth: $Pu(OH)^{+}_{3\,(aq)} + H_2O \leftrightarrow Pu(OH)^{0}_{4\,(aq)} + H^+$ (4)

Johnson and Toth point out, however, that in interpreting the formation of the Pu(IV) intrinsic colloid, it makes better sense to include the implied waters of hydration that surround metal cations in solution. Hydrolysis equations (1) through (4) can be rewritten as follows, where n equals 4:

first: $[Pu(H_2O)_m]^{n+} \leftrightarrow [Pu(OH)(H_2O)_{m-1}]^{n-1} + H^+$ (5)

second: $[Pu(H_2O)_{m-1}]^{n-1} \leftrightarrow [Pu(OH)(H_2O)_{m-2}]^{n-2} + H^+$ (6)

third: $[Pu(H_2O)_{m-2}]^{n-2} \leftrightarrow [Pu(OH)(H_2O)_{m-3}]^{n-3} + H^+$ (7)

fourth: $[Pu(H_2O)_{m-3}]^{n-3} \leftrightarrow [Pu(OH)(H_2O)_{m-4}]^{n-4} + H^+$ (8)

From the literature, it is clear that polymerization occurs nearly immediately after the first hydrolysis occurs (5). Johnson and Toth suggest the following reaction involving polymerization of two hydrolyzed species by loss of water (oxolation):

$$2\{[(H_2O)_{d-2}Pu(OH)(H_2O)]^{+(y-1)}\} \leftrightarrow$$
$$[(H_2O)_{d-2}Pu(OH)(OH)Pu(H_2O)_{d-2}]^{+2(y-1)} + 2H_2O \quad (9)$$

Aging or maturation of polymer then occurs by loss of water (olation) as follows:

$$Pu(OH)(OH)Pu(OH)(OH)Pu(OH)(OH)\cdots] \rightarrow [Pu(O)Pu(O)Pu(O)\cdots]_n + 3nH_2O \quad (10)$$

Maiti et al. (1989) and Laul et al. (1985) describe similar reactions, but it appears as though they believe that the third hydrolysis reaction occurs, because they use the $Pu(OH)^{+}_{3\,(aq)}$ ion in their proposed polymerization reaction. Use of that ion does not appear to be consistent with observations by many workers that polymerization occurs immediately after the first hydrolysis reaction.

As the actinide polyelectrolytes mature through the olation process to become closer in composition to an actinide-oxide mineral, they will be kinetically destabilized by the high ionic strengths of the WIPP brines, and will not be mobile. Further, the solubilities of the mature solid phase cannot be exceeded. In fairly long-term experiments, Nitsche et al. (1992, 1994) showed that the concentration of Pu(IV) intrinsic colloid stabilized at about 10^{-8} M. It is not known whether the form was Pu(IV) polyelectrolyte or Pu(IV) mineral fragment type colloid.

Intrinsic Colloids of other Actinides

Reference is made to a variety of intrinsic colloids of other actinides, but no systematic investigations of their formation and behaviors appear to have been made. Plutonium is apparently unique in its propensity to form an intrinsic colloid. No mention is made in the literature of maturation of polyelectrolytes of other actinides to form mineral fragment type colloidal particles as plutonium does.

In general, the tendency of actinides to hydrolyze and to polymerize to form intrinsic colloids follows the order:

$$An^{4+} >> An(VI)O_2^{2+} > An^{3+} > An(V)O_2^{+} \qquad (11)$$

where An represents an actinide element (Cleveland, 1979a,b; Choppin, 1983; Kim, 1992; Lieser et al., 1991, p. 119). The order of oxidation states in the equation above results from the ionic charge to ionic radius ratios. The tendency for hydrolysis of $An(VI)O_2^{2+}$ is greater than for An^{3+} because the effective charge on the central cation on the linear $[O\text{-}An\text{-}O]^{2+}$ ion is 3.3±0.1, slightly greater than 3. This trend generally holds true for the actinide elements in general, because of the very small changes in ionic radii among the actinide elements (this is the oxidation state analogy; refer to Novak, 1996). There are differences in the behaviors of the actinides from element to element that stem from very subtle changes in the charge to radius ratio and the nature of the configuration of the f molecular orbital.

Considering Pu as an example, hydrolysis becomes significant for Pu^{4+}, $Pu(VI)O_2^{2+}$, Pu^{3+}, and $Pu(V)O_2^{+}$ at pH values of <1, 4-5, 6-8, and 9-10, respectively (Choppin, 1983). On the basis of the hydrolysis trend, it is not likely that An(III) and An(V) actinides will form actinide intrinsic colloids. That group includes Pu^{3+}, Am^{3+}, $Pu(V)O_2^{+}$, and $Np(V)O_2^{+}$. There are suggestions in the literature, however, that Am^{3+} may form an intrinsic colloid, which is surprising because it does not undergo hydrolysis until relatively high pH values. Thorium does not follow the trend described by equation (11) because its large size makes it resistant to hydrolysis (Cotton and Wilkinson, 1988). Nevertheless, thermodynamic data suggest that in almost all environments (near neutral or higher pH) thorium exists as $Th(OH)^{0}_{4(aq)}$. Moreover, thorium has been reported to form a polymer (Kraus, 1956; Johnson and Toth, 1978), although as discussed below, should be referred to as an oligomer.

Examples can be found in the literature of polymeric species of many of the actinides of importance to WIPP (see e.g., Baes and Mesmer, 1976; Kim, 1992). It is important, however, to note the sizes of polymers described in the literature. It is well known that as polyvalent metals, the actinides can form polynuclear species, but they are largely lower polymers (i.e., oligomers) such as dimers, trimers, tetramers, and hexamers (see, e.g., Choppin, 1983, p. 46). However, in terms of physical transport behavior, lower polymers will behave no differently than dissolved monomeric species. In contrast, the higher polymers, such as the Pu(IV)-polymer, may reach colloidal sizes (1 nm to 1 μm) and will have different hydrodynamic properties than the sub-colloidal-sized dissolved species. Johnson and Toth (1978) reported a molecular weight of 4000 for a Th polymer. Assuming that it consisted of $Th(OH)_4$, that polymer would consist of about 13 thorium metal ions (i.e., the degree of polymerization number, N). That observation is consistent with Kraus (1956), in which he quotes an N value of about 9 for Th polyelectrolyte.

Empirical evidence published in the literature does not always support the suggestion that Am, as a trivalent cation, will form an intrinsic colloidal particle. Avogadro and de Marsily (1984) suggested that, like Pu, Am is a likely candidate to form an insoluble hydroxide. Buckau et al. (1986) reported the formation of Am(III) intrinsic colloids at near neutral pH conditions, with a particle size greater than 1 nm. In their study of the hydrolysis of Am(III) over a pH range from 3 to 13.5, however, Kim et al. (1984a) found only monomers of Am. Regardless of whether Am(III) intrinsic colloids will form under highly idealized laboratory environments, it would be highly unlikely that they would form in a geologic system, because of the tremendously strong sorption properties of the Am(III) ion.

Experimental

Because of the absence of conclusive evidence in the literature that intrinsic colloids of Th, U, Np, and Am develop to sizes large enough to affect transport behavior, the focus of the experimental program was on Pu. A variety of screening experiments were conducted at Lawrence Livermore National Laboratory (LLNL; contract number AG-4965, Cynthia E. A. Palmer, LLNL PI) to test phenomena described in the published literature, under WIPP-relevant conditions:

- Critical coagulation concentration for mature Pu(IV) mineral fragment type colloid (refer to description of experiment AIC-1 in Papenguth and Behl, 1996);
- formation of Pu(IV) colloid, from oversaturation and undersaturation in the absence of carbon dioxide (AIC-8 and AIC-9, respectively);
- inhibition of Pu(IV) polymerization due to organic complexants (AIC-2);
- depolymerization of Pu-colloid due to organic complexants (AIC-2b);

- polyelectrolyte chain termination by non-actinide metal cations (AIC-4); and
- sorption effects of WIPP repository substrates on Pu(IV) colloid (AIC-5).

The last four experiments listed above provide evidence that, under some conditions at the WIPP, the Pu(IV)-colloid is less likely to form or is sorbed. To parameterize the WIPP PA calculations, however, the first two experiments listed above were used. Both sets of experiments (AIC-1, AIC-8/9) can essentially be viewed as solubility experiments. The critical coagulation experiments are solubility experiments conducted from undersaturation conditions, in which the in-growth of free Pu(IV) is observed (and are therefore equivalent to AIC-9). In both sets of experiments (AIC-1, AIC-8/9), the Pu solution concentration is measured as a function of time for as long as 5 weeks, as steady-state concentration is being reached. The two sets of experiments were anticipated to provide information to resolve the question of kinetic versus thermodynamic stability control on the formation and development of the Pu(IV) colloid. That question was not resolved, but the data still provide the necessary information for parameterizing the WIPP PA calculations. The values for the parameters submitted to PA were derived from the following experiments:

number	experiment	starting material	approx. pcH	[NaCl]	duration
AIC-1	c.c.c. (equivalent to undersaturation experiment AIC-9)	Pu(IV)-colloid; aged 1-month: ~2 x 10^{-4} M	4 7 10	0.001 m 0.01 m 0.1 m 0.8 m 3.0 m 5.0 m	3 to 5 weeks
AIC-8	oversaturation	Pu(IV) aquo ion: ~1 x 10^{-4} M	3 7 11	0.05 m 0.5 m 1.0 m 5.0 m	4 weeks

The data from those experiments are plotted in Figure 1 along with regression lines for data collected by Rai et al. (1980) for Pu(OH)$_4$ (amorphous) and PuO$_2$ and Rai and Swanson (1981) for Pu(IV)-polymer under acidic pH conditions. The current WIPP Project position is that MgO backfill will be added to control pCO$_2$. With MgO backfill, the pcH of the repository brine is expected to be about 9.3 (refer to Wang, 1996; also see Novak and Moore, 1996; Siegel, 1996). As shown in Figure 1, the regression line calculated from the LLNL data suggests that at a pcH of 9.3 the solubility of Pu(IV)-polymer is approximately 5 x 10^{-10} M. Because the extrapolated concentration is less than the minimum analytical detection limit (ADL) of 1 x 10^{-9} M, the ADL value was selected for use in WIPP PA calculations. The LLNL results are consistent with the extrapolated relationships based on published results of Rai et al. (1980) and Rai and Swanson (1981).

Interpreted Results

Parameter values (CONCINT) describing the amount of actinide element bound by actinide intrinsic colloidal particles were determined from the information described above. For the Pu(IV)-polymer, the minimum ADL was selected. In the absence of conclusive evidence that intrinsic colloids of other actinides form, or form polymers rather than oligomers, the concentration of Th-, U-, Np-, and Am-intrinsic colloids was set to zero.

Geochemical conditions in the Culebra are not conducive to the formation of a new supplementary population of actinide intrinsic colloids. In particular, the concentration of actinide ions is reduced. Therefore, the source term for actinide intrinsic colloids only reflects what would form in the WIPP repository.

Summary

Interpreted values for CONCINT are summarized in Attachments C, E, and F.

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Figure 1.

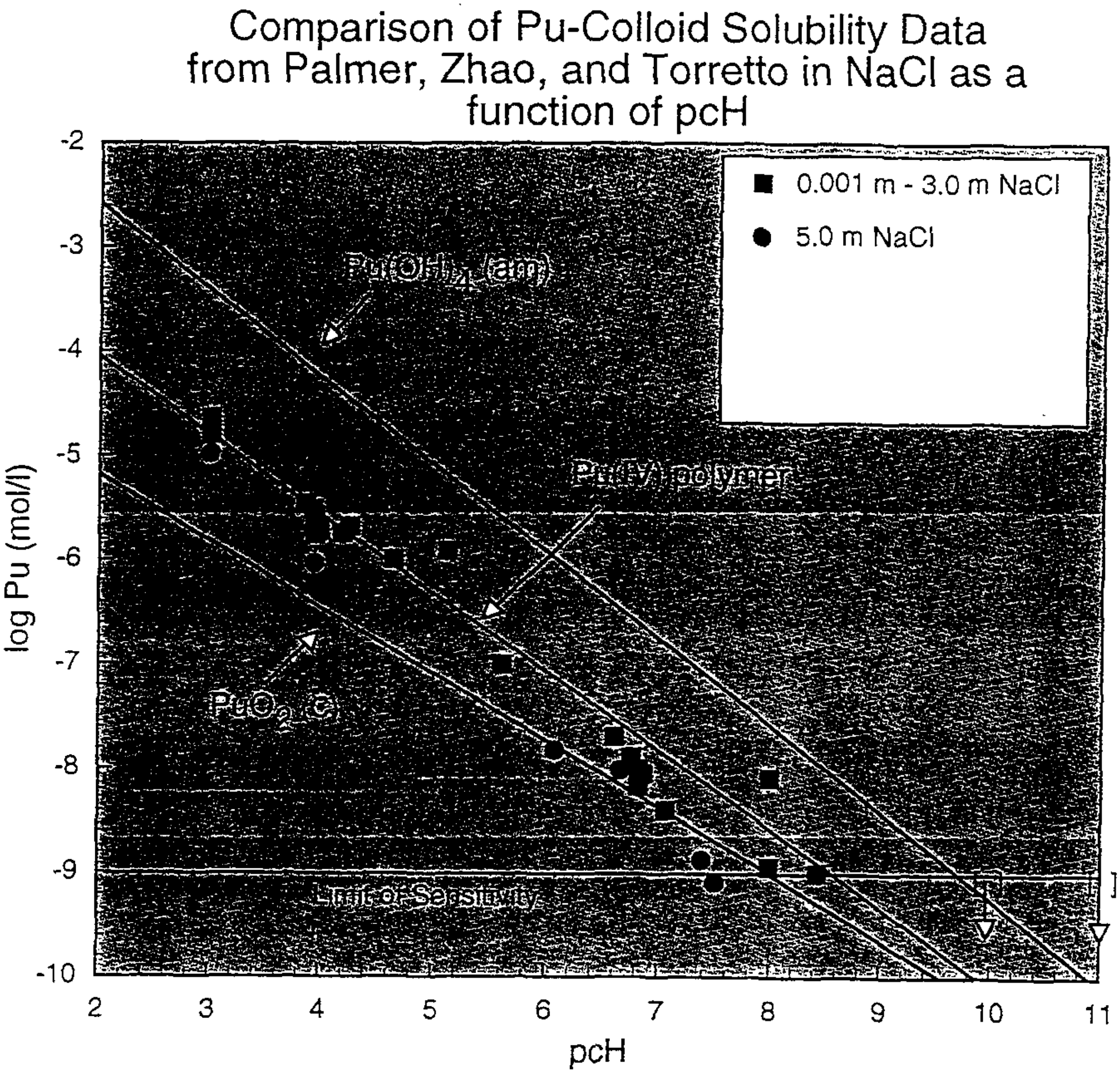

Figure 1: Solubility of Pu(IV)-polymer as a function of pcH+. Open brackets with arrows pointing down indicate that Pu concentration is below the Limit of Sensitivity. Note: Solubility lines for $Pu(OH)_4$ and PuO_2 are extrapolated from Rai, Serne, and Moore, *Soil Sci. Soc. Am. J.*, **44**, 490, (1980). Solubility line for Pu(IV) polymer is extrapolated from Rai and Swanson, *Nuc. Tech.*, **54**, 107, (1981)

Attachment B:

Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 3/29/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

In order to properly model the transport of radionuclides within the Salado formation, we will need information about the possible transport of these radionuclide on colloids. In this memo we request the maximum mobilized radionuclide concentration and/or the proportionality constant defining the moles mobilized on colloid per moles in solution, for each transported element and colloid type. We are planning to transport Am, Pu, U, and Th, and may also transport Cm, Np, Ra, and Sr. If we transport Ra and Sr, we are planning to model them as very soluble, and not sorbed, so I believe modeling of colloids for them will not be necessary. For Cm solubility, we will be using the Am(III) model. If you believe that Cm colloids also behave similarly to Am colloids, we could extend the chemical analogy to the colloid behavior. If you agree with these simplifications then we will need the parameters for Am, Pu, U, Th and Np only.

Suggested names for database entry:
IDMTRL: Am, Pu, U, Th, Np

IDPRAM:

CONCINT	for concentration of actinide on mobilized intrinsic colloid
CONCMIN	for concentration of actinide on mobilized mineral fragments
CAPHUM	for maximum concentration of actinide on humic colloids
CAPMIC	for maximum concentration of actinide on microbe colloids
PROPHUM	for moles actinide mobilized on humic colloids per moles dissolved
PROPMIC	for moles actinide mobilized on microbe colloids per moles dissolved

You will need to provide a distribution for each material-parameter pair, but that distribution may be "CONSTANT" for most of the numbers. Eight sampling slots have been reserved for the most important of these parameters that have non-constant distributions.

cc:
Mary-Alena Martell
Hong-Nian Jow
E. James Nowak
James L. Ramsey
Amy S. Johnson
Martin S. Tierney
W. George Perkins
J. T. Schneider
Richard V. Bynum
Ali A. Shinta
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment C:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Sandia National Laboratories
Albuquerque, New Mexico 87185

date: 29 March 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters

This memorandum summarizes best estimates for the mobile colloidal actinide source term for input to the WIPP Compliance Certification Application. The use of material and parameter identification codes is consistent with your letter to me dated 29 March 1996 requesting parameter values. In the attached table, I have provided best estimates for the following material-parameter combinations:

IDMTRL: Th, U, Np, Pu, Am

IDPRAM:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids
	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
	CAPHUM	maximum concentration of actinide associated with mobile humic colloids
	CAPMIC	maximum concentration of actinide associated with mobile microbes
	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids
	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes

As a first approximation, the colloidal behavior of curium can be simulated be using parameter values for americium. The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1320	E. James Nowak, 6831 EJN
MS 1320	R. Vann Bynum, 6831
MS 1341	John T. Holmes, 6748
MS 1341	Laurence H. Brush, 6748
MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748 wgp
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt O. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851

SWCF-A:WBS1.1.10.2.1

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CONCMIN	Th	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
CONCMIN	U	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
CONCMIN	Np	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
CONCMIN	Pu	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
CONCMIN	Am	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
PROPHUM	Th	6.4e+00	6.4e+00	6.4e+00	moles colloidal humic-bound Th per moles dissolved Th	constant	2,3
PROPHUM	U	1.4e+00	1.6e-01	2.0e+00	moles colloidal humic-bound U per moles dissolved U	triangular	2,3,4
PROPHUM	Np	4.0e+00	4.0e+00	4.0e+00	moles colloidal humic-bound Np per moles dissolved Np	constant	2,3
PROPHUM	Pu	5.9e+00	5.9e+00	5.9e+00	moles colloidal humic-bound Pu per moles dissolved Pu	constant	2,3
PROPHUM	Am	2.5e+00	1.9e-01	3.9e+00	moles colloidal humic-bound Am per moles dissolved Am	triangular	2,3,4

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CAPHUM	Th	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
CAPHUM	U	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
CAPHUM	Np	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
CAPHUM	Pu	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
CAPHUM	Am	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7
Notes:							
general	The colloidal actinide source term is added to the dissolved actinide source term.						
general	None of the parameters are correlated.						
1	If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.						
2	Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.						
3	Proportionality constants are to be used with the sum of actinide oxidation species for each actinide element (uncomplexed only, i.e., without organic ligand contribution).						
4	If a distribution is not used for humic-bound U or Am, use the maximum concentration as a constant value.						
5	The maximum ("cap") values are in units comparable to molarity rather than molality.						
6	CAPHUM is compared to the concentration of the respective humic-bound actinide element.						
7	CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e. the sum of dissolved plus colloidal actinide).						

Attachment D:

Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 4/2/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

YiFeng Wang has revised his recommendation to use 2 invariant points in the PA calculation. He now recommends that we use the $Mg(OH)_2 + MgCO_3$ invariant point for all calculations. If this invalidates the assumptions that you used to prepare colloid concentration or proportion parameters please indicate as soon as possible which parameters are affected, and as soon as possible after that provide a memo documenting the new values.

cc:
Mary-Alena Martell
Amy S. Johnson
Hong-Nian Jow
Martin S. Tierney
J. T. Schneider
Richard V. Bynum
E. James Nowak
W. George Perkins
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment E:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 18 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 1

This memorandum summarizes the revised best estimates for the mobile colloidal-actinide source term for input to the WIPP Compliance Certification Application. Values presented herein supersede the values provided to you on 29 March 1996 (Papenguth, 1996) in response to your memorandum of 29 March 1996 (Stockman, 1996a). The present memorandum addresses your request for modifications stated in your memorandum dated 2 April 1996 (Stockman, 1996b).

In the attached table, I have summarized the complete set of parameters and values for the mobile colloidal-actinide source term. Revised values for maximum actinide concentration values for humic substances and constants describing actinide concentrations associated with mineral-fragment-type colloidal particles are included. New values (i.e., corresponding to new idpram's and idmtrl's) for proportionality constants describing actinide concentrations associated with humic substances are also included.

The revisions described herein for humic substances reflect a shift in approach from proportionality constants describing actinide-humic concentration by element, to proportionality constants describing actinide-humic concentration by actinide oxidation state. That change affects treatment of actinide elements that will have multiple oxidation states in the WIPP repository [e.g., U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV)]. A second modification in approach, is that I now provide values for two cases: (1) a Castile brine in equilibrium with brucite and magnesite; and (2) a Salado brine in equilibrium with brucite and magnesite. For humic substances, the following material-parameter combinations apply:

IDMTRL: PHUMOX3 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 3;

	PHUMOX4	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4;
	PHUMOX5	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5; and
	PHUMOX6	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6.
IDPRAM:	PHUMCIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite);
	PHUMSIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite).

The revisions made for actinide concentration associated with mineral-fragment-type colloidal particles were made to include the potential contribution of actinide-mineral colloids formed in the Culebra. To accomplish that, the original repository source term values (Papenguth, 1996) have been doubled. That approach is not necessary for humic substances or actinide intrinsic colloids [i.e., Pu(IV)-polymer], because their concentrations are limited by solubilities. Concentrations of actinides associated with microbes are limited by the steady-state population of microbes in the repository, which will not increase when introduced to the Culebra.

The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, SNL technical memorandum dated 29 March 1996 to Christine T. Stockman.

Stockman, C.T., 1996a, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 29 March 1996 to Hans W. Papenguth.

Stockman, C.T., 1996b, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 2 April 1996 to Hans W. Papenguth.

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MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
revised (new)	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
revised	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
revised	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
revised	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
revised	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

Attachment F:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 22 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 2

In my rush to complete and distribute Revision 1 (Papenguth, 1996), I made mistakes on the minimum and maximum values for actinide concentrations associated with mineral-fragment-type colloidal particles. The attached Table contains the correct values.

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL technical memorandum dated 18 April 1996 to Christine T. Stockman.

copy to:

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MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

Title 40 CFR Part 191
Compliance Certification Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.6

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WPO #35856

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 7 May 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Parameter Record Package for Colloidal Actinide Source Term Parameters

Attached is the Parameter Record Package for the WIPP PA parameters describing actinide concentrations associated with mobile **microbes**. This Package is one of four describing the concentration of actinides associated with the four colloidal particle types. The complete set of Packages consists of the following:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy with Attachments to:

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MS 1320	W. George Perkins, 6748
DOE/CAO	Robert A. Stroud

SWCF-A:WBS:1.1.10.2.1: Colloid Characterization and Transport

SWCF-A:WPO#35856: Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy without Attachments to:

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MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1328	Mary-Alena Martell, 6749
MS 1341	John T. Holmes, 6748

Parameter Record Package for Mobile-Colloidal Actinide Source Term.
Part 4. Microbes

The parameter values in this package are based on data which were collected under the guidance of the Principal Investigator for the Waste Isolation Pilot Plant (WIPP) Colloid Research Program, Hans W. Papenguth, for input to the WIPP Data Entry Form and for use in WIPP Performance Assessment (PA) calculations.

I. *Parameter No. (id):* Not applicable.

II. *Data/Parameter:* Not applicable.

III. *Parameter id (idpram):* PROPMIC and CAPMIC.

IV. *Material:* Microbes and the actinides Th, U, Np, Pu, and Am.

V. *Material Identification (idmtrl):* Th, U, Np, Pu, and Am.

VI. *Units:* For proportionality constants (PROPMIC), the units are "moles microbe-bound actinide per moles of dissolved actinide." For the maximum concentration of each actinide associated with mobile microbes (CAPMIC), the units are "moles microbe-bound actinide per liter of dispersion."

VII. *Distribution Information.*

A. *Category:* The development of parameter values and their distributions is described in Attachment A. Summaries of the parameter values are presented in Attachments C, E, and F. Constant CAPMIC values are supplied for Th, U, Np, and Pu. CAPMIC values for Am are not available (refer to Attachment A, page 6). Constant PROPMIC values are supplied for all five actinide elements listed above.

B. *Mean:* See Attachments A, C, E, and F.

C. *Median:* Not applicable.

D. *Standard Deviation:* Not applicable.

E. *Maximum:* See Attachments A, C, E, and F.

F. *Minimum:* See Attachments A, C, E, and F.

G. *Number of data points:* Not applicable.

VIII. *Data Collection and Interpretation Information.*

A. *Data Source Information:* WIPP observational data and literature.

B. *Data Collection (for WIPP observational data).*

1. *Data Collection or Test Method:* Experiments were conducted at Brookhaven National Laboratory (BNL; contract number AP-2273; A. J. Francis, BNL PI) and at Los Alamos National Laboratory (LANL; contract number AP-2272; Inés

R. Triay, LANL PI). Work conducted at LANL was done as a collaborative effort under the guidance of the BNL PI. Descriptions of experiments conducted at those institutions are described in Attachment A.

2. *Assumptions Made During Testing:* See Attachment A.

3. *Standard Error of Measurement of Tests Performed:* See Attachment A.

4. *Form of Raw Data:* Data on actinide bioaccumulation by microbes is reported in actinide concentration or counts per unit volume. Data on actinide toxicity effects is reported in actinide concentration or counts per unit volume and cell population in cells per unit volume or in optical density.

5. *References Related to Data Collection:* See Attachment A.

6. *QA Status of Data:*

   a. *Are all of the data qualified?* Yes.

   b. *Were data qualified by QAP 20-3?* No. Data packages will be submitted for work conducted at BNL and LANL (see VIII,B,1 above for contract numbers), under File code WBS 1.1.10.2.1.

   c. *Were the data the subject of audit/surveillance by SNL or DOE?* Yes. LANL (contract number AP-2272) was audited by SNL (EA96-11) and by DOE/CAO (S-96-08). BNL (contract number AP-2273) is scheduled to be audited by SNL (EA96-19) in May 1996. DOE/CAO conducted a surveillance of BNL (S-96-08).

   d. *Were the data collected under an SNL approved QA program?* Yes. Data were collected under SNL WIPP QAPD, Rev. P, effective October 1, 1992, and SNL WIPP QAPD, Rev. R, effective July 31, 1995. LANL conducted work under an approved QAPP prepared especially for their program (WIPP Colloid and Bacterial Transport Project, CST-CBT-QAP1-001/0). BNL conducted work under an approved QAPP prepared especially for their program (Examination of the Role of Microorganisms in Colloidal Transport of Actinides under WIPP Repository Relevant Test Conditions). Data were collected under a test plan for the WIPP Colloid Research Program (Papenguth and Behl, 1996). Detailed descriptions of the experiments and interpretation listed herein will be published in a SAND report. Documents related to data collection at BNL and LANL will be archived in the Sandia WIPP Central Files (SWCF; File code WBS 1.1.10.2.1).

C. *Interpretation of Data.*

1. *Was the interpretation made by reference to previous work.* No.

2. *Was the interpretation made by using newly performed calculations?* Yes.

3. *Form of Interpreted Data.* List of interpreted values.

4. *Assumptions Made During Interpretation.* See Attachment A.

5. *Name of Code(s)/Software used to Interpret Data:* Not applicable.

6. *QA Status of Code(s) used to Interpret Data:* Not applicable.

    a. *Was the code qualified under QAP 19-1?* Not applicable.

    b. *Was the code qualified under QAP 9-1?* Not applicable.

7. *References Related to Data Interpretation:* See XI below and Attachment A.

8. *For interpretations made by using a newly performed calculations provide documentation that you followed the requirements of QAP 9-1 Appendix B.* The data analysis is controlled by Analysis Plan for the Colloid Research Program, AP-004 (Behl and Papenguth, 1996).

9. *For routine calculations (not using code) did you follow requirements of QAP 9-5?* Yes.

IX. *Correlation with other Parameters:* Parameter values describing the concentration of actinides associated with mobile humic substances are linked to solubility of the dissolved actinides, with a maximum value which cannot be exceeded.

X. *Limitations or qualifications for usage of data by Performance Assessment (PA):* None.

XI. *References cited above:*

Behl, Y.K., and Papenguth, H.W., 1996, Analysis Plan for the WIPP Colloid Research Program WBS #1.1.10.2.1, SNL Analysis Plan AP-004.

Papenguth, H.W., and Behl, Y.K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

XII. *Attachments:*

Attachment A: Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Microbes.

Attachment B: Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Attachment C: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Attachment D: Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Attachment E: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Attachment F: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

XIII. *Distribution*

SWCF-A:WPO# 35856: Mobile-Colloidal Actinide Source Term. 4. Microbes.
SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.

Attachment A:

Papenguth, Hans W., 1996, Rationale for Definition of Parameter Values for Microbes.

Attachment A.
Rationale for Definition of Parameter Values for Microbes

Hans W. Papenguth

Introduction

The actinide source term at the WIPP is defined as the sum of contributions from dissolved actinide species and mobile colloidal actinide species. The dissolved actinide source term has been defined elsewhere (Novak, 1996; Novak and Moore, 1996; Siegel, 1996). It is important to note that colloidal actinides which are not suspended in the aqueous phase (i.e., not mobile) are not included in the colloidal actinide source term. Colloidal actinides may become immobilized by several mechanisms, including precipitation followed by coagulation and gravitational settling (humic substances and actinide intrinsic colloids), adhesion to fixed substrates (microbes), and flocculation or coagulation of colloidal particles followed by gravitational settling (mineral fragments). Sorption of colloidal actinides onto fixed substrates will also reduce the mobile colloidal actinide source term, but no credit is currently being taken for reduction by that means.

To facilitate quantification of the colloidal actinide source term, as well as an efficient experimental approach, the source term has been divided into four components according to colloid types. On the basis of (1) the behavior of colloidal particles in high ionic strength electrolytes, (2) the way in which colloidal particles interact with actinide ions, and (3) the transport behaviors of colloidal particles, four colloidal particle types are recognized (Papenguth and Behl, 1996): mineral fragments, actinide intrinsic colloids, humic substances, and microbes.

The focus of this document is on the quantification of the actinide concentration mobilized by microbes. In terms of the WIPP performance assessment (PA) calculations, the rationale for selecting the values corresponding to the following parameter designators is discussed:

idpram:	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes; and
	CAPMIC	maximum (cap) concentration of actinide associated with mobile microbes
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Potentially important colloidal sized microorganisms include bacteria, fungi, yeast, and protozoa. Fungi and yeast are not important for the WIPP Site because of the anticipated anoxic environment of the repository. For the WIPP Site, the focus is on the halophilic and halotolerant microbes that have been identified at the Site (Brush, 1990; Francis and Gillow, 1994). Microbes are important to consider in performance assessments of the WIPP because they may significantly affect the characteristics of the waste stored at the WIPP, and also participate in transport of actinides in the event of human intrusion. Microbes are known to actively bioaccumulate actinides intracellularly as well as act as substrates for passive extracellular sorption.

At the WIPP Site, concentrations of naturally occurring microbes are on the order of 10^4 to 10^7 cells per milliliter (Francis and Gillow, 1994, Table 1). In the presence of nutrients provided by WIPP waste constituents, including nitrates, sulfates, and cellulosic materials such as protective clothing and wood, the population of microbes is likely to increase. Lysis, a natural phenomenon whereby cells die and release their cell constituents to the solution, also provides a source of nutrients to microbes.

When introduced to nutrient, microbes typically follow a predictable growth curve (defined by the number population of microbes plotted as a function of time), consisting of an initial period of inactivity ("very early log phase") ranging up to several days, followed by a sharp increase in growth ("early log phase"). That level of growth is sustained for one or more days ("log phase") during which time microbial metabolites, including carboxylic acids, enzymes, and exocellular polymers, are generated. The growth rate eventually begins to decline ("late log phase") due to the effects of those metabolites, limitations in nutrients or substrates, or population dynamics, and reaches a steady-state population ("stationary phase"). Viable microbes may aggregate to form clusters.

Experimental

Several types of experiments were conducted to evaluate the impact of microbes in support of the WIPP Colloid Research Program (refer to descriptions in Papenguth and Behl, 1996): (1) evaluation of indigenous concentrations of microbes; (2) quantification of mobile concentrations under nutrient- and substrate-rich conditions; (3) quantification and characterization of actinide bioaccumulation by microbes; and (4) evaluation of toxicity effects of actinide elements on microbe growth.

Experiments were conducted at Brookhaven National Laboratory (BNL; contract number AP-2273; A. J. Francis, BNL PI) and as a collaborative effort between BNL and Los Alamos National Laboratory (LANL; contract number AP-2272; Inés R. Triay, LANL PI). Evaluation of indigenous concentrations was a collaborative effort between BNL and LANL. Quantification of mobile concentrations was conducted at BNL. The bioaccumulation and toxicity work was conducted at BNL or LANL depending on actinide element. Thorium and uranium were investigated at BNL. The other actinide elements of interest, neptunium, plutonium, and americium, were investigated at LANL under the guidance of BNL personnel.

Experiments to determine the mobile concentrations of microbes remaining suspended in the fluid column were conducted similarly to experiments previously conducted in support of the WIPP Gas Generation Program (Brush, 1990; Francis and Gillow, 1994). Bacterial cultures were introduced to a solution containing nutrient and substrate, and sealed. Bacteria population was monitored over periods of several weeks or more using measurements of optical density or by direct counting of aliquots of fixed cells. An important change in protocol from previous experiments, however, is that instead of filtering the entire contents of the vessels, only the mobile cells remaining suspended in the fluid column were counted. Results of the experiments showed that the mobile concentration of microbes was a couple orders-of-magnitude less than the total concentration of microbes. The existence of indigenous microbes in Salado groundwaters has been demonstrated in previous work (Francis and Gillow, 1994). As part of the WIPP Colloid Research Program, samples of Culebra groundwater were carefully collected from the H-19 hydropad, processed, and characterized for indigenous microbes. Concentrations of naturally occurring microbes were on the order of 10^5 cells per milliliter, determined using direct counting methods.

The evaluation of indigenous concentrations of microbes and quantification of mobile concentrations provided important supporting evidence for quantifying the microbial actinide source term and for evaluating microbe-facilitated transport of actinides in the Culebra. However, the basis for developing the actual parameter values to be used in PA calculations was established with bioaccumulation and toxicity experiments, referred to herein as filtration experiments. Those experiments were conducted by combining microbe cultures with various concentrations and complexes of ^{232}Th, ^{238}U, ^{237}Np, ^{239}Pu, or ^{243}Am. The actinide reagents used were thorium nitrate, thorium EDTA, uranyl(VI) nitrate, uranyl(VI) citrate, neptunyl(V) EDTA, plutonyl(V) perchlorate, plutonyl(V) EDTA, and americium EDTA. For those experiments, a pure bacterial culture (WIPP-1A) and a mixed bacterial culture (BAB) were used. Most of the experiments were conducted with the WIPP-1A culture, because of the fast growth of that pure culture. The WIPP-1A mixed culture typically reaches steady-state concentration within several days, whereas the BAB pure culture requires several weeks. Because of the rapid response of the WIPP-1A culture, most of the experiments in support of the WIPP Colloid Research Program were conducted with that culture to expedite the research program. A complementary set of experiments were repeated with the BAB mixed culture, to evaluate the representativeness of the pure culture. Experiments were conducted over periods of 11 to 15 days for the WIPP-1A microbe culture, and up to 21 days for the BAB culture. Each experiment consisted of a subset of two or three replicate test vessels, which were sampled during the overall test interval, to provide time sequence data. In addition, replicate test vessels which were not inoculated with microbes were included in each experiment to provide a control. Sequential filtration with 0.03 µm, 0.4 µm, and 10 µm filter pore sizes was conducted on each vessel. The following size fractions were obtained:

fluid column sample	**particle size**	**actinide association with:**
not filtered	all	all forms listed below
0.22 µm syringe filter, filtrate	< 0.22 µm	dissolved; lysed microbes
10 µm filter, filter rentenate	> 10 µm	clumped microbes
10 µm filter, filtrate	< 10 µm	dissolved; dispersed microbes; lysed microbes
0.4 µm filter, filter rentenate	= 0.4 to 10 µm	dispersed microbes
0.4 µm filter, filtrate	< 0.4 µm	dissolved; lysed microbes
0.03 µm filter, filter rentenate	= 0.03 to 0.4 µm	lysed microbes
0.03 µm filter, filtrate	< 0.03 µm	dissolved; lysed microbes

In addition to the potential actinide associations listed above, there was some evidence of the formation of inorganic precipitates in some of the experiments. The nutrient used in many experiments was phosphate (1 g PO_4^{3-}/L), which is known to coprecipitate actinide cations. The inoculated control samples provided the means to evaluate the extent of that experimental artifact. The control samples also provided the means to assess the extent of sorption of actinides onto test vessels, sampling, and filtration equipment. All sequential filters were composed of the same material, which simplifies assessment of sorption on the filtration equipment.

The toxicity experiments were conducted as a component of the filtration experiments described above, by varying the actinide concentration, and comparing growth curves measured by optical density and/or by direct cell counting. To increase the total concentration of actinides in solution, EDTA was added in some experiments in a one-to-one molar ratio with the actinide element. That approach was taken for some Pu experiments, and all of the Th, Np, and Am experiments.

Interpretation of Experimental Results

Proportionality constants (PROPMIC) describing the amount of actinide element bound to mobile microbes were determined from the data listed above. In addition, maximum concentrations of actinides that could be associated with microbes (CAPMIC) were determined from the experimental data. Those two parameters are suitable for use in PA calculations, when coupled with dissolved actinide solubility values.

The 0.4 µm filter rententate and 0.03 µm filtrate (acquired from the inoculated vessels, not the uninoculated control vessels) were selected to represent the microbial actinide and dissolved actinide concentrations, respectively. The ratio between the microbial actinide and dissolved actinide, both expressed in molarity, represents the proportionality constant value used for the PROPMIC parameter. The 0.4 µm filter rententate was selected to represent the microbial fraction because nearly all of the bacteria biomass was associated with that filter. A small concentration of actinides was associated with suspected biomass trapped on the 10 µm filter, as clumped microbes, and on the 0.03 µm filter, as lysed microbes. The contribution of actinides associated biomass consisting of clumped and lysed microbes was typically at least one order-of-magnitude less than the actinide concentration associated with the dispersed microbes collected on the 0.4 µm filter. The concentration of dissolved actinides measured from the 0.03 filter filtrate was used in the ratio because it provides the best indication of final dissolved actinide concentration. The individual proportionality constants for the filtration experiments are summarized in Table 1. Representative values for PROPMIC were developed from the individual proportionality constants on an element-by-element basis. Results of experiments using the BAB culture were disregarded, because of their lower uptake of actinides (especially plutonium), and because of the limited number of experiments conducted with that culture. For the WIPP-1A culture, the first sampling period (2 to 4 days, but generally 3 days) was disregarded in determining proportionality constants because steady state population had not yet been reached. The remaining values were averaged arithmetically (refer to comment column in Table 1).

The filtration experiments discussed above (see Table 1) also provided the basis for determining CAPMIC values. Final cell population numbers in the test vessels were estimated using measurements of optical density at a wavelength of 600 nm or by direct counting with epifluorescent microscopy. The magnitude of the toxicity effects were estimated by comparing final cell numbers obtained from a series of test vessels with varying actinide concentration. The direct counting technique provided the most dependable measure of cell number and was used where available. The CAPMIC value is defined as the actinide concentration in molarity at which no growth was observed. For cases where growth clearly diminished as actinide concentration increased, but the actinide concentration was not great enough to stop growth, CAPMIC values were determined by linear extrapolation of population numbers, and then adding an order-of-magnitude to account for uncertainty. It appears that the toxicity effects are due to chemical toxicity rather than radiotoxicity. Because of the high radiation levels of americium and safety considerations in the laboratory facility used, the molar concentration could not be increased to the point at which toxicity effects could be observed. Consequently no CAPMIC value is currently available for americium. The experimental basis for determination of CAPMIC values and comments on the determination of parameter values are summarized in Table 2.

The experiments conducted do not provide sufficient information to enable us to formulate a distribution of values for PROPMIC and CAPMIC. Therefore, single values for PROPMIC and CAPMIC are provided to the PA Department. Uncertainties due to analytical precision are small compared to uncertainties in knowledge of the microbe culture which might predominate in the WIPP repository or in the Culebra in an intrusion scenario. The proportionality factor approach coupled with the plus or minus one order-of-magnitude uncertainty in actinide solubilities results in a plus or minus one order-of-magnitude uncertainty in the concentration of actinides bound by mobile microbes.

Summary

Interpreted values for PROPMIC and CAPMIC are summarized in Attachments C, E, and F.

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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.

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Siegel, M. D., 1996, Solubility parameters for use in the CCA NUTS and GRIDFLOW calculations. SNL Technical memorandum dated 29 March 1996 to Martin S. Tierney.

Table 1.—Microbe filtration results.

date of experiment	actinide	form	initial target actinide concentration (M)	microbe culture	sampling time (days)	0.4 µm filter, filter retentate, inoculated vessel	uncertainty	0.03 µm filter, filtrate, inoculated vessel	uncertainty	proportionality constant (microbial An/dissolved An in M/M)	comments related to selection of PROPMIC values
PLUTONIUM											
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-05	WIPP-1A	3	3.59E-07	not available	1.30E-06	not available	0.2762	disregard
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-05	WIPP-1A	8	3.67E-08	not available	5.80E-07	not available	0.0633	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-05	WIPP-1A	15	7.85E-09	not available	1.66E-07	not available	0.0473	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	3	1.81E-07	not available	6.85E-08	not available	2.6423	disregard
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	8	7.55E-09	not available	3.05E-08	not available	0.2475	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	15	2.69E-09	not available	1.07E-08	not available	0.2514	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-07	WIPP-1A	3	7.28E-09	not available	1.94E-08	not available	0.3753	disregard
28-Nov-95	Pu-239	Pu(V) EDTA	1.00E-07	WIPP-1A	15	1.11E-10	not available	5.82E-08	not available	0.0019	include in mean for Pu
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	2	3.16E-08	4.59E-10	1.38E-08	1.34E-09	2.2899	disregard
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	8	1.44E-09	9.50E-11	6.02E-09	1.11E-10	0.2392	include in mean for Pu
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	WIPP-1A	11	9.24E-10	1.70E-10	6.33E-09	3.22E-10	0.1460	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-05	WIPP-1A	3	2.54E-07	not available	1.63E-06	not available	0.1558	disregard
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-05	WIPP-1A	8	5.18E-07	not available	1.16E-06	not available	0.4466	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-05	WIPP-1A	15	2.87E-08	not available	1.83E-06	not available	0.0157	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-06	WIPP-1A	3	2.43E-07	not available	9.94E-08	not available	2.4447	disregard
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-06	WIPP-1A	8	1.17E-08	not available	4.08E-08	not available	0.2868	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-06	WIPP-1A	15	1.00E-09	not available	2.01E-08	not available	0.0498	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-07	WIPP-1A	3	1.15E-08	not available	2.29E-08	not available	0.5022	disregard
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-07	WIPP-1A	8	2.93E-09	not available	1.43E-09	not available	2.0490	include in mean for Pu
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00E-07	WIPP-1A	15	7.65E-11	not available	1.07E-07	not available	0.0007	include in mean for Pu
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	BAB	3	2.52E-10	4.28E-11	5.68E-08	3.19E-10	0.0044	disregard
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	BAB	9	1.45E-09	1.14E-10	3.89E-08	5.96E-10	0.0373	disregard
12-Feb-96	Pu-239	Pu(V) EDTA	1.00E-06	BAB	21	1.22E-09	2.00E-10	5.46E-08	5.45E-10	0.0223	disregard
PROPMIC(Pu):	mean										3.0e-01
	standard deviation										5.44e-01
	number of samples										1.3e+01

Table 1.—Microbe filtration results.

date of experiment	actinide	form	initial target actinide concentration (M)	microbe culture	sampling time (days)	0.4 µm filter, filter retentate, inoculated vessel	uncertainty	0.03 µm filter, filtrate, inoculated vessel	uncertainty	proportionality constant (microbial An/dissolved An in M/M)	comments related to selection of PROPMIC values
AMERICIUM											
11-Mar-96	Am-243	Am EDTA	5.00E-07	WIPP-1A	3	1.82E-08	1.15E-10	1.84E-09	2.12E-10	9.8913	disregard
11-Mar-96	Am-243	Am EDTA	5.00E-07	WIPP-1A	7	6.32E-09	2.52E-10	3.35E-09	6.65E-10	1.8866	include in mean for Am
11-Mar-96	Am-243	Am EDTA	5.00E-07	WIPP-1A	11	1.22E-08	5.33E-10	2.28E-09	1.05E-10	5.3509	include in mean for Am
PROPMIC(Am):	mean										3.6e+00
	standard deviation										2.45e+00
	number of samples										2.0e+00
NEPTUNIUM											
29-Mar-96	Np-237	Np(V) EDTA	5.00E-05	WIPP-1A	3	6.24E-06	1.58E-07	8.04E-06	4.11E-06	0.7761	disregard
29-Mar-96	Np-237	Np(V) EDTA	5.00E-05	WIPP-1A	7	2.33E-06	1.24E-06	1.98E-07	8.89E-09	11.7677	include in mean for Np
29-Mar-96	Np-237	Np(V) EDTA	5.00E-05	WIPP-1A	11	not available	not available	not available	not available	not available	disregard
PROPMIC(Np):	mean										1.2e+01
	standard deviation										not applicable
	number of samples										1.0e+00
THORIUM											
11-Mar-96	Th-232	Th EDTA	1.00E-03	WIPP-1A	7	4.90E-04	1.41E-04	2.72E-04	9.14E-05	1.8015	include in mean for Th
11-Mar-96	Th-232	Th EDTA	1.00E-03	WIPP-1A	13	6.95E-04	7.55E-05	1.55E-04	6.10E-06	4.4839	include in mean for Th
PROPMIC(Th):	mean										3.1e+00
	standard deviation										1.90e+00
	number of samples										2.0e+00
URANIUM											
9-Feb-96	U-238	U(VI) nitrate	1.00E-03	WIPP-1A	4	5.30E-07	3.18E-08	2.93E-04	1.06E-06	0.0018	disregard
9-Feb-96	U-238	U(VI) nitrate	1.00E-03	WIPP-1A	13	2.11E-06	2.61E-07	9.83E-04	1.68E-05	0.0021	include in mean for U
22-Feb-96	U-238	U(VI) nitrate	1.00E-03	BAB	5	2.17E-06	1.64E-07	1.24E-03	4.20E-06	0.0018	disregard
22-Feb-96	U-238	U(VI) nitrate	1.00E-03	BAB	13	2.22E-06	1.89E-07	1.16E-03	4.20E-06	0.0019	disregard
PROPMIC(U):	mean										2.1e-03
	standard deviation										not applicale
	number of samples										1

Table 2.—Microbe toxicity results.

date of experiment	actinide	form	initial target actinide concentration (M)	0.2 µm filter, filtrate (actinide solubility; M)	final cell number (cells/mL)	final optical density at 600 nm (units)	final pH	magnitude of toxicity (relative to no actinide control)	toxic concentration - observed (M)	toxic concentration - extrapolated (M)	comments related to selection of CAPMIC values	
THORIUM												
13-Mar-96	control (none)	not applicable	not applicable	not applicable	not analyzed	0.567	8.08	not applicable				
13-Mar-96	Th-232	Th(IV) nitrate	4.30e-04	0 (ppt.)	not analyzed	0.645	8.22	none				
13-Mar-96	Th-232	Th(IV) nitrate	1.10e-03	0 (ppt.)	not analyzed	0.58	8.28	none				
13-Mar-96	Th-232	Th(IV) nitrate	2.20e-03	0 (ppt.)	not analyzed	0.352 (ppt.)	6.05	extreme	1.90e-03		use for Th	
13-Mar-96	Th-232	Th(IV) nitrate	4.30e-03	0 (ppt.)	not analyzed	0.427 (ppt.)	5.76	extreme	3.46e-03		disregard, toxicity observed at lower value	
13-Mar-96	Th-232	Th(IV) EDTA	4.30e-04	3.41e-04	not analyzed	0.063	6.45	inconclusive				
13-Mar-96	Th-232	Th(IV) EDTA	1.10e-03	1.01e-03	4.24e+06	0.071	6.13	moderate				
13-Mar-96	Th-232	Th(IV) EDTA	2.20e-03	1.90e-03	not analyzed	0.004	6.08	extreme	2.20e-03		disregard, toxicity observed at lower value	
13-Mar-96	Th-232	Th(IV) EDTA	4.30e-03	3.46e-03	not analyzed	0	6.32	extreme	4.30e-03		disregard, toxicity observed at lower value	
URANIUM												
17-Oct-95	control (none)	not applicable	not applicable	not applicable	2.62e+08	0.541	8.1	not applicable	not applicable	not applicable		
17-Oct-95	U-238	U(VI) nitrate	4.20e-04	4.20e-04	2.57e+08	0.543	8.04	none				
17-Oct-95	U-238	U(VI) nitrate	1.10e-03	1.00e-03	3.08e+08	0.539	7.94	none				
17-Oct-95	U-238	U(VI) nitrate	2.10e-03	0 (ppt.)	2.24e+05	0.272	6.26	extreme	2.10e-03		use for U	
17-Oct-95	U-238	U(VI) nitrate	4.20e-03	0 (ppt.)	2.02e+05	0.533	5.9	extreme	4.20e-03		disregard, toxicity observed at lower value	
17-Oct-95	U-238	U(VI) citrate	4.20e-04	4.20e-04	2.77e+08	0.514	8.01	none				
17-Oct-95	U-238	U(VI) citrate	1.10e-03	1.10e-03	2.39e+08	0.508	7.96	none				
17-Oct-95	U-238	U(VI) citrate	2.10e-03	0 (ppt.)	2.58e+05	0.318	6.11	extreme	2.10e-03		use for U	
17-Oct-95	U-238	U(VI) citrate	4.20e-03	0 (ppt.)	1.93e+05	0.344	5.91	extreme	4.20e-03		disregard, toxicity observed at lower value	
NEPTUNIUM												
19-Mar-96	control (none)	not applicable	not applicable	not applicable	not analyzed	0.8	8.04	none				
19-Mar-96	Np-237	Np(V) EDTA	5.00e-06	2.70e-06	not analyzed	0.788	8.02	none				
19-Mar-96	Np-237	Np(V) EDTA	5.00e-05	2.53e-05	not analyzed	0.802	7.95	none				
19-Mar-96	Np-237	Np(V) EDTA	5.00e-04	2.65e-04	not analyzed	0.141	6.57	, but some growth	2.65e-04		use for Np, but increase by one order of magnitude because of some growth	
PLUTONIUM												
28-Nov-95	control (none)	not applicable	not applicable	not applicable	3.40e+08	0.672	8.157	not applicable	not applicable	not applicable		
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00e-07	5.01e-08	3.20e+08	0.683	8.197	none				
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00e-06	6.90e-07	1.40e+08	0.453	8.327	moderate				
28-Nov-95	Pu-239	Pu(V) perchlorate	1.00e-05	8.80e-06	5.50e+07	0.237	7.94	extreme		7.71e-06	disregard, toxicity observed at lower value	
28-Nov-95	Pu-239	Pu(V) EDTA	1.00e-07	5.50e-08	2.80e+08	0.691	8.223	none				
28-Nov-95	Pu-239	Pu(V) EDTA	1.00e-06	6.20e-07	1.20e+08	0.499	8.387	moderate				
28-Nov-95	Pu-239	Pu(V) EDTA	1.00e-05	8.00e-06	9.80e+07	0.532	8.363	extreme		6.83e-06	use for Pu, but increase by one order of magnitude	
AMERICIUM												
5-Mar-96	control (none)	not applicable	not applicable	not applicable	not analyzed	0.89	7.93	not applicable				
5-Mar-96	Am-243	Am(III) EDTA	5.00e-08	2.62e-08	not analyzed	0.864	7.98	none				
5-Mar-96	Am-243	Am(III) EDTA	5.00e-07	3.36e-07	not analyzed	0.821	8.04	none				
5-Mar-96	Am-243	Am(III) EDTA	5.00e-06	2.65e-06	not analyzed	0.79	8.04	slight	>2.65E-06		Inconclusive; Am concentrations not sufficiently high	

Attachment B:

Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 3/29/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

In order to properly model the transport of radionuclides within the Salado formation, we will need information about the possible transport of these radionuclide on colloids. In this memo we request the maximum mobilized radionuclide concentration and/or the proportionality constant defining the moles mobilized on colloid per moles in solution, for each transported element and colloid type. We are planning to transport Am, Pu, U, and Th, and may also transport Cm, Np, Ra, and Sr. If we transport Ra and Sr, we are planning to model them as very soluble, and not sorbed, so I believe modeling of colloids for them will not be necessary. For Cm solubility, we will be using the Am(III) model. If you believe that Cm colloids also behave similarly to Am colloids, we could extend the chemical analogy to the colloid behavior. If you agree with these simplifications then we will need the parameters for Am, Pu, U, Th and Np only.

Suggested names for database entry:
IDMTRL: Am, Pu, U, Th, Np

IDPRAM:

CONCINT	for concentration of actinide on mobilized intrinsic colloid
CONCMIN	for concentration of actinide on mobilized mineral fragments
CAPHUM	for maximum concentration of actinide on humic colloids
CAPMIC	for maximum concentration of actinide on microbe colloids
PROPHUM	for moles actinide mobilized on humic colloids per moles dissolved
PROPMIC	for moles actinide mobilized on microbe colloids per moles dissolved

You will need to provide a distribution for each material-parameter pair, but that distribution may be "CONSTANT" for most of the numbers. Eight sampling slots have been reserved for the most important of these parameters that have non-constant distributions.

cc:
Mary-Alena Martell
Hong-Nian Jow
E. James Nowak
James L. Ramsey
Amy S. Johnson
Martin S. Tierney
W. George Perkins
J. T. Schneider
Richard V. Bynum
Ali A. Shinta
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment C:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 29 March 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters

This memorandum summarizes best estimates for the mobile colloidal actinide source term for input to the WIPP Compliance Certification Application. The use of material and parameter identification codes is consistent with your letter to me dated 29 March 1996 requesting parameter values. In the attached table, I have provided best estimates for the following material-parameter combinations:

IDMTRL: Th, U, Np, Pu, Am

IDPRAM:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids
	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
	CAPHUM	maximum concentration of actinide associated with mobile humic colloids
	CAPMIC	maximum concentration of actinide associated with mobile microbes
	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids
	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes

As a first approximation, the colloidal behavior of curium can be simulated be using parameter values for americium. The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1320	E. James Nowak, 6831 EJN
MS 1320	R. Vann Bynum, 6831
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MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748 wgp
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt O. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851

SWCF-A:WBS1.1.10.2.1

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CONCMIN	Th	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
CONCMIN	U	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
CONCMIN	Np	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
CONCMIN	Pu	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
CONCMIN	Am	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
PROPHUM	Th	6.4e+00	6.4e+00	6.4e+00	moles colloidal humic-bound Th per moles dissolved Th	constant	2,3
PROPHUM	U	1.4e+00	1.6e-01	2.0e+00	moles colloidal humic-bound U per moles dissolved U	triangular	2,3,4
PROPHUM	Np	4.0e+00	4.0e+00	4.0e+00	moles colloidal humic-bound Np per moles dissolved Np	constant	2,3
PROPHUM	Pu	5.9e+00	5.9e+00	5.9e+00	moles colloidal humic-bound Pu per moles dissolved Pu	constant	2,3
PROPHUM	Am	2.5e+00	1.9e-01	3.9e+00	moles colloidal humic-bound Am per moles dissolved Am	triangular	2,3,4

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CAPHUM	Th	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
CAPHUM	U	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
CAPHUM	Np	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
CAPHUM	Pu	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
CAPHUM	Am	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the sum of actinide oxidation species for each actinide element (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used for humic-bound U or Am, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e. the sum of dissolved plus colloidal actinide).

Attachment D:

Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 4/2/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

YiFeng Wang has revised his recommendation to use 2 invariant points in the PA calculation. He now recommends that we use the $Mg(OH)_2 + MgCO_3$ invariant point for all calculations. If this invalidates the assumptions that you used to prepare colloid concentration or proportion parameters please indicate as soon as possible which parameters are affected, and as soon as possible after that provide a memo documenting the new values.

cc:
Mary-Alena Martell
Amy S. Johnson
Hong-Nian Jow
Martin S. Tierney
J. T. Schneider
Richard V. Bynum
E. James Nowak
W. George Perkins
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment E:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 18 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 1

This memorandum summarizes the revised best estimates for the mobile colloidal-actinide source term for input to the WIPP Compliance Certification Application. Values presented herein supersede the values provided to you on 29 March 1996 (Papenguth, 1996) in response to your memorandum of 29 March 1996 (Stockman, 1996a). The present memorandum addresses your request for modifications stated in your memorandum dated 2 April 1996 (Stockman, 1996b).

In the attached table, I have summarized the complete set of parameters and values for the mobile colloidal-actinide source term. Revised values for maximum actinide concentration values for humic substances and constants describing actinide concentrations associated with mineral-fragment-type colloidal particles are included. New values (i.e., corresponding to new idpram's and idmtrl's) for proportionality constants describing actinide concentrations associated with humic substances are also included.

The revisions described herein for humic substances reflect a shift in approach from proportionality constants describing actinide-humic concentration by element, to proportionality constants describing actinide-humic concentration by actinide oxidation state. That change affects treatment of actinide elements that will have multiple oxidation states in the WIPP repository [e.g., U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV)]. A second modification in approach, is that I now provide values for two cases: (1) a Castile brine in equilibrium with brucite and magnesite; and (2) a Salado brine in equilibrium with brucite and magnesite. For humic substances, the following material-parameter combinations apply:

IDMTRL: PHUMOX3 proportionality constant for concentration of actinides associated with mobile <u>hum</u>ic substances, for actinide elements with <u>ox</u>idation state <u>3</u>;

	PHUMOX4	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4;
	PHUMOX5	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5; and
	PHUMOX6	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6.
IDPRAM:	PHUMCIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite);
	PHUMSIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite).

The revisions made for actinide concentration associated with mineral-fragment-type colloidal particles were made to include the potential contribution of actinide-mineral colloids formed in the Culebra. To accomplish that, the original repository source term values (Papenguth, 1996) have been doubled. That approach is not necessary for humic substances or actinide intrinsic colloids [i.e., Pu(IV)-polymer], because their concentrations are limited by solubilities. Concentrations of actinides associated with microbes are limited by the steady-state population of microbes in the repository, which will not increase when introduced to the Culebra.

The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, SNL technical memorandum dated 29 March 1996 to Christine T. Stockman.

Stockman, C.T., 1996a, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 29 March 1996 to Hans W. Papenguth.

Stockman, C.T., 1996b, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 2 April 1996 to Hans W. Papenguth.

copy to:

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MS 1341	Kurt W. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
revised (new)	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
revised	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
revised	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
revised	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
revised	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

Attachment F:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 22 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 2

In my rush to complete and distribute Revision 1 (Papenguth, 1996), I made mistakes on the minimum and maximum values for actinide concentrations associated with mineral-fragment-type colloidal particles. The attached Table contains the correct values.

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL technical memorandum dated 18 April 1996 to Christine T. Stockman.

copy to:

MS 1328	Hong-Nian Jow, 6741
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MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.7

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WPO # 35855

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 7 May 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Parameter Record Package for Colloidal Actinide Source Term Parameters

Attached is the Parameter Record Package for the WIPP PA parameters describing actinide concentrations associated with mobile **humic substances**. This Package is one of four describing the concentration of actinides associated with the four colloidal particle types. The complete set of Packages consists of the following:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy with Attachments to:

MS 1320	Hans W. Papenguth, 6748
MS 1320	W. George Perkins, 6748
MS 1341	Robert C. Moore, 6748
DOE/CAO	Robert A. Stroud

SWCF-A:WBS:1.1.10.2.1: Colloid Characterization and Transport
SWCF-A:WPO#:35855: Mobile-Colloidal-Actinide Source Term. 3. Humic Substances.

copy without Attachments to:

MS 1320	E. James Nowak, 6831
MS 1324	Susan A. Howarth, 6115
MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1328	Mary-Alena Martell, 6749
MS 1341	John T. Holmes, 6748

Parameter Record Package for Mobile-Colloidal Actinide Source Term.
Part 3. Humic Substances

The parameter values in this package are based on data which were collected under the guidance of the Principal Investigator for the Waste Isolation Pilot Plant (WIPP) Colloid Research Program, Hans W. Papenguth, for input to the WIPP Data Entry Form and for use in WIPP Performance Assessment (PA) calculations.

I. *Parameter No. (id):* Not applicable.

II. *Data/Parameter:* Not applicable.

III. *Parameter id (idpram):* PROPHUM, PHUMCIM, PHUMSIM, and CAPHUM.

IV. *Material:* Humic substances, which include fulvic acid, aliphatic humic acid, and aromatic humic acid, and the actinides Th, U, Np, Pu, and Am.

V. *Material Identification (idmtrl):* Th, U, Np, Pu, and Am (for PROPHUM and CAPHUM); PHUMOX3, PHUMOX4, PHUMOX5, and PHUMOX6 (for PHUMCIM and PHUMSIM).

VI. *Units:* For proportionality constants (PROPHUM, PHUMCIM and PHUMSIM), the units are "moles colloidal humic-bound actinide per moles of dissolved actinide." For the maximum concentration of each actinide associated with mobile humic colloids (CAPHUM), the units are "moles colloidal humic-bound actinide per liter of dispersion."

VII. *Distribution Information.*

A. *Category:* The development of parameter values and their distributions is described in Attachment A. Summaries of the parameter values are presented in Attachments C, E, and F. Constant CAPHUM values are supplied for all five of the actinide elements listed. Constant PROPHUM values are supplied for Th, Np, and Pu. Constant PHUMCIM and PHUMSIM values are supplied for PHUMOX4. Triangular distributions are supplied for PROPHUM values for U and Am. Triangular distributions are supplied for PHUMCIM and PHUMSIM values for PHUMOX3, PHUMOX5, and PHUMOX6. In the event that those triangular distributions of parameter values cannot be sampled in the PA calculations, the maximum value should be selected. The decision of whether to use the distribution or the constant value is to be made by the PA Department.

B. *Mean:* See Attachments A, C, E, and F. (Note that for triangular distributions, the apices of the triangle are defined by the minimum value, the most likely value, and the maximum value; refer to Attachments).

C. *Median:* Not applicable.

D. *Standard Deviation:* Not applicable.

E. *Maximum:* See Attachments A, C, E, and F.

F. *Minimum:* See Attachments A, C, E, and F.

G. *Number of data points:* Not applicable.

VIII. *Data Collection and Interpretation Information.*

A. *Data Source Information:* WIPP observational data and literature.

B. *Data Collection (for WIPP observational data).*

1. *Data Collection or Test Method:* Experiments were conducted at Florida State University (FSU; contract number AH-5590; Greg R. Choppin, FSU PI), at Colorado School of Mines (CSM; contract number AR-9240; Bruce D. Honeyman, CSM PI), and at SNL (Hans W. Papenguth and co-workers). Descriptions of experiments conducted at those institutions are included in Attachment A.

2. *Assumptions Made During Testing:* See Attachment A.

3. *Standard Error of Measurement of Tests Performed:* See Attachment A.

4. *Form of Raw Data:* Solubilities of humic substances were reported in units of mg/L. Complexation of actinides by humic substances were described in terms of stability constants. Humic substance site binding density was reported in units of milliequivalents of OH^- per gram of humic substance.

5. *References Related to Data Collection:* See Attachment A.

6. *QA Status of Data:*

    a. *Are all of the data qualified?* Yes.

    b. *Were data qualified by QAP 20-3?* No. Data packages will be submitted for work conducted at FSU, CSM, and at SNL (see VIII,B,1 above for contract numbers), under File code WBS 1.1.10.2.1.

    c. *Were the data the subject of audit/surveillance by SNL or DOE?* Yes. Florida State University (contract number AH-5590) was audited by SNL (94-03 and EA95-02) and is scheduled to be audited again in May 1996 (EA96-15). Colorado School of Mines (contract number AR-9240) is working under the SNL WIPP QA Program.

    d. *Were the data collected under an SNL approved QA program?* Yes. Data were collected under SNL WIPP QAPD, Rev. P, effective October 1, 1992, and SNL WIPP QAPD, Rev. R, effective July 31, 1995. Data were collected under a test plan for the WIPP Colloid Research Program (Papenguth and Behl, 1996). Detailed descriptions of the experiments and interpretation listed herein will be published in a SAND report. Documents related to data collection at SNL, Florida State University, and the Colorado School of Mines will be archived in the Sandia WIPP Central Files (SWCF; File code WBS 1.1.10.2.1).

C. *Interpretation of Data.*

1. *Was the interpretation made by reference to previous work.* No.

2. *Was the interpretation made by using newly performed calculations?* Yes.

3. *Form of Interpreted Data.* List of interpreted values.

4. *Assumptions Made During Interpretation.* See Attachment A.

5. *Name of Code(s)/Software used to Interpret Data:* Not applicable.

6. *QA Status of Code(s) used to Interpret Data:* Not applicable.

   a. *Was the code qualified under QAP 19-1?* Not applicable.

   b. *Was the code qualified under QAP 9-1?* Not applicable.

7. *References Related to Data Interpretation:* See XI below and Attachment A.

8. *For interpretations made by using a newly performed calculations provide documentation that you followed the requirements of QAP 9-1 Appendix B.* The data analysis is controlled by Analysis Plan for the Colloid Research Program, AP-004 (Behl and Papenguth, 1996).

9. *For routine calculations (not using code) did you follow requirements of QAP 9-5?* Yes.

IX. *Correlation with other Parameters:* Parameter values describing the concentration of actinides associated with mobile humic substances are linked to solubility of the dissolved actinides, with a maximum value which cannot be exceeded.

X. *Limitations or qualifications for usage of data by Performance Assessment (PA):* None.

XI. *References cited above:*

Behl, Y.K., and Papenguth, H.W., 1996, Analysis Plan for the WIPP Colloid Research Program WBS #1.1.10.2.1, SNL Analysis Plan AP-004.

Papenguth, H.W., and Behl, Y.K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

XII. *Attachments:*

Attachment A: Papenguth, Hans W., and Moore, Robert C., 1996, Rationale for Definition of Parameter Values for Humic Substances.

Attachment B: Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Attachment C: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Attachment D: Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Attachment E: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Attachment F: Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

XIII. *Distribution*

SWCF-A:WPO# 35855: Mobile-Colloidal Actinide Source Term. 3. Humic Substances.

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.

Attachment A:

Papenguth, Hans W., and Moore, Robert C., 1996, Rationale for Definition of Parameter Values
for Humic Substances.

Attachment A.
Rationale for Definition of Parameter Values for Humic Substances

Hans W. Papenguth and Robert C. Moore

Introduction

The actinide source term at the WIPP is defined as the sum of contributions from dissolved actinide species and mobile colloidal actinide species. The dissolved actinide source term has been defined elsewhere (Novak, 1996; Novak and Moore, 1996; Siegel, 1996). It is important to note that colloidal actinides which are not suspended in the aqueous phase (i.e., not mobile) are not included in the colloidal actinide source term. Colloidal actinides may become immobilized by several mechanisms, including precipitation followed by coagulation and gravitational settling (humic substances and actinide intrinsic colloids), adhesion to fixed substrates (microbes), and flocculation or coagulation of colloidal particles followed by gravitational settling (mineral fragments). Sorption of colloidal actinides onto fixed substrates will also reduce the mobile colloidal actinide source term, but no credit is currently being taken for reduction by that means.

To facilitate quantification of the colloidal actinide source term, as well as an efficient experimental approach, the source term has been divided into four components according to colloid types. On the basis of (1) the behavior of colloidal particles in high ionic strength electrolytes, (2) the way in which colloidal particles interact with actinide ions, and (3) the transport behaviors of colloidal particles, four colloidal particle types are recognized (Papenguth and Behl, 1996): mineral fragments, actinide intrinsic colloids, humic substances, and microbes.

In this document, we focus on the quantification of the actinide concentration mobilized by humic substances. In terms of the WIPP performance assessment (PA) calculations, we discuss the rationale for selecting the values corresponding to the following parameter designators:

idpram:	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids;
	PHUMCIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite);
	PHUMSIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite); and

	CAPHUM	maximum (cap) concentration of actinide associated with mobile humic colloids.
idmtrl:	Th	thorium [i.e., Th(IV)];
	U	uranium [i.e., U(IV) and U(VI)];
	Np	neptunium [i.e., Np(IV) and Np(V)];
	Pu	plutonium [i.e., Pu(III) and Pu(IV)];
	Am	americium [i.e., Am(III)];
	PHUMOX3	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 3 [i.e., Pu(III) and Am(III)];
	PHUMOX4	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4 [i.e., Th(IV), U(IV), Np(IV), and Pu(IV)];
	PHUMOX5	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5 [i.e., Np(V)]; and
	PHUMOX6	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6 [i.e., U(VI)].

Humic substances are defined as high-molecular-weight organic compounds generally present as anions in natural waters. Humic substances may consist of humic acids, which may be aliphatic or aromatic, or fulvic acids. The difference between humic acids and fulvic acids is largely an operational distinction; humic acids can be precipitated at pH values below about 2, whereas fulvic acids are soluble over the entire pH range. Fulvic acids generally have lower molecular weights than humic acids. The dominant functional group which may react with dissolved actinides are carboxyl groups, but phenolic hydroxyl and alcoholic hydroxyl groups also contribute to complexation. At the WIPP, humic substances may be introduced to the repository as a constituent of soil-bearing waste or may be a constituent of the organic carbon component of Castile, Salado, or Culebra groundwaters. Probably more importantly, humic substances may form from condensation reactions between microbial metabolites (e.g., carboxylic acids), cellulosic degradation products, and the extracellular polymers associated with microbes. Because of the general lack of knowledge in the scientific community regarding the formation and humic substances form, we have not attempted to directly quantify the amounts of humic substances likely to be introduced to the WIPP or that would form in situ. Instead, we have elected to bound the contribution of humic-bound actinides through quantification of humic-actinide complexation behavior coupled with quantification of solubilities of humic substances in WIPP-relevant brines. Regardless of the source of humic substances, the total concentration is limited by the solubility of humic substances in WIPP brines. The chemical nature of humic substances generated in situ cannot be predicted either, but can be bounded by the three types of humic substances.

To determine the concentration of actinides associated with humic substances, four pieces of information are required: (1) the concentration of reactive humic substance in the aqueous phase (i.e., humic solubility); (2) the binding capacity of the humic substance; (3) actinide uptake (i.e., actinide complexation constants); and (4) concentrations of actinide ions in the aqueous phase (i.e., actinide solubility). The quantification of actinide solubilities (4) is described in Novak (1996) and results are summarized in Siegel (1996). In the remainder of this document, we focus on the determination of items (1) through (3), the interpretation of that information, and the development of parameter values suitable for PA calculations.

Experimental

In general, humic substances encompass a broad variety of high-molecular-weight organic compounds. The range of their chemical behaviors, however, is covered by consideration of three types: aliphatic humic acid (generally terrestrial); aromatic humic acid (generally marine); and fulvic acid. In our work, the following humic substances were used:

FA-Suw:	fulvic acid isolated from the Suwannee River purchased from the International Humic Substances Society, Golden, Colorado;
HA_{al}-LBr:	aliphatic humic acid isolated from sediments collected from Lake Bradford, Florida, prepared by Florida State University;
HA_{al}-Ald:	aliphatic humic acid purchased from Aldrich Chemical Co., purified by Florida State University;
HA_{ar}-Gor:	aromatic humic acid isolated from groundwaters near Gorleben, Germany, obtained from Professor J.-I. Kim, Institut für Radiochemie, München; and
HA_{ar}-Suw:	aromatic humic acid isolated from the Suwannee River purchased from the International Humic Substances Society, Golden, Colorado.

Solubilities of humic substances were measured at SNL (Hans W. Papenguth and coworkers) and at the Colorado School of Mines (CSM; contract number AR-9240; Bruce D. Honeyman, CSM PI). At SNL, solubilities were measured in experiments which were conducted over periods of several weeks. The concentrations of humic substances remaining in the fluid column was determined using a scanning fluorometer, carbon coulometer, and UV/Visible light spectrophotometer, in WIPP-relevant brine simulants with FA-Suw, HA_{al}-LBr, HA_{al}-Ald, and HA_{ar}-Suw. In addition to spectroscopic data, visible inspection proved valuable. In over saturation experiments, humic substances were dissolved in deionized water under basic pH conditions to enhance dissolution and then added as a spike to a brine solution. In undersaturation experiments, humic substances were added directly to brine solutions and allowed to dissolve until an equilibrium was reached. In either case, an equilibrium was reached between dissolved (i.e., ionic) and precipitated humic substances. The precipitated humic substances coagulated and settled by gravity. The kinetics of precipitation were sufficiently slow that several weeks were required for equilibrium to be reached. Brine solutions consisted of a NaCl matrix with various concentrations of Ca^{2+} and Mg^{2+}. The concentration of Na^+ in the brine had little effect on solubility except at very high concentrations, but the concentration of the divalent cations had a significant impact on humic substance solubilities. Consequently, experiments were conducted with a NaCl background electrolyte concentration with concentrations of Ca and Mg ranging from 10 mM each (representative of natural WIPP brines) to 500 mM each (representative of CaO or MgO backfill scenarios). At SNL, solubilities between approximately 1.5 mg/L and 2.0 mg/L were observed in systems containing 10 mM or greater Ca^{2+} and Mg^{2+}. For the calculations described below, the higher solubility value of 2.0 mg/L was used.

At the CSM, three humic substances (FA-Suw, HA_{al}-LBr, and HA_{ar}-Suw) were labeled with ^{14}C so that concentrations in WIPP-relevant brines could be tracked with liquid scintillation counting. That technique was anticipated to provide better analytical results because it is free from spectral interference problems of spectroscopic techniques. Because of slow precipitation kinetics, the duration of the experiment of only one week was not sufficient for equilibrium to be reached. Consequently, we elected to use the SNL results, which were conducted over a period of several weeks.

Site-binding capacity values were determined by titration at Florida State University for two humic substances (HA_{al}-LBr and HA_{al}-Ald). Those values were supplemented with values for a variety of humic substances compiled from published literature. In general, site-binding capacities for humic substances are between 3 and 6 meq OH^-/g, but in isolated cases are as low as about 1.5 and as high as about 9.5 meq OH^-/g. For the calculations described below, we used values of 4.65, 5.38, and 5.56 meq OH-/g for aliphatic humic acid, aromatic humic acid, and fulvic acid, respectively. The aliphatic humic acid value was determined from HA_{al}-LBr at FSU. The aromatic humic acid value was from Gorleben (Gohy-573). The fulvic acid value represents the mean of 11 published values for fulvic acids collected in Europe (Ephraim et al., 1995).

Actinide complexation factors for Am(III) and U(VI) binding on three humic substances (FA-Suw, HA_{al}-LBr, and HA_{ar}-Gor) were measured at Florida State University (FSU; contract number AH-5590; Greg R. Choppin, FSU PI). Complexation measurements were made at measured pH_{obs} values of approximately 4.8 and 6, conditions at which the humic substances are highly deprotonated, and actinides U and Am have not undergone hydrolysis reactions. Those conditions were chosen to maximize complexation between the humic substances and those actinide elements. Measurements were made in NaCl media with ionic strengths of approximately 3 and 6 molal. Those experiments were completed prior to the WIPP Project establishing the position that MgO backfill would be emplaced to scrub CO_2 and fix pcH at about 9.3. The experiments conducted at FSU represent worst-case scenarios designed to provide high-end estimates of actinide uptake by humic substances. Actinide complexation by humic substances generally decreases at basic pH values because of the reduction in actinide-complex charges due to hydrolysis reactions. In addition, the high concentrations of Mg^{2+} in solution due to the presence of MgO backfill will compete with actinides for binding sites on humic substances and reduce the actinide uptake. FSU reported the first and second stability constants defined as follows (square brackets represent concentration):

$$\mathrm{An} + \mathrm{HS} \leftrightarrow \mathrm{AnHS}; \qquad b_{1;\mathrm{An}} = \frac{[\mathrm{AnHS}]}{[\mathrm{An}]\,[\mathrm{HS}]} \tag{1}$$

$$\mathrm{An} + 2(\mathrm{HS}) \leftrightarrow \mathrm{An(HS)_2}; \qquad b_{2;\mathrm{An}} = \frac{[\mathrm{An(HS)_2}]}{[\mathrm{An}]\,[\mathrm{HS}]^2} \tag{2}$$

where:

HS = humic substance (eq OH^-/L, i.e., site-binding capacity incorporated)
An = actinide element
$b_{1;An}$ = first stability constant, for 1:1 An:humic binding
$b_{2;An}$ = second stability constant, for 1:2 An:humic binding

For the calculations described below, complexation constants were selected from the most relevant experimental conditions, which were pH_{obs} 6 and 6 molal NaCl. The following stability constants reported by FSU were used (reported as log values):

humic substance	Am^{3+}; b_1	Am^{3+}; b_2	$U(VI)O_2^{2+}$; b_1	$U(VI)O_2^{2+}$; b_2
HA_{al}-LBr	6.09±0.05	10.46±0.12	5.91±0.16	10.43±0.19
HA_{ar}-Gor	6.02±0.04	10.41±0.10	5.35±0.15	8.98±0.26
FA-Suw	4.6±0.3	8.95±0.45	not measured	not measured

The FSU results show that there is little difference in Am(III) and $U(VI)O_2^{2+}$ uptake by aliphatic and aromatic humic acids, but that uptake by fulvic acid is significantly less. The FSU results also show that an increase of NaCl ionic strength from 3 to 6 has little effect on actinide uptake. Those observations aid in justifying the use of published stability constants for other actinide elements experimentally determined at lower ionic strengths and for other humic substances. On the basis of the similarities in stability constants for Am(III) and $U(VI)O_2^{2+}$ for the humic acids, we have used the Am(III) stability constant for FA-Suw for $U(VI)O_2^{2+}$ on FA-Suw.

Stability constants for Th(IV) with several humic and fulvic acids were reported by Nash and Choppin (1979). In NaCl media at pH values between 3.95 and 5.03, those authors reported log stability constants between 9.7 and 13.2. Under basic conditions expected in the WIPP repository, it is likely that complexation of Th(IV) will be markedly less, because the dominant Th(IV)-bearing aqueous species will be $Th(OH)_4^0$ (Novak and Moore, 1996). As far as we know, no investigations of Th-complex binding on humic substances have been made. For the calculations described herein, we have elected to use published results from Baskaran et al. (1992) describing the distribution of Th(IV) in sea water. From that work, a ratio of dissolved versus colloidal Th(IV) of 6.349 was calculated, assuming that the solubility of colloidal organic material in sea water is equivalent to our measured value of humic substances in WIPP-relevant brines (i.e., 2.0 mg/L). The nature of the humic substances is likely to be dominated by aromatic humic acid, but may also contain fulvic acid.

For the calculations described herein, we use a log stability constant for $Np(V)O_2^+$ of 3.67 measured at pH 9 for a Gorleben humic acid (Gohy-573; Kim and Sekine, 1991). Results presented in Rao and Choppin (1995) for Lake Bradford humic acid and a Gorleben humic acid (Gohy-573) show little effect of pH on Np(V) stability constants, presumably because of the lack of hydrolysis of reactions for Np(V) over the pH range those authors studied. The Gorleben humic acid is aromatic in nature.

No published stability constants were found for plutonium. For the calculations described herein, we use an oxidation state analogy for the plutonium oxidation species, which we believe is conservative. Allard et al. (1980) have shown that at pH 9, Pu(IV) undergoes hydrolysis reactions to a greater extent than Th(IV), which should result in reduced complexation of Pu(IV).

We also used an oxidation state analogy to develop parameter values for elements expected to have multiple oxidation states in the WIPP repository. Oxidation speciation of the actinide elements was evaluated as part of the dissolved actinide source term program. Weiner (1996) has concluded that in the WIPP repository, the following species will be present: Th(IV); U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV); and Am(III). The relative concentrations of oxidation species of a particular element are designated by their respective solubility values. The substitutions made following the oxidation state analogy are summarized in the following table:

required binding constant	substitute	source of data
Th(IV)	Th(IV)	Baskaran et al. (1992)
U(IV)	Th(IV)	Baskaran et al. (1992)
U(VI)	U(VI)	WIPP-specific data, FSU
Np(IV)	Th(IV)	Baskaran et al. (1992)
Np(V)	Np(V)	Kim and Sekine (1991)
Pu(III)	Am(III)	WIPP-specific data, FSU
Pu(IV)	Th(IV)	Baskaran et al. (1992)
Am(III)	Am(III)	WIPP-specific data, FSU

To compensate for the effects of competition for actinide complexation by the high concentrations of calcium and magnesium in repository brines in the presence of MgO backfill, stability constants for Ca^{2+} and Mg^{2+} were used in simultaneously solved equations (described below). Stability constants for Ca^{2+} and Mg^{2+} at basic pH values are not available, but several published reports provide values in the acidic range. Choppin and Shanbhag reported log stability constants of 2.25 to 3.32 for Ca^{2+} in 0.1m $NaClO_4$ at pH 3.9 and 5.0 for an aliphatic humic acid (Aldrich humic acid). Schnitzer and Skinner (1966) reported log binding constants ranging from 2.2 to 3.72 for Ca^{2+} in low ionic strength solutions over a pH range of 3.5 to 5.0 for fulvic acid. For Mg^{2+}, Schnitzer and Skinner (1966) reported log stability constants ranging from 1.23 to approximately 2.0 under the same experimental conditions. For our calculations, we used a log stability constant of 2.0 for the sum of Ca^{2+} and Mg^{2+} concentrations, which we believe is a conservative value.

Binding of Ca^{2+} and Mg^{2+} to humic substances is described in the same way as equation (1) above:

$$(Ca+Mg) + HS \leftrightarrow (CaMg)HS; \qquad b_{1;Ca,Mg} = \frac{[(Ca+Mg)HS]}{[Ca+Mg]\,[HS]} \qquad (3)$$

where:

$b_{1;CaMg}$ = first stability constant, for 1:1 (Ca+Mg):humic binding (note that no second stability constants exists for divalent cation binding)

Interpretation of Experimental and Literature Results

Proportionality constants (PROPHUM, PHUMCIM, and PHUMSIM) describing the amount of actinide element bound to humic substances were determined from the data listed above, coupled with dissolved actinide concentrations. In addition, maximum theoretical concentrations of actinides that could be associated with humic substances (CAPHUM) were calculated from the data above.

The concentration of an actinide element of a given oxidation state was calculated by simultaneous solution of equations (1) and (3), combined with a mass-balance expression:

$$[HS_{tot}] = [AnHS] + [(CaMg)HS] + [HS] \tag{4}$$

where:

$[HS_{tot}]$ = total concentration of humic substance
$[HS]$ = concentration of uncomplexed humic substance
$[AnHS]$ = concentration of humic complexed with an actinide element
$[(CaMg)HS]$ = concentration of humic complexed with divalent cations

Equation (2) describing the effect of two humic substances binding with one actinide ion was disregarded for these calculations, because its contribution to the total humic-bound actinide concentrations was negligible.

Rearranging equations (1) and (3) provides:

$$[AnHS] = b_{1;An}\,[An]\,[HS] \tag{5}$$

$$[(CaMg)HS] = b_{1;CaMg}\,[Ca+Mg]\,[HS] \tag{6}$$

Substituting equations (5) and (6) into equation (4) results in:

$$[HS_{tot}] = b_{1;An}\,[An]\,[HS] + b_{1;Ca,Mg}\,[Ca+Mg]\,[HS] + [HS] \tag{7}$$

Rearranging equation (7) provides:

$$[HS] = \frac{[HS_{tot}]}{b_{1;An}\,[An] + b_{1;CaMg}\,[Ca+Mg] + 1} \tag{8}$$

Equations (5), (6), and (8) were used to calculate humic-bound actinide concentrations ([AnHS]). The resulting AnHS concentration values were then summed for actinide elements with multiple oxidation states, and then divided by the dissolved concentration of the respective actinide element. The final forms of the parameter values PROPHUM, PHUMCIM, and PHUMSIM are proportionality constants in units of "moles humic-bound colloidal actinide per mole of dissolved actinide." In WIPP PA calculations, the proportionality values may be multiplied by the dissolved actinide concentration expressed in molarity or molality, depending on what the desired final unit should be. Note, however, that dissolved actinide element concentration to be used in that calculation must not include complexes containing commercial organic complexants (e.g., EDTA).

Depending on the intrusion scenario, the WIPP repository may be dominated by Castile brine or by intergranular Salado brine, resulting in different actinide solubilities. In addition to brine type, commercial organic complexants such as EDTA affect actinide solubilities. Finally, actinide solubilities are dependent on the mineral assemblage (either brucite plus magnesite, or portlandite plus calcite) buffering the system. On the basis of those scenarios, Siegel (1996) provided solubility parameters for the following eight brine compositions:

idpram	brine	invariant point	organic complexants
SOLSIM	Salado	$Mg(OH)_2$-$MgCO_3$-CO_2	absent
SOLSIC	Salado	$Ca(OH)_2$-$CaCO_3$-CO_2	absent
SOLCIM	Castile	$Mg(OH)_2$-$MgCO_3$-CO_2	absent
SOLCIC	Castile	$Ca(OH)_2$-$CaCO_3$-CO_2	absent
SOLSOM	Salado	$Mg(OH)_2$-$MgCO_3$-CO_2	present
SOLSOC	Salado	$Ca(OH)_2$-$CaCO_3$-CO_2	present
SOLCOM	Castile	$Mg(OH)_2$-$MgCO_3$-CO_2	present
SOLCOC	Castile	$Ca(OH)_2$-$CaCO_3$-CO_2	present

In determining the concentration of humic-bound actinides, we assume that dissolved actinides complexed with commercial organic complexants are not available for interaction with humic substances. Therefore the brines listed above with organic complexants present can be disregarded herein. Wang (1996) conducted calculations which demonstrate that the brines buffered by portlandite plus calcite will not be present in the WIPP repository. Therefore, those brines can be disregarded. For determination of humic-bound actinide concentrations, therefore, we are left with two brine types, designated by SOLSIM and SOLCIM above. The solubilities of actinides of oxidation states III, IV, V, and VI in those brines were provided by Siegel (1996) (solubility values are listed in molality):

IDPRAM:	IDMTRL: SOLMOD3	IDMTRL: SOLMOD4	IDMTRL: SOLMOD5	IDMTRL: SOLMOD6
SOLSIM	4.4e-6	5.0e-6	2.6e-6	1.0e-5
SOLCIM	4.1e-7	6.8e-9	2.5e-6	1.0e-5

In our calculations described herein, those values were used. Concentrations of Ca^{2+} and Mg^{2+} in those two brines were obtained from Novak and Moore (1996).

Calculations are summarized in three tables. Tables 1a and 1b are calculations using equations (5), (6), and (8) to determine humic-bound actinide concentrations ([AnHS]) for one or more humic substance type for Am(III), Th(IV), Np(V), and U(VI). In Tables 2a through 2f, results of Tables 1a and 1b are transferred to facilitate summing humic-bound actinide concentrations for actinide elements with multiple oxidation species. The oxidation state analogy is most heavily drawn on for plutonium, because stability constants for Pu(III) or Pu(IV) are not available.

In Table 3, results of Tables 2a through 2f are summarized according to brine type and humic substance type. Table 3 was used to formulate the final PROPHUM, PHUMCIM, and PHUMSIM parameter values provided to PA. For americium and uranium (i.e., III and VI oxidation states, respectively), for which the greatest amount of information is available, we have calculated a "most-likely value" for humic-bound actinide concentration by taking the largest values for fulvic acid, aromatic humic acid, and aliphatic humic, and calculated the arithmetic mean. We recommend that a triangular distribution be established about that "most-likely value." The "minimum value" and "maximum value" correspond to the largest humic-bound actinide concentrations associated with fulvic acid and aliphatic humic acid, respectively. For thorium, plutonium, and neptunium (i.e., IV, V, and V oxidation states, respectively), for which less information is available, we have used the largest humic-bound actinide value for each as the "most-likely value." No distribution is recommended for those three actinide elements. For uranium and americium, in the event that the distributions of parameter values cannot be sampled in the PA calculations, we recommend that the maximum value be used as a constant value. The decision of whether to use the distribution or the constant value is to be made by the PA Department.

The PROPHUM idpram, used in conjunction with idmtrls Th, U, Np, Pu, or U, is designed to be used to calculate actinide-humic concentration by element. The PHUMCIM and PHUMSIM idpram's, used in conjunction with idmtrls PHUMOX3, PHUMOX4, PHUMOX5, or PHUMOX6, provides the means to calculate actinide-humic concentrations by actinide oxidation state and for different brine intrusion scenarios. The latter approach may be more analogous to the approach used to determine concentrations of dissolved actinide elements in the repository. For example, in an E1 scenario under "reducing conditions" in the WIPP repository, PHUMCIM would be used with the following idmtrls to determine actinide-humic concentrations: thorium = PHUMOX4; uranium = PHUMOX4; neptunium = PHUMOX4; plutonium = PHUMOX3; and americium = PHUMOX3. For an E2 scenario under "oxidizing conditions" in the WIPP repository, PHUMSIM would be used with the following idmtrls to determine actinide-humic concentrations: thorium = PHUMOX4; uranium = PHUMOX6; neptunium = PHUMOX5; plutonium = PHUMOX4; and americium = PHUMOX3.

Uncertainties due to analytical precision are small compared to uncertainties in knowledge of the dominant humic substance type, site binding densities, and actinide solubilities. The proportionality factor approach coupled with the plus or minus one order-of-magnitude uncertainty in actinide solubilities results in a plus or minus one order-of-magnitude uncertainty in the concentration of actinides bound by mobile humic substances.

The CAPHUM parameter simply represents the theoretical maximum concentration of actinides that can be bound by a humic substance. Based on a solubility limit concentration of humic substances of 2.0 mg/L, and the highest site-binding capacity (for fulvic acids) of 5.56 meq OH^-/g, the theoretical maximum is 1.1×10^{-5} eq/L (refer to Tables 1a and b, column 4). Assuming the conservative case in which actinide species are monovalent, the maximum theoretical concentration of actinides that can be bound by humic substances is 1.1×10^{-5} molar. Note that that number is conservative, because it assumes a pool of humic substances is available for each actinide element, when in reality, actinide elements will compete for the same pool of humic substances. CAPHUM is intended to be used in an expression such as the following:

$$[\mathrm{AnHS}] = \mathrm{MIN}(\text{AnHS value calculated using PROPHUM, 1.1e-5}) \qquad (9)$$

Summary

Interpreted values for PROPHUM, PHUMCIM, PHUMSIM, and CAPHUM are summarized in Attachments C, E, and F.

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Table 1a. Complexation of actinides with humic substances in Castile brine in the presence of magnesium oxide backfill.

	pH	Am(III)	Th(IV)	Np(V)	U(VI)	Mg+Ca
Dissolved Actinide Concentration (molality)	9.24	4.12E-07	6.78E-09	2.53E-06	1.00E-05	5.76E-02

Actinide	Type of humic Substance	humic substance total amount mg/L	humic substance meq OH⁻/g	humic substance total capacity eq/L	$\beta_{1;An}$	$\beta_{1;(MgCa)}$	[HS] $_{free}$ molality	[An-HS] molality	[(MgCa)-HS] molality	Check sum: humic substance total cap. eq/L
Am(III)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	1.64E-06	2.69E-08	9.45E-06	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	1.23E+06	1.00E+02	1.28E-06	6.49E-07	7.37E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	1.05E+06	1.00E+02	1.50E-06	6.45E-07	8.62E-06	1.08E-05
Th(IV)	Constant ratio of humic bound actinide conc. to dissolved actinide conc. of 6.34 used in all calculations.									
Np(V)	Lake Bradford Humic Acid	2	4.65	9.30E-06	3.16E+02	1.00E+02	1.38E-06	1.10E-09	7.92E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	4.68E+03	1.00E+02	1.59E-06	1.88E-08	9.17E-06	1.08E-05
U(VI)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	1.55E-06	6.18E-07	8.95E-06	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	8.13E+05	1.00E+02	6.25E-07	5.08E-06	3.60E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	2.24E+05	1.00E+02	1.20E-06	2.68E-06	6.89E-06	1.08E-05

Table 1b. Complexation of actinides with humic substances in Salado brine in the presence of magnesium oxide backfill.

	pH	Am(III)	Th(IV)	Np(V)	U(VI)	Mg+Ca
Dissolved Actinide Concentration (molality)	8.69	4.39E-06	4.98E-06	2.64E-06	1.00E-05	5.42E-01

Actinide	Type of humic Substance	humic substance total amount mg/L	humic substance meq OH⁻/g	humic substance total capacity eq/L	$\beta_{1;An}$	$\beta_{1;(MgCa)}$	$[HS]_{free}$ molality	[An-HS] molality	[(MgCa)-HS] molality	Check sum: humic substance total cap. eq/L
Am(III)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	*3.98E+04*	*1.00E+02*	*2.01E-07*	*3.51E-08*	*1.09E-05*	*1.11E-05*
	Lake Bradford Humic Acid	2	4.65	9.30E-06	1.23E+06	1.00E+02	1.53E-07	8.29E-07	8.32E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	1.05E+06	1.00E+02	1.80E-07	8.27E-07	9.75E-06	1.08E-05
Th(IV)	Constant ratio of humic bound actinide conc. to dissolved actinide conc. of 6.34 used in all calculations.									
Np(V)	Lake Bradford Humic Acid	2	4.65	9.30E-06	3.16E+02	1.00E+02	1.68E-07	1.41E-10	9.13E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	4.68E+03	1.00E+02	1.95E-07	2.41E-09	1.06E-05	1.08E-05
U(VI)	Suwannee River Fulvic Acid	2	5.56	1.11E-05	3.98E+04	1.00E+02	2.00E-07	7.96E-08	1.08E-05	1.11E-05
	Lake Bradford Humic Acid	2	4.65	9.30E-06	8.13E+05	1.00E+02	1.47E-07	1.19E-06	7.98E-06	9.30E-06
	Gorleben Humic Acid	2	5.38	1.08E-05	2.24E+05	1.00E+02	1.87E-07	4.19E-07	1.02E-05	1.08E-05

Table 2a. Concentration of dissolved and fulvic acid complexed actinide for each oxidation state in Castile brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				moles fulvic acid bound actinide/ moles dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		6.78E-09		1.00E-05	6.2E-02.
Fulvic-U concentration		*		6.18E-07	
Np					
dissolved concentration		6.78E-09	2.53E-06		*
Fulvic-Np concentration		*	*		
Pu					
dissolved concentration	4.12E-07	6.78E-09			*
Fulvic-Pu concentration	*	*			
Am					
dissolved concentration	4.12E-07				6.5E-02
Fulvic-Am concentration	2.69E-08				
Th					
dissolved concentration		6.78E-09			*
Fulvic-Th concentration		*			

* no available information

Table 2b. Concentration of dissolved and fulvic acid complexed actinide for each oxidation state *in Salado brine in the presence of magnesium oxide backfill.*

Actinide	Oxidation State				mole fulvic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		4.98E-06		1.00E-05	8.0E-03
Fulvic-U concentration		*		7.96E-08	
Np					
dissolved concentration		4.98E-06	2.64E-06		*
Fulvic-Np concentration		*	*		
Pu					
dissolved concentration	4.39E-06	4.98E-06			*
Fulvic-Pu concentration	*	*			
Am					
dissolved concentration	4.39E-06				8.0E-03
Fulvic-Am concentration	3.51E-08				
Th					
dissolved concentration		4.98E-06			*
Fulvic-Th concentration		*			

* no available information

Table 2c. Concentration of dissolved and Gorleben humic acid (aromatic) complexed actinide for each oxidation state in Castile brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		6.78E-09		1.00E-05	2.7E-01
Humic-U concentration		4.30E-08		2.68E-06	
Np					
dissolved concentration		6.78E-09	2.53E-06		2.4E-02
Humic-Np concentration		4.30E-08	1.88E-08		
Pu					
dissolved concentration	4.12E-07	6.78E-09			1.6E+00
Humic-Pu concentration	6.45E-07	4.30E-08			
Am					
dissolved concentration	4.12E-07				1.6E+00
Humic-Am concentration	6.45E-07				
Th					
dissolved concentration		6.78E-09			6.3E+00
Humic-Th concentration		4.30E-08			

Table 2d. Concentration of dissolved and Gorleben humic acid (aromatic) complexed actinide for each oxidation state in Salado brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State (III)	(IV)	(V)	(VI)	mole humic acid bound actinide/ mole dissolved actinide concentration
U					
dissolved concentration		4.98E-06		1.00E-05	2.1E+00
Humic-U concentration		3.16E-05		4.19E-07	
Np					
dissolved concentration		4.98E-06	2.64E-06		4.1E+00
Humic-Np concentration		3.16E-05	2.41E-09		
Pu					
dissolved concentration	4.39E-06	4.98E-06			3.5E+00
Humic-Pu concentration	8.27E-07	3.16E-05			
Am					
dissolved concentration	4.39E-06				1.9E-01
Humic-Am concentration	8.27E-07				
Th					
dissolved concentration		4.98E-06			6.3E+00
Humic-Th concentration		3.16E-05			

Table 2e. Concentration of dissolved and Lake Bradford humic acid (aliphatic) complexed actinide for each oxidation state in Castile brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		6.78E-09		1.00E-05	5.1E-01
Humic-U concentration		4.30E-08		5.08E-06	
Np					
dissolved concentration		6.78E-09	2.53E-06		1.7E-02
Humic-Np concentration		4.30E-08	1.10E-09		
Pu					
dissolved concentration	4.12E-07	6.78E-09			1.7E+00
Humic-Pu concentration	6.49E-07	4.30E-08			
Am					
dissolved concentration	4.12E-07				1.6E+00
Humic-Am concentration	6.49E-07				
Th					
dissolved concentration		6.78E-09			6.3E+00
Humic-Th concentration		4.30E-08			

Table 2f. Concentration of dissolved and Lake Bradford humic acid (aliphatic) complexed actinide for each oxidation state in Salado brine in the presence of magnesium oxide backfill.

Actinide	Oxidation State				mole humic acid bound actinide/ mole dissolved actinide concentration
	(III)	(IV)	(V)	(VI)	
U					
dissolved concentration		4.98E-06		1.00E-05	2.2E+00
Humic-U concentration		3.16E-05		1.19E-06	
Np					
dissolved concentration		4.98E-06	2.64E-06		4.1E+00
Humic-Np concentration		3.16E-05	1.41E-10		
Pu					
dissolved concentration	4.39E-06	4.98E-06			3.5E+00
Humic-Pu concentration	8.29E-07	3.16E-05			
Am					
dissolved concentration	4.39E-06				1.9E-01
Humic-Am concentration	8.29E-07				
Th					
dissolved concentration		4.98E-06			6.3E+00
Humic-Th concentration		3.16E-05			

Table 3. Summary of humic substance actinide complexation in Castile and Salado brines in the presence of magnesium oxide backfill.

Actinide	Brine/ Backfill	Ratio of humic bound actinide to dissolved actinide concentration Suwannee River Fulvic Acid	Gorleben Humic Acid	Lake Bradford Humic Acid
U	Castile/Mg	6.2E-02	2.7E-01	5.1E-01
	Salado/Mg	8.0E-03	2.1E+00	2.2E+00
Pu	Castile/Mg	*	1.6E+00	1.7E+00
	Salado/Mg	*	3.5E+00	3.5E+00
Am	Castile/Mg	6.5E-02	1.6E+00	1.6E+00
	Salado/Mg	8.0E-03	1.9E-01	1.9E-01
Th	Castile/Mg	*	6.3E+00	6.3E+00
	Salado/Mg	*	6.3E+00	6.3E+00
Np	Castile/Mg	*	2.4E-02	1.7E-02
	Salado/Mg	*	4.1E+00	4.1E+00

* no available information

Attachment B:

Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 3/29/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

In order to properly model the transport of radionuclides within the Salado formation, we will need information about the possible transport of these radionuclide on colloids. In this memo we request the maximum mobilized radionuclide concentration and/or the proportionality constant defining the moles mobilized on colloid per moles in solution, for each transported element and colloid type. We are planning to transport Am, Pu, U, and Th, and may also transport Cm, Np, Ra, and Sr. If we transport Ra and Sr, we are planning to model them as very soluble, and not sorbed, so I believe modeling of colloids for them will not be necessary. For Cm solubility, we will be using the Am(III) model. If you believe that Cm colloids also behave similarly to Am colloids, we could extend the chemical analogy to the colloid behavior. If you agree with these simplifications then we will need the parameters for Am, Pu, U, Th and Np only.

Suggested names for database entry:
IDMTRL: Am, Pu, U, Th, Np

IDPRAM:

CONCINT	for concentration of actinide on mobilized intrinsic colloid
CONCMIN	for concentration of actinide on mobilized mineral fragments
CAPHUM	for maximum concentration of actinide on humic colloids
CAPMIC	for maximum concentration of actinide on microbe colloids
PROPHUM	for moles actinide mobilized on humic colloids per moles dissolved
PROPMIC	for moles actinide mobilized on microbe colloids per moles dissolved

You will need to provide a distribution for each material-parameter pair, but that distribution may be "CONSTANT" for most of the numbers. Eight sampling slots have been reserved for the most important of these parameters that have non-constant distributions.

cc:
Mary-Alena Martell
Hong-Nian Jow
E. James Nowak
James L. Ramsey
Amy S. Johnson
Martin S. Tierney
W. George Perkins
J. T. Schneider
Richard V. Bynum
Ali A. Shinta
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment C:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 29 March 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters

This memorandum summarizes best estimates for the mobile colloidal actinide source term for input to the WIPP Compliance Certification Application. The use of material and parameter identification codes is consistent with your letter to me dated 29 March 1996 requesting parameter values. In the attached table, I have provided best estimates for the following material-parameter combinations:

IDMTRL: Th, U, Np, Pu, Am

IDPRAM:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids
	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
	CAPHUM	maximum concentration of actinide associated with mobile humic colloids
	CAPMIC	maximum concentration of actinide associated with mobile microbes
	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids
	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes

As a first approximation, the colloidal behavior of curium can be simulated be using parameter values for americium. The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy to:

MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1320	E. James Nowak, 6831 EJN
MS 1320	R. Vann Bynum, 6831
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MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748 wgp
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt O. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851

SWCF-A:WBS1.1.10.2.1

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CONCMIN	Th	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
CONCMIN	U	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
CONCMIN	Np	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
CONCMIN	Pu	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
CONCMIN	Am	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
PROPHUM	Th	6.4e+00	6.4e+00	6.4e+00	moles colloidal humic-bound Th per moles dissolved Th	constant	2,3
PROPHUM	U	1.4e+00	1.6e-01	2.0e+00	moles colloidal humic-bound U per moles dissolved U	triangular	2,3,4
PROPHUM	Np	4.0e+00	4.0e+00	4.0e+00	moles colloidal humic-bound Np per moles dissolved Np	constant	2,3
PROPHUM	Pu	5.9e+00	5.9e+00	5.9e+00	moles colloidal humic-bound Pu per moles dissolved Pu	constant	2,3
PROPHUM	Am	2.5e+00	1.9e-01	3.9e+00	moles colloidal humic-bound Am per moles dissolved Am	triangular	2,3,4

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CAPHUM	Th	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
CAPHUM	U	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
CAPHUM	Np	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
CAPHUM	Pu	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
CAPHUM	Am	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general	The colloidal actinide source term is added to the dissolved actinide source term.
general	None of the parameters are correlated.
1	If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.
2	Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.
3	Proportionality constants are to be used with the sum of actinide oxidation species for each actinide element (uncomplexed only, i.e., without organic ligand contribution).
4	If a distribution is not used for humic-bound U or Am, use the maximum concentration as a constant value.
5	The maximum ("cap") values are in units comparable to molarity rather than molality.
6	CAPHUM is compared to the concentration of the respective humic-bound actinide element.
7	CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e. the sum of dissolved plus colloidal actinide).

Attachment D:

Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 4/2/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

YiFeng Wang has revised his recommendation to use 2 invariant points in the PA calculation. He now recommends that we use the $Mg(OH)_2 + MgCO_3$ invariant point for all calculations. If this invalidates the assumptions that you used to prepare colloid concentration or proportion parameters please indicate as soon as possible which parameters are affected, and as soon as possible after that provide a memo documenting the new values.

cc:
Mary-Alena Martell
Amy S. Johnson
Hong-Nian Jow
Martin S. Tierney
J. T. Schneider
Richard V. Bynum
E. James Nowak
W. George Perkins
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment E:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 18 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 1

This memorandum summarizes the revised best estimates for the mobile colloidal-actinide source term for input to the WIPP Compliance Certification Application. Values presented herein supersede the values provided to you on 29 March 1996 (Papenguth, 1996) in response to your memorandum of 29 March 1996 (Stockman, 1996a). The present memorandum addresses your request for modifications stated in your memorandum dated 2 April 1996 (Stockman, 1996b).

In the attached table, I have summarized the complete set of parameters and values for the mobile colloidal-actinide source term. Revised values for maximum actinide concentration values for humic substances and constants describing actinide concentrations associated with mineral-fragment-type colloidal particles are included. New values (i.e., corresponding to new idpram's and idmtrl's) for proportionality constants describing actinide concentrations associated with humic substances are also included.

The revisions described herein for humic substances reflect a shift in approach from proportionality constants describing actinide-humic concentration by element, to proportionality constants describing actinide-humic concentration by actinide oxidation state. That change affects treatment of actinide elements that will have multiple oxidation states in the WIPP repository [e.g., U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV)]. A second modification in approach, is that I now provide values for two cases: (1) a Castile brine in equilibrium with brucite and magnesite; and (2) a Salado brine in equilibrium with brucite and magnesite. For humic substances, the following material-parameter combinations apply:

IDMTRL: PHUMOX3 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 3;

	PHUMOX4	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4;
	PHUMOX5	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5; and
	PHUMOX6	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6.
IDPRAM:	PHUMCIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite);
	PHUMSIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite).

The revisions made for actinide concentration associated with mineral-fragment-type colloidal particles were made to include the potential contribution of actinide-mineral colloids formed in the Culebra. To accomplish that, the original repository source term values (Papenguth, 1996) have been doubled. That approach is not necessary for humic substances or actinide intrinsic colloids [i.e., Pu(IV)-polymer], because their concentrations are limited by solubilities. Concentrations of actinides associated with microbes are limited by the steady-state population of microbes in the repository, which will not increase when introduced to the Culebra.

The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, SNL technical memorandum dated 29 March 1996 to Christine T. Stockman.

Stockman, C.T., 1996a, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 29 March 1996 to Hans W. Papenguth.

Stockman, C.T., 1996b, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 2 April 1996 to Hans W. Papenguth.

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MS 1320	Malcolm D. Siegel, 6748
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MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
revised (new)	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
revised	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
revised	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
revised	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
revised	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

Attachment F:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 22 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 2

In my rush to complete and distribute Revision 1 (Papenguth, 1996), I made mistakes on the minimum and maximum values for actinide concentrations associated with mineral-fragment-type colloidal particles. The attached Table contains the correct values.

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL technical memorandum dated 18 April 1996 to Christine T. Stockman.

copy to:

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MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7
	Notes:							
	general	The colloidal actinide source term is added to the dissolved actinide source term.						
	general	None of the parameters are correlated.						
	1	If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.						
	2	Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.						
	3	Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).						
	4	If a distribution is not used, use the maximum concentration as a constant value.						
	5	The maximum ("cap") values are in units comparable to molarity rather than molality.						
	6	CAPHUM is compared to the concentration of the respective humic-bound actinide element.						
	7	CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).						

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.8

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WPO # 35850

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 7 May 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Parameter Record Package for Colloidal Actinide Source Term Parameters

Attached is the Parameter Record Package for the WIPP PA parameters describing actinide concentrations associated with mobile **mineral fragment type colloids**. This Package is one of four describing the concentration of actinides associated with the four colloidal particle types. The complete set of Packages consists of the following:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy with Attachments to:

MS 1320	Hans W. Papenguth, 6748
MS 1320	W. George Perkins, 6748
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

[redacted]

copy without Attachments to:

MS 1320	E. James Nowak, 6831
MS 1324	Susan A. Howarth, 6115
MS 1328	Hong-Nian Jow, 6741
MS 1328	Amy S. Johnson, 6741
MS 1328	Martin S. Tierney, 6741
MS 1328	Mary-Alena Martell, 6749
MS 1341	John T. Holmes, 6748

Parameter Record Package for Mobile-Colloidal Actinide Source Term.
Part 1. Mineral Fragment Type Colloids

The parameter values in this package are based on data which were collected under the guidance of the Principal Investigator for the Waste Isolation Pilot Plant (WIPP) Colloid Research Program, Hans W. Papenguth, for input to the WIPP Data Entry Form and for use in WIPP Performance Assessment (PA) calculations.

I. *Parameter No. (id):* Not applicable.

II. *Data/Parameter:* Not applicable.

III. *Parameter id (idpram):* CONCMIN.

IV. *Material:* Mineral fragment type colloidal particles and the actinides Th, U, Np, Pu, and Am.

V. *Material Identification (idmtrl):* Th, U, Np, Pu, and Am.

VI. *Units:* For CONCMIN, the units are "moles colloidal mineral-fragment-bound actinide per liter of dispersion."

VII. *Distribution Information.*

A. *Category:* The development of parameter values and their distributions is described in Attachment A. Summaries of the parameter values are presented in Attachments C, E, and F. Triangular distributions are supplied for CONCMIN values for each of the five actinide elements (idmtrl). In the event that those triangular distributions of parameter values cannot be sampled in the PA calculations, the maximum value should be selected. The decision of whether to use the distribution or the constant value is to be made by the PA Department.

B. *Mean:* See Attachments A, C, E, and F. (Note that for triangular distributions, the apices of the triangle are defined by the minimum value, the most likely value, and the maximum value; refer to Attachments).

C. *Median:* Not applicable.

D. *Standard Deviation:* Not applicable.

E. *Maximum:* See Attachments A, C, E, and F.

F. *Minimum:* See Attachments A, C, E, and F.

G. *Number of data points:* Not applicable.

VIII. *Data Collection and Interpretation Information.*

A. *Data Source Information:* WIPP observational data and literature.

B. *Data Collection (for WIPP observational data).*

1. *Data Collection or Test Method:* Experiments were conducted at SNL (Hans W. Papenguth and co-workers). Descriptions of experiments conducted at those institutions are described in Attachment A.

2. *Assumptions Made During Testing:* See Attachment A.

3. *Standard Error of Measurement of Tests Performed:* See Attachment A.

4. *Form of Raw Data:* Measurements of residual concentrations of colloidal particles are reported in number population.

5. *References Related to Data Collection:* See Attachment A.

6. *QA Status of Data:*

   a. *Are all of the data qualified?* Yes.

   b. *Were data qualified by QAP 20-3?* No. Data packages will be submitted for work conducted, under File code WBS 1.1.10.2.1.

   c. *Were the data the subject of audit/surveillance by SNL or DOE?* Yes.

   d. *Were the data collected under an SNL approved QA program?* Yes. Data were collected under SNL WIPP QAPD, Rev. P, effective October 1, 1992, and SNL WIPP QAPD, Rev. R, effective July 31, 1995. Data were collected under a test plan for the WIPP Colloid Research Program (Papenguth and Behl, 1996. Detailed descriptions of the experiments and interpretation listed herein will be published in a SAND report. Documents related to data collection at SNL will be archived in the Sandia WIPP Central Files (SWCF; File code WBS 1.1.10.2.1).

C. *Interpretation of Data.*

1. *Was the interpretation made by reference to previous work.* No.

2. *Was the interpretation made by using newly performed calculations?* Yes.

3. *Form of Interpreted Data.* List of interpreted values.

4. *Assumptions Made During Interpretation.* See Attachment A.

5. *Name of Code(s)/Software used to Interpret Data:* Not applicable.

6. *QA Status of Code(s) used to Interpret Data:* Not applicable.

   a. *Was the code qualified under QAP 19-1?* Not applicable.

   b. *Was the code qualified under QAP 9-1?* Not applicable.

7. *References Related to Data Interpretation:* See XI below and Attachment A.

8. *For interpretations made by using a newly performed calculations provide documentation that you followed the requirements of QAP 9-1 Appendix B.* The

data analysis is controlled by Analysis Plan for the Colloid Research Program, AP-004 (Behl and Papenguth, 1996).

9. *For routine calculations (not using code) did you follow requirements of QAP 9-5?* Yes.

IX. *Correlation with other Parameters:* Parameter values describing the concentration of actinides associated with mobile humic substances are linked to solubility of the dissolved actinides, with a maximum value which cannot be exceeded.

X. *Limitations or qualifications for usage of data by Performance Assessment (PA):* None.

XI. *References cited above:*

Behl, Y.K., and Papenguth, H.W., 1996, Analysis Plan for the WIPP Colloid Research Program WBS #1.1.10.2.1, SNL Analysis Plan AP-004.

Papenguth, H.W., and Behl, Y.K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

XII. *Attachments:*

Attachment A:	Papenguth, Hans W., and Aguilar, Richard, 1996, Rationale for Definition of Parameter Values for Mineral Fragment Type Colloidal Particles.
Attachment B:	Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.
Attachment C:	Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.
Attachment D:	Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.
Attachment E:	Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.
Attachment F:	Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

XIII. *Distribution*

SWCF-A:WPO# 35850: Mobile-Colloidal Actinide Source Term. 1. Mineral Fragment Colloids.

SWCF-A:WBS 1.1.10.2.1: Colloid Characterization and Transport.

Attachment A:

Papenguth, Hans W., and Aguilar, Richard, 1996, Rationale for Definition of Parameter Values for Mineral Fragment Type Colloids.

Attachment A.

Rationale for Definition of Parameter Values for Mineral Fragment Type Colloids

Hans W. Papenguth and Richard Aguilar

Introduction

The actinide source term at the WIPP is defined as the sum of contributions from dissolved actinide species and mobile colloidal actinide species. The dissolved actinide source term has been defined elsewhere (Novak, 1996; Novak and Moore, 1996; Siegel, 1996). It is important to note that colloidal actinides which are not suspended in the aqueous phase (i.e., not mobile) are not included in the colloidal actinide source term. Colloidal actinides may become immobilized by several mechanisms, including precipitation followed by coagulation and gravitational settling (humic substances and actinide intrinsic colloids), adhesion to fixed substrates (microbes), and flocculation or coagulation of colloidal particles followed by gravitational settling (mineral fragments). Sorption of colloidal actinides onto fixed substrates will also reduce the mobile colloidal actinide source term, but no credit is currently being taken for reduction by that means.

To facilitate quantification of the colloidal actinide source term, as well as an efficient experimental approach, the source term has been divided into four components according to colloid types. On the basis of (1) the behavior of colloidal particles in high ionic strength electrolytes, (2) the way in which colloidal particles interact with actinide ions, and (3) the transport behaviors of colloidal particles, four colloidal particle types are recognized (Papenguth and Behl, 1996): mineral fragments, actinide intrinsic colloids, humic substances, and microbes.

In this document, we focus on the quantification of the actinide concentration mobilized by mineral fragment type colloidal particles. In terms of the WIPP performance assessment (PA) calculations, we discuss the rationale for selecting the values corresponding to the following parameter designators:

idpram:	CONCMIN	<u>conc</u>entration of actinide associated with mobile <u>min</u>eral fragment colloids.
idmtrl:	Th	thorium;
	U	uranium;
	Np	neptunium;
	Pu	plutonium; and
	Am	americium.

Mineral fragment type colloidal particles may be present in naturally occurring groundwaters, and they may be released from the host rock due to disruption of fragile aggregates by changes in ionic strength or hydrodynamic forces, dissolution of a more soluble surrounding matrix, mechanical grinding of mineral surfaces, or mechanical disruption of secondary minerals present at mineral surfaces. Under certain conditions, such as extreme changes in ionic strength of the groundwater or by physical disruption due to natural or human-induced events, mineral fragment type colloidal particles could also be produced within the Culebra. In an intrusion scenario at the WIPP, mixing of repository brines with Culebra brines is likely to result in mineral precipitation which may include coprecipitation of actinide-bearing mineral fragment type colloidal particles. Within the repository, mineral fragment type colloidal particles may form from corrosion of iron-bearing waste and the steel packaging materials. In addition, Portland cement based matrixes will be attacked and will produce mineral fragment type colloidal particles. Bentonite, which may be a constituent of drilling mud is itself a potential source of mineral fragment type colloidal material that should be considered for actinide transport.

In terms of colloidal actinide transport, mineral fragment type colloids act as carriers, in that actinide ions sorb onto the surfaces of the colloids. Because each mineral substrate has a different affinity for actinides, quantification of actinide concentrations associated with the wide range of mineralogies likely to be present at the WIPP is insurmountable. Instead, we elected to use a bounding approach based on residual concentrations of colloidal particles in WIPP-relevant brines coupled with estimates of reasonable maximum concentrations of actinides which could be sorbed onto the colloid surfaces. That approach requires three pieces of information: (1) the number population of mineral fragment type colloidal particles in the aqueous phase; (2) the geometric surface area of individual colloidal particles; and (3) the site-binding capacity of the mineral surface. In the remainder of this document, we focus on the determination of items (1) through (3), the interpretation of that information, and the development of parameter values suitable for PA calculations.

Experimental

Hydrophobic colloidal particles, such as mineral fragments, are kinetically stabilized and destabilized by electrostatic forces (refer to detailed discussion in Papenguth and Behl, 1996, Sections 2.5.1 and 2.6). In an aqueous dispersant, hydrophobic colloidal particles are attracted to one another by van der Waals forces. That electrostatic attraction is countered by repulsive forces generated by a cloud of counterions surrounding each particle. In a kinetically stable colloidal dispersion colloidal particles are usually repelled from one another before they get close enough to become agglomerated. However, as the ionic strength of the dispersion is increased, the thickness of the cloud of counterions is compressed, allowing closer particle-particle interaction. The net effect is that as colloidal particles come into proximity with one another in the dispersion, a greater chance for sticking exists, and so the rate of agglomeration increases. That phenomenon is very effective at removing colloidal particles from suspension even at fairly low ionic strengths over periods of hours to days.

The kinetic stability of the mineral-fragment-type colloids in WIPP-relevant brines was evaluated in coagulation series experiments. Colloidal dispersions of mineral fragments were prepared by mechanical disaggregation of representative mineral, rock samples, and other materials or by chemical precipitation from laboratory reagents. Brine simulants were prepared which covered the ranges of ionic strengths observed in WIPP brines. The brines were sequentially diluted with deionized water by factors of 10 and adjusted to acidic, neutral, and basic pH conditions to evaluate the effects of ionic strength and pH on kinetic stability. At the ionic strength referred to as the critical coagulation concentration (c.c.c.), colloidal particles will rapidly coagulate, forming agglomerates large enough to settle by gravitational forces. The number population of colloidal particles remaining in suspension in the various dispersions was measured over time to assess their stability as a function of solution ionic strength and time.

Colloidal dispersions were prepared for the following minerals or materials: bentonite, kaolinite, montmorillonite, vermiculite, illite, anhydrite, calcium carbonate, magnesite, hematite (mechanically disaggregated), hematite (chemical precipitate), limonite, goethite, magnetite, quartz, siderite, brucite, strontianite, diatomaceous earth, pyrite, and cellulosic materials (Masslinn paper towels and Scott paper towels). The brine solutions used included a Salado-like brine simulant (SPC brine) and a Culebra brine simulant (H-17). For c.c.c. experiments, sequential dilutions of those brines were made which spanned approximately five orders-of-magnitude. Brine simulants consisting of 0.5M NaCl or $CaCl_2$ were also used. For the residual concentration measurements which were used as the basis for the PA deliverables described herein, the one order-of-magnitude dilution (i.e., 10 percent of original strength) of the Salado-like brine and the Culebra brine simulants were used. That reduction in ionic strength provides a degree of conservatism in the results.

C.c.c. experiments for the various concentrations of WIPP brine simulants were conducted under acidic (observed pH generally ranging from 3 to 4), neutral (pH 6 to 8), and basic (pH 9 to 12) conditions. Following the introduction of an aliquot of dispersed colloidal particles to a series of test tubes containing the sequentially diluted brine, colloidal particle concentrations remaining near the top of the fluid columns (residual concentration) were measured as a function of time. The degree of coagulation and settling was quantified using an inductively coupled argon-plasma atomic emission spectrophotometer (ICP-AES), nephelometry, and direct particle counting.

Most of the experiments conducted relating to the kinetic stability of mineral fragment colloidal particles were qualitative to semi-quantitative, and were focused on evaluating whether a c.c.c.

existed. For the final experiments, however, we used a state-of-the-art particle spectrometer designed for semiconductor fabrication plants, which require extremely pure processing water, and use a similar instrument to ascertain purity. Our final experiments were conducted over an extended period of time using that more sensitive analytical technique to determine the number and size of colloids in the brine suspensions. Those experiments were conducted in a similar fashion to previous experiments for bentonite (Aldrich Chemical Co.), goethite, and hematite (mechanically disaggregated), but in a relatively dilute (and therefore conservative) brine simulant consisting of 0.1 M NaCl. Residual particle concentrations made with the particle spectrometer compared favorably with measurements made with spectroscopic techniques made at similar experiment times. Generally after the first day of the c.c.c. experiments, the majority (greater than 99 percent) of the colloidal particles had already settled out of suspension. With the more sensitive particle spectrometer, however, residual concentrations of colloidal particles were observed to continue to decrease. For experiments analyzed by spectroscopic or light-scattering techniques, final residual colloid number populations remaining suspended in the test vessels were determined by multiplying the initial colloid number populations determined at the start of our experiments by the fraction of suspended colloids remaining at the final reading. Using the particle spectrometer, final number populations were measured directly.

Discussion

Parameter values (CONCMIN) describing the amount of actinide element bound by mineral fragment type colloidal particles were determined from the information described above, combined with estimates of adsorption site densities.

Actinides sorbed to the surfaces of colloidal particles can be estimated using ranges of values for adsorption site densities taken from published surface complexation modeling research. The actinide concentration contained by a single mineral fragment type colloidal particle is calculated by considering the geometrical surface area of a spherical particle:

$$[An]_p = \frac{\pi D^2 N_s}{N_A} \qquad (1)$$

where:

$[An]_p$ = concentration of an adsorbed actinide element (moles/particle)
D = spherical colloidal particle diameter (nm)
N_s = adsorption site density (sites/nm^2)
N_A = Avogadro constant

An adsorption site density of 1 site/nm^2 was used for N_s in the above equation, a value which we believe is conservative. With that site density, 10 nm and 1 μm diameter particles could have a maximum of about 10^{-22} and 10^{-18} moles actinide per particle, respectively. To obtain an estimate of the maximum actinide concentrations that could be associated with the colloids, the estimates of residual colloid number populations (particles per liter of dispersion) were multiplied by the estimated maximum actinide transport capacity described by equation (1). Our use of a uniform adsorption site density is a conservative approach, because the actual sorption on mineral surfaces should be described by some kind of isotherm which will result in less than 100 percent coverage.

Interpreted Results

Final residual colloid number populations quantified by spectrophotometry or nephelometry showed that mineral fragment type colloidal particles are kinetically destabilized by brines similar in composition to those present at the WIPP Site. Colloid number population values were, with a few exceptions, reduced to less than 5 percent of the initial values within 1 day. Conservative estimates of maximum actinide concentrations associated with those residual colloid populations are on the order of 10^{-7} to 10^{-9} moles actinide per liter of dispersion.

The final experiments, which utilized the particle spectrometer to measure the quantity of colloids remaining in suspension offered the most sensitive estimates. Moreover, those experiments were conducted for substantially longer periods of time than the semi-quantitative c.c.c. experiments. Those experimental results are the following:

Mineral	Time of final reading (days)	Estimated actinide concentration (moles/L dispersion)
hematite	12.8	1.6×10^{-8}
goethite	12.9	9.5×10^{-10}
bentonite	12.8	1.6×10^{-10}
geometric mean		1.3×10^{-9}

We believe that the experimental results using the particle spectrometer, although only reflecting three distinct colloids (hematite, goethite, and bentonite), are representative of other mineral fragment type colloidal particles in terms of their behavior in brine solutions. The geometric mean was assumed to be a more representative average of the final colloid concentrations than the arithmetic mean because of the very small final colloid concentrations (which, for this particular case, is also conservative).

Mineral fragment type colloidal particles are unique among the four colloidal particle types addressed for WIPP, because their concentrations are not generally linked to solubility, as are actinide intrinsic colloids and humic substances, or to a maximum supportable population in the case of microbes. Consequently, in an intrusion scenario at the WIPP, as dissolved actinide elements are introduced to the Culebra, it is possible that those dissolved actinides could sorb onto a separate population of indigenous mineral fragments, producing a supplemental source term. To account for that possibility, we recommend multiplying the geometric mean value listed above by a factor of two, producing a final "most-likely value" of 2.6×10^{-9} moles actinide per liter of dispersion.

To capture uncertainty, mainly stemming from knowledge of the adsorption site density value, we recommend a triangular distribution with "minimum values" and "maximum values" spanning one order of magnitude about the geometric mean.

Summary

Interpreted values for CONCMIN are summarized in Attachments C, E, and F. In those values, we have incorporated conservatism in two ways. First, we have increased the experimental results by a factor of two to account for the possibility that the indigenous mineral fragment colloidal particles in the Culebra could sorb dissolved actinides (see Attachment F). Second, we have essentially multiplied the total concentration of actinides carried by mineral fragment colloidal particles by a factor of five, because we have assumed a separate population of colloidal particles for each actinide element. No consideration of competition for sorption sites is incorporated into our calculation approach. We believe that the value used for adsorption site density is conservative, but reasonable. The triangular distribution of one-order-of-magnitude about the "most-likely value" essentially captures our uncertainty in site density values. If the WIPP PA Department elects to not use the triangular distribution in their calculations, we recommend that the "maximum values" be used as constant values.

References

Novak, C. F., 1996, The Waste Isolation Pilot Plant (WIPP) Actinide Source Term Program: Test Plan for the Conceptual Model and the Dissolved Concentration Submodel, Albuquerque, New Mexico, Sandia National Laboratories, SAND95-1895 (submitted).

Novak, C. F., and Moore, R. C., 1996, Estimates of dissolved Concentration for +III, +IV, +V, and +VI Actinides in a Salado and a Castile Brine under Anticipated Repository Condtions. SNL Technical memorandum dated 28 March 1996 to Malcolm D. Siegel.

Papenguth, H. W., and Behl, Y. K., 1996, Test Plan for Evaluation of Colloid-Facilitated Actinide Transport at the Waste Isolation Pilot Plant, SNL Test Plan TP 96-01.

Siegel, M. D., 1996, Solubility parameters for use in the CCA NUTS and GRIDFLOW calculations. SNL Technical memorandum dated 29 March 1996 to Martin S. Tierney.

Attachment B:

Stockman, Christine T., 1996, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 29 March 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 3/29/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

In order to properly model the transport of radionuclides within the Salado formation, we will need information about the possible transport of these radionuclide on colloids. In this memo we request the maximum mobilized radionuclide concentration and/or the proportionality constant defining the moles mobilized on colloid per moles in solution, for each transported element and colloid type. We are planning to transport Am, Pu, U, and Th, and may also transport Cm, Np, Ra, and Sr. If we transport Ra and Sr, we are planning to model them as very soluble, and not sorbed, so I believe modeling of colloids for them will not be necessary. For Cm solubility, we will be using the Am(III) model. If you believe that Cm colloids also behave similarly to Am colloids, we could extend the chemical analogy to the colloid behavior. If you agree with these simplifications then we will need the parameters for Am, Pu, U, Th and Np only.

Suggested names for database entry:
IDMTRL: Am, Pu, U, Th, Np

IDPRAM:

CONCINT	for concentration of actinide on mobilized intrinsic colloid
CONCMIN	for concentration of actinide on mobilized mineral fragments
CAPHUM	for maximum concentration of actinide on humic colloids
CAPMIC	for maximum concentration of actinide on microbe colloids
PROPHUM	for moles actinide mobilized on humic colloids per moles dissolved
PROPMIC	for moles actinide mobilized on microbe colloids per moles dissolved

You will need to provide a distribution for each material-parameter pair, but that distribution may be "CONSTANT" for most of the numbers. Eight sampling slots have been reserved for the most important of these parameters that have non-constant distributions.

cc:
Mary-Alena Martell
Hong-Nian Jow
E. James Nowak
James L. Ramsey
Amy S. Johnson
Martin S. Tierney
W. George Perkins
J. T. Schneider
Richard V. Bynum
Ali A. Shinta
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment C:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters. SNL Technical Memorandum dated 29 March 1996 to Christine T. Stockman.

Sandia National Laboratories
Albuquerque, New Mexico 87185

date: 29 March 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters

This memorandum summarizes best estimates for the mobile colloidal actinide source term for input to the WIPP Compliance Certification Application. The use of material and parameter identification codes is consistent with your letter to me dated 29 March 1996 requesting parameter values. In the attached table, I have provided best estimates for the following material-parameter combinations:

IDMTRL: Th, U, Np, Pu, Am

IDPRAM:	CONCINT	concentration of actinide associated with mobile actinide intrinsic colloids
	CONCMIN	concentration of actinide associated with mobile mineral fragment colloids
	CAPHUM	maximum concentration of actinide associated with mobile humic colloids
	CAPMIC	maximum concentration of actinide associated with mobile microbes
	PROPHUM	proportionality constant for concentration of actinides associated with mobile humic colloids
	PROPMIC	proportionality constant for concentration of actinides associated with mobile microbes

As a first approximation, the colloidal behavior of curium can be simulated be using parameter values for americium. The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

copy to:

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MS 1328	Martin S. Tierney, 6741
MS 1320	E. James Nowak, 6831 EJN
MS 1320	R. Vann Bynum, 6831
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MS 1341	Laurence H. Brush, 6748
MS 1341	Robert C. Moore, 6748
MS 1341	W. Graham Yelton, 6748
MS 1320	W. George Perkins, 6748 wgp
MS 1320	John W. Kelly, 6748
MS 1320	Daniel A. Lucero, 6748
MS 1320	Craig F. Novak, 6748
MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt O. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851

SWCF-A:WBS1.1.10.2.1

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CONCMIN	Th	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
CONCMIN	U	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
CONCMIN	Np	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
CONCMIN	Pu	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
CONCMIN	Am	1.3e-09	1.3e-10	1.3e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
PROPHUM	Th	6.4e+00	6.4e+00	6.4e+00	moles colloidal humic-bound Th per moles dissolved Th	constant	2,3
PROPHUM	U	1.4e+00	1.6e-01	2.0e+00	moles colloidal humic-bound U per moles dissolved U	triangular	2,3,4
PROPHUM	Np	4.0e+00	4.0e+00	4.0e+00	moles colloidal humic-bound Np per moles dissolved Np	constant	2,3
PROPHUM	Pu	5.9e+00	5.9e+00	5.9e+00	moles colloidal humic-bound Pu per moles dissolved Pu	constant	2,3
PROPHUM	Am	2.5e+00	1.9e-01	3.9e+00	moles colloidal humic-bound Am per moles dissolved Am	triangular	2,3,4

Mobile-Colloidal-Actinide Source Term—Concentration/Proportionality Constants

Parameter	Material	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
CAPHUM	Th	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
CAPHUM	U	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
CAPHUM	Np	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
CAPHUM	Pu	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
CAPHUM	Am	1.5e-05	1.5e-05	1.5e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.
general None of the parameters are correlated.
1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.
2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.
3 Proportionality constants are to be used with the sum of actinide oxidation species for each actinide element (uncomplexed only, i.e., without organic ligand contribution).
4 If a distribution is not used for humic-bound U or Am, use the maximum concentration as a constant value.
5 The maximum ("cap") values are in units comparable to molarity rather than molality.
6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.
7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e. the sum of dissolved plus colloidal actinide).

Attachment D:

Stockman, Christine T., 1996, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations. SNL Technical Memorandum dated 2 April 1996 to Hans W. Papenguth.

Sandia National Laboratories
Operated for the U.S. Department of Energy by
Sandia Corporation

Albuquerque, New Mexico 87185-

date: 4/2/96

to: Hans W. Papenguth

Christine T. Stockman

from: Christine T. Stockman

subject: Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations

YiFeng Wang has revised his recommendation to use 2 invariant points in the PA calculation. He now recommends that we use the $Mg(OH)_2 + MgCO_3$ invariant point for all calculations. If this invalidates the assumptions that you used to prepare colloid concentration or proportion parameters please indicate as soon as possible which parameters are affected, and as soon as possible after that provide a memo documenting the new values.

cc:
Mary-Alena Martell
Amy S. Johnson
Hong-Nian Jow
Martin S. Tierney
J. T. Schneider
Richard V. Bynum
E. James Nowak
W. George Perkins
SWCF-A:WBS1.2.07.1.1:PDD:QA:GENERAL

Attachment E:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL Technical Memorandum dated 18 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 18 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 1

This memorandum summarizes the revised best estimates for the mobile colloidal-actinide source term for input to the WIPP Compliance Certification Application. Values presented herein supersede the values provided to you on 29 March 1996 (Papenguth, 1996) in response to your memorandum of 29 March 1996 (Stockman, 1996a). The present memorandum addresses your request for modifications stated in your memorandum dated 2 April 1996 (Stockman, 1996b).

In the attached table, I have summarized the complete set of parameters and values for the mobile colloidal-actinide source term. Revised values for maximum actinide concentration values for humic substances and constants describing actinide concentrations associated with mineral-fragment-type colloidal particles are included. New values (i.e., corresponding to new idpram's and idmtrl's) for proportionality constants describing actinide concentrations associated with humic substances are also included.

The revisions described herein for humic substances reflect a shift in approach from proportionality constants describing actinide-humic concentration by element, to proportionality constants describing actinide-humic concentration by actinide oxidation state. That change affects treatment of actinide elements that will have multiple oxidation states in the WIPP repository [e.g., U(IV) and U(VI); Np(IV) and Np(V); Pu(III) and Pu(IV)]. A second modification in approach, is that I now provide values for two cases: (1) a Castile brine in equilibrium with brucite and magnesite; and (2) a Salado brine in equilibrium with brucite and magnesite. For humic substances, the following material-parameter combinations apply:

IDMTRL: PHUMOX3 proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 3;

	PHUMOX4	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 4;
	PHUMOX5	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 5; and
	PHUMOX6	proportionality constant for concentration of actinides associated with mobile humic substances, for actinide elements with oxidation state 6.
IDPRAM:	PHUMCIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Castile brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite);
	PHUMSIM	proportionality constant for concentration of actinides associated with mobile humic colloids, in Salado brine, actinide solubilities are inorganic only (no man-made ligands), brine is in equilibrium with Mg-bearing minerals (brucite and magnesite).

The revisions made for actinide concentration associated with mineral-fragment-type colloidal particles were made to include the potential contribution of actinide-mineral colloids formed in the Culebra. To accomplish that, the original repository source term values (Papenguth, 1996) have been doubled. That approach is not necessary for humic substances or actinide intrinsic colloids [i.e., Pu(IV)-polymer], because their concentrations are limited by solubilities. Concentrations of actinides associated with microbes are limited by the steady-state population of microbes in the repository, which will not increase when introduced to the Culebra.

The basis for the values summarized in the attached table is described in the following record packages for WBS 1.1.10.2.1:

WPO#	Parameter Record Package Name
35850	Mobile-Colloidal-Actinide Source Term. 1. Mineral Fragment Colloids
35852	Mobile-Colloidal-Actinide Source Term. 2. Actinide Intrinsic Colloids
35855	Mobile-Colloidal-Actinide Source Term. 3. Humic Substances
35856	Mobile-Colloidal-Actinide Source Term. 4. Microbes

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, SNL technical memorandum dated 29 March 1996 to Christine T. Stockman.

Stockman, C.T., 1996a, Request for colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 29 March 1996 to Hans W. Papenguth.

Stockman, C.T., 1996b, Request for any modifications to the colloid parameters for use in NUTS, GRIDFLOW and direct brine release calculations, SNL technical memorandum dated 2 April 1996 to Hans W. Papenguth.

copy to:

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MS 1328	Martin S. Tierney, 6741
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MS 1320	Hans W. Papenguth, 6748
MS 1320	Malcolm D. Siegel, 6748
MS 1324	Susan A. Howarth, 6115
MS 1341	Kurt W. Larson, 6747
MS 1341	Ruth F. Weiner, 6747
MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-09	2.6e-09	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
revised (new)	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
revised (new)	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
revised (new)	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
revised	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
revised	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
revised	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
revised	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

Attachment F:

Papenguth, Hans W., 1996, Colloidal Actinide Source Term Parameters, Revision 2. SNL Technical Memorandum dated 22 April 1996 to Christine T. Stockman.

Sandia National Laboratories

Albuquerque, New Mexico 87185

date: 22 April 1996

to: Christine T. Stockman, MS-1328 (Org. 6749)

Hans W. Papenguth

from: Hans W. Papenguth, MS-1320 (Org. 6748)

subject: Colloidal Actinide Source Term Parameters, Revision 2

In my rush to complete and distribute Revision 1 (Papenguth, 1996), I made mistakes on the minimum and maximum values for actinide concentrations associated with mineral-fragment-type colloidal particles. The attached Table contains the correct values.

References

Papenguth, H.W., 1996, Colloidal Actinide Source Term Parameters, Revision 1. SNL technical memorandum dated 18 April 1996 to Christine T. Stockman.

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MS 1324	Richard Aguilar, 6851
DOE/CAO	Robert A. Stroud

SWCF-A:WBS1.1.10.2.1

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
revised	CONCMIN	Th	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Th per liter of dispersion	triangular	1
revised	CONCMIN	U	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound U per liter of dispersion	triangular	1
revised	CONCMIN	Np	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Np per liter of dispersion	triangular	1
revised	CONCMIN	Pu	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Pu per liter of dispersion	triangular	1
revised	CONCMIN	Am	2.6e-09	2.6e-10	2.6e-08	moles colloidal mineral-fragment-bound Am per liter of dispersion	triangular	1
	CONCINT	Th	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Th per liter of dispersion	constant	
	CONCINT	U	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal U per liter of dispersion	constant	
	CONCINT	Np	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Np per liter of dispersion	constant	
	CONCINT	Pu	1.0e-09	1.0e-09	1.0e-09	moles actinide-intrinsic colloidal Pu per liter of dispersion	constant	
	CONCINT	Am	0.0e+00	0.0e+00	0.0e+00	moles actinide-intrinsic colloidal Am per liter of dispersion	constant	
	PHUMSIM	PHUMOX3	1.3e-01	8.0e-03	1.9e-01	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMSIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMSIM	PHUMOX5	4.8e-04	5.3e-05	9.1e-04	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMSIM	PHUMOX6	5.6e-02	8.0e-03	1.2e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4
	PHUMCIM	PHUMOX3	1.1e+00	6.5e-02	1.6e+00	moles colloidal humic-bound actinide (III) per moles dissolved actinide (III)	triangular	2,3,4
	PHUMCIM	PHUMOX4	6.3e+00	6.3e+00	6.3e+00	moles colloidal humic-bound actinide (IV) per moles dissolved actinide (IV)	constant	2,3
	PHUMCIM	PHUMOX5	3.9e-03	4.3e-04	7.4e-03	moles colloidal humic-bound actinide (V) per moles dissolved actinide (V)	triangular	2,3,4
	PHUMCIM	PHUMOX6	2.8e-01	6.2e-02	5.1e-01	moles colloidal humic-bound actinide (VI) per moles dissolved actinide (VI)	triangular	2,3,4

Status	Parameter (IDPRAM)	Material (IDMTRL)	Most Likely Value	Minimum Value	Maximum Value	Units	Distribution Type	Notes
	CAPHUM	Th	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Th per liter of dispersion	constant	5,6
	CAPHUM	U	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound U per liter of dispersion	constant	5,6
	CAPHUM	Np	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Np per liter of dispersion	constant	5,6
	CAPHUM	Pu	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Pu per liter of dispersion	constant	5,6
	CAPHUM	Am	1.1e-05	1.1e-05	1.1e-05	moles colloidal humic-bound Am per liter of dispersion	constant	5,6
	PROPMIC	Th	3.1e+00	3.1e+00	3.1e+00	moles microbial Th per moles dissolved Th	constant	2,3
	PROPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles microbial U per moles dissolved U	constant	2,3
	PROPMIC	Np	1.2e+01	1.2e+01	1.2e+01	moles microbial Np per moles dissolved Np	constant	2,3
	PROPMIC	Pu	3.0e-01	3.0e-01	3.0e-01	moles microbial Pu per moles dissolved Pu	constant	2,3
	PROPMIC	Am	3.6e+00	3.6e+00	3.6e+00	moles microbial Am per moles dissolved Am	constant	2,3
	CAPMIC	Th	1.9e-03	1.9e-03	1.9e-03	moles total mobile Th per liter	constant	5,7
	CAPMIC	U	2.1e-03	2.1e-03	2.1e-03	moles total mobile U per liter	constant	5,7
	CAPMIC	Np	2.7e-03	2.7e-03	2.7e-03	moles total mobile Np per liter	constant	5,7
	CAPMIC	Pu	6.8e-05	6.8e-05	6.8e-05	moles total mobile Pu per liter	constant	5,7
	CAPMIC	Am	not currently available	not currently available	not currently available	moles total mobile Am per liter	constant	5,7

Notes:

general The colloidal actinide source term is added to the dissolved actinide source term.

general None of the parameters are correlated.

1 If a distribution is not used for mineral-fragment-bound actinides, use the maximum concentration as a constant value.

2 Proportionality constants may be used with actinide solubility expressed in molarity or molality, depending on the desired final units.

3 Proportionality constants are to be used with the inorganic actinide solubility value (uncomplexed only, i.e., without organic ligand contribution).

4 If a distribution is not used, use the maximum concentration as a constant value.

5 The maximum ("cap") values are in units comparable to molarity rather than molality.

6 CAPHUM is compared to the concentration of the respective humic-bound actinide element.

7 CAPMIC is compared to the total concentration of the respective actinide element in the mobile system (i.e., the sum of dissolved plus colloidal actinide).

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NFORMATION ONL

Estimate of Repository pH and f_{CO2} Distribution for the Long-Term WIPP Performance Assessment

WBS 1.1.09.1.1 (BC)
March 29, 1996

Performed by:
Y. Wang
WIPP Chemical and Disposal
Room Processes Department
Date: 3/29/96

Organizational Approval:
J. T. Holmes
Manager
WIPP Chemical and Disposal
Room Processes Department
Date: 4/1/96

Technical Reviewer: Chris Craft
C. C. Crafts
WIPP Chemical and Disposal
Room Processes Department
Date: 4/1/96

WPO 37415

Sandia National Laboratories

Albuquerque, New Mexico 87185-1341

date: March 29, 1996

to: Martin S. Tierney (Org. 6741)

Christine T. Stockman (Org. 6749)

from: Yifeng Wang (Org. 6748)

subject: Estimate of Repository pH and f_{CO2} Distribution for the Long-Term WIPP Performance Assessment (PA)

In my memo to M. D. Siegel (Wang, 1996), I justified that, due to the addition of MgO backfill, WIPP brine pH and f_{CO2} will be determined mainly by two chemical invariant points: $Mg(OH)_2 + MgCO_3$ or $Ca(OH)_2 + CaCO_3$. I thus suggested that actinide solubility be calculated only for these two invariant points. In this memo, I want to define the likelihood for the occurrence of each invariant point in WIPP repository over 10000 years.

I assume that 2×10^9 moles of MgO will be added to the repository for controlling brine chemistry (Bynum, per comm., 3/26/1996) and 8×10^6 moles of $Ca(OH)_2$ will be present as a cementious material in the waste (Drez, 1996; Storz, 1996). Since the quantities of MgO and $Ca(OH)_2$ are fixed, the pH and f_{CO2} will be a function only of the amount of CO_2 produced by microbial reaction , the volume of brine in the repository, and the type of brine. With computer code EQ3/6 (Wolery, 1992; Wolery & Daveler, 1992), I conducted titration calculations for each WIPP brine (ERDA-6 and Brine-A) with various amounts of $Mg(OH)_2$ and CO_2. In the calculations, $Ca(OH)_2$ was added in proportion to MgO. Furthermore, in order to avoid the numerical problem caused by water consumption, $Mg(OH)_2$, instead of MgO, was used in the calculations. The brine compositions were from Brush (1990). Based on the calculations, the distribution of the chemical invariant points was constructed as a function of moles of CO_2 /kg H_2O and moles of $Mg(OH)_2$/kg H_2O for each brine (Figures 1 and 2). For Castile brine ERDA-6, the transition from one invariant point to another is very sharp (Figure 1), while, for Salado brine Brine-A, a transition region (III) exists due to the formation of Mg-oxychlorite (Figure 2). The transition region and region I have very similar pH values. Note that pH in this memo always refers to pmH = $-\log [H^+]$.

From Figures 1 and 2, the following conclusions can be drawn:

(1) The biodegradation of a small percentage of total cellulosics will produce sufficient CO_2 to react all $Ca(OH)_2$ in the waste (see dash lines region I in both Figure1 and 2). Therefore, for the cases with microbial gas generation, the brine chemistry will be controlled mainly by $Mg(OH)_2 + MgCO_3$ invariant point

(2) Without CO_2 production, in order for Salado brine to reach region II, the ratio of $Mg(OH)_2$/kg H_2O needs to be larger than 400, corresponding to the brine volume of 5000 m^3 (Figure 2). This brine volume is small and may only account for a few percents of total pore volume in the repository. Therefore, the brine chemistry in E2 scenario is unlikely to be controlled by the $Ca(OH)_2 + CaCO_3$ chemical invariant point, although this control may be in effect for some undisturbed cases.

(3) Figure 1 indicates that the brine chemistry will be controlled by $Ca(OH)_2 + CaCO_3$ in an E1 scenario with no CO_2 production. But, this may not be true, if there is enough Salado brine (> 5000 m^3) in the repository to react with all $Ca(OH)_2$ before human intrusion; for these cases, the brine chemistry will not be controlled by $Ca(OH)_2 + CaCO_3$.

Because the volumes of the brine in the repository and the brine released can not be predetermined, it is difficult to give a good estimate of the relative probability of being in region I versus region II. However, based on the above discussion, I expect that, given the current inventory estimate of $Ca(OH)_2$, the overall chance for a WIPP brine to be in region II is low. Considering that actinide solubility is higher at $Mg(OH)_2 + MgCO_3$ (Novak & Moore, 1996, *I recommend using the actinide solubility calculated for* $Mg(OH)_2 + MgCO_3$ *invariant point for all PA calculations.* This recommendation is conservative.

Figure 1. Chemical-Invariant-Point Distribution for Castile Brine (ERDA-6) as a Function of CO_2 Produced and $Mg(OH)_2$ Added per Kilograms of Water. Since MgO and $Ca(OH)_2$ are fixed, the ratio of $Mg(OH)_2/H_2O = 2x10^9$ moles/kg of total water in the repository. The ratio of $Ca(OH)_2$/kg H_2O = 0.004*$Mg(OH)_2$/kg H_2O. The dash line is the CO_2/H_2O ratio corresponding to 8% of cellulosics biodegraded.

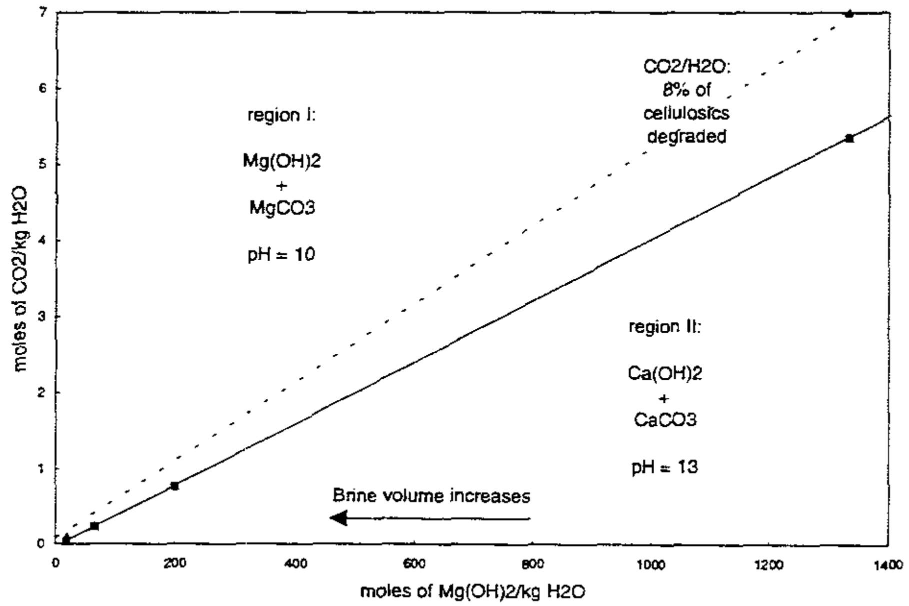
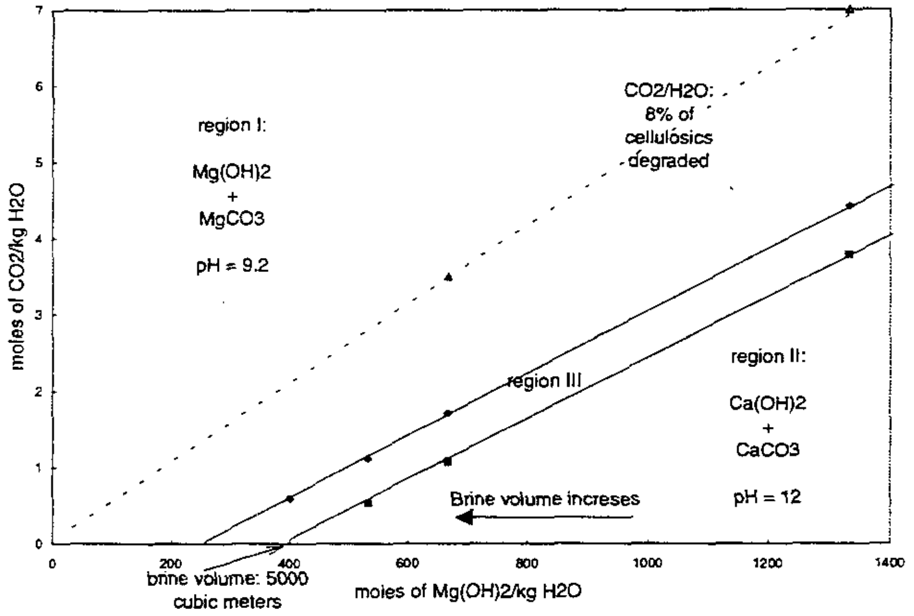


Figure 2. Chemical-Invariant-Point Distribution for Salado brine (Brine-A) as a Function of CO_2 Produced and $Mg(OH)_2$ Added per Kilograms of Water. Since MgO and $Ca(OH)_2$ are fixed, the ratio of $Mg(OH)_2/H2O = 2x10^9$ moles/kg of total water in the repository. The ratio of $Ca(OH)_2$/kg H_2O = 0.004*$Mg(OH)_2$/kg H_2O. The dash line is the CO_2/H_2O ratio corresponding to 8% of cellulosics biodegraded. Region III can be combined into region I, because they have similar pH values.



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From Estimates of Gas Generation 30819

Sandia National Laboratories
Albuquerque, New Mexico 87185-1341

INFORMATION ONLY

date: March 18, 1996

to: Malcolm D. Siegel (Org. 6748)

from: Yifeng Wang (Org. 6748)

subject: Define Chemical Conditions for FMT Actinide Solubility Calculations

Reflecting the recent decision of adding MgO as a backfill to control WIPP repository chemistry, this memorandum is to define the chemical conditions for FMT actinide solubility calculations for WIPP performance assessment (PA). The decision of adding backfill will significantly simplify the FMT calculations. In the original plan, the actinide solubility was supposed to be calculated for the whole ranges of brine chemical conditions (pH, CO_2 fugacity) and the results would be submitted to PA as lookup tables. However, due to the addition of MgO, we now only need to calculate the actinide solubility for two chemical invariant points, and the full-range lookup tables are no longer needed.

To define WIPP brine pH and CO_2 fugacity (f_{CO2}), I have conducted the titration calculations for both Salado brine (Brine-A) and Castile brine (ERDA-6) with computer code EQ3/6 (Wolery, 1992; Wolery & Daveler, 1992). In the calculations, I have assumed (1) that the repository chemistry will be mainly controlled by microbial CO_2 production and the dissolution of MgO backfill and $Ca(OH)_2$ originally present in the waste as a cementious material and (2) that the amount of MgO added will be sufficient to remove all CO_2 from gaseous and liquid phases. The brine chemical composition used in the calculations are from Brush (1990, tables 2-2 and 2-3). The calculation results are shown in Figures 1 and 2. Note that pH in this memo always refers to $pmH = -\log[H^+]$.

The calculation results show (1) that adding sufficient MgO to the repository will buffer brine pH at 10 for Castile brine (ERDA-6) and 9.2 for Salado brine (Brine-A), after all CO_2 in the gaseous and liquid phases are consumed, and (2) that the presence of $Ca(OH)_2$ in the waste may bring pH to 13 for Castile brine and 12 for Salado brine (Figures 1 and 2). Thermodynamic calculation shows that the reaction:

$$MgCO_3 + Ca(OH)_2 \rightarrow Mg(OH)_2 + CaCO_3 \qquad \Delta G = -9.4 \text{ kcal/mole (Drever, 1982)}$$

will proceed until all $MgCO_3$ is consumed. Thus, the effect of $Ca(OH)_2$ on pH will depend will only on the ratio of $Ca(OH)_2$ to water, regardless of how much MgO will be added. Figure 1 and 2 indicates that the brine pH and f_{CO2} will be essentially determined by either of two chemical invariant points:

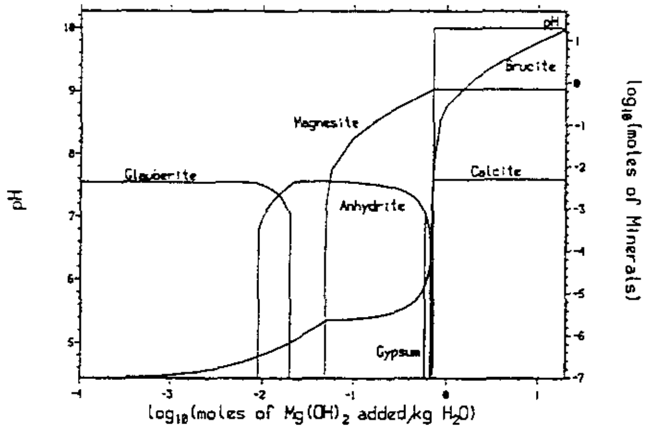
(1) $MgCO_3 + Mg(OH)_2$ — pH = 10 for Castile brine and 9.2 for Salado brine
(2) $CaCO_3 + Ca(OH)_3$ — pH = 13 for Castile brine and 12 for Salado brine.

The transition between the two invariant is sudden.

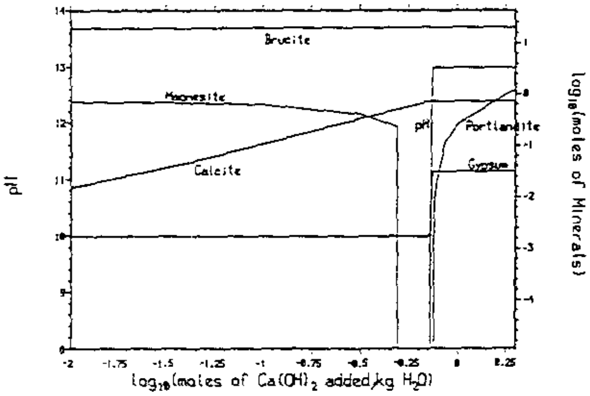
From the calculation results, I suggest using FMT to calculate the actinide solubility only for the two chemical invariant points for each brine. The solubility in the transition zone between the two invariant points will be determined, if needed, by a linear interpolation method. In FMT calculations, the chemical invariant points can be obtained by adding sufficient amounts of $Mg(OH)_2$ and $Ca(OH)_2$ to the brines and they are characterized by the presence of a typical mineral set: either $MgCO_3 + Mg(OH)_2$ or $CaCO_3 + Ca(OH)_2$.

In a separate memo to PA, I will provide the relationship between the brine chemistry and its controlling factors such as the quantity of CO_2 produced, the amount $Ca(OH)_2$ present, and the brine volume. This relationship will allow us to determine the probability of the chemical system falling at each chemical invariant point or the transition zone between the two invariant points.

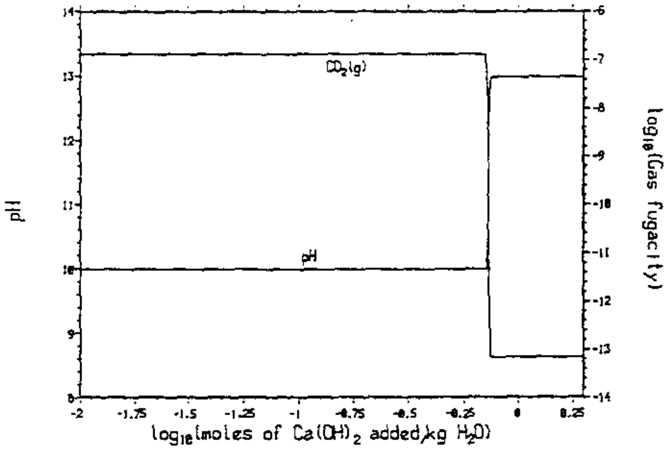
Figure 1. (A) Castile brine (ERDA-6) titrated with $Mg(OH)_2$. (B) and (C) The resulting system in (A) is further titrated with $Ca(OH)_2$. Note a sudden transition from $MgCO_3 + Mg(OH)_2$ to $CaCO_3 + Ca(OH)_2$ regions.



A

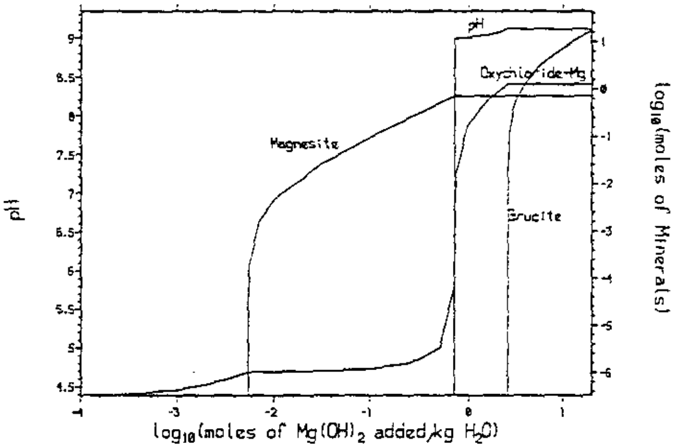

Brucite
Magnesite
Calcite
pH
Portlandite
Gypsum
pH
log10(moles of Minerals)
log10(moles of Ca(OH)2 added/kg H2O)
14
13
12
11
10
9
8
1
0
-1
-2
-3
-4
-2
-1.75
-1.5
-1.25
-1
-0.75
-0.5
-0.25
0
0.25

B


CO2(g)
pH
pH
log10(Gas fugacity)
log10(moles of Ca(OH)2 added/kg H2O)
14
13
12
11
10
9
8
-6
-7
-8
-9
-10
-11
-12
-13
-14
-2
-1.75
-1.5
-1.25
-1
-0.75
-0.5
-0.25
0
0.25

C

Figure 2. (A) Salado brine (Brine-A) titrated with $Mg(OH)_2$. (B) and (C) The resulting system in (A) is further titrated with $Ca(OH)_2$. Note a sudden transition from $MgCO_3$ + $Mg(OH)_2$ to $CaCO_3$ + $Ca(OH)_2$ regions



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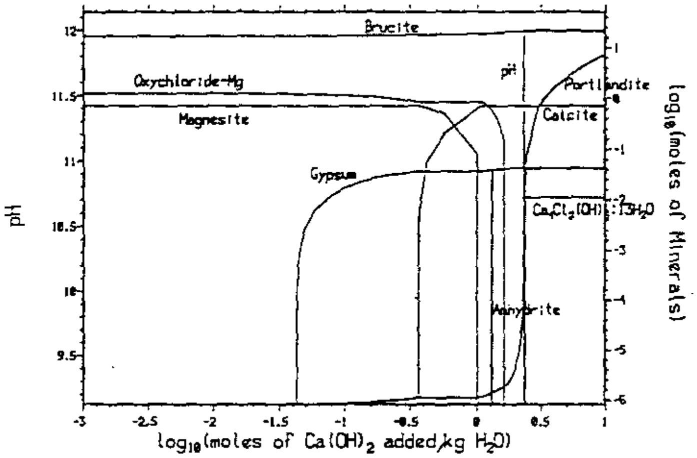

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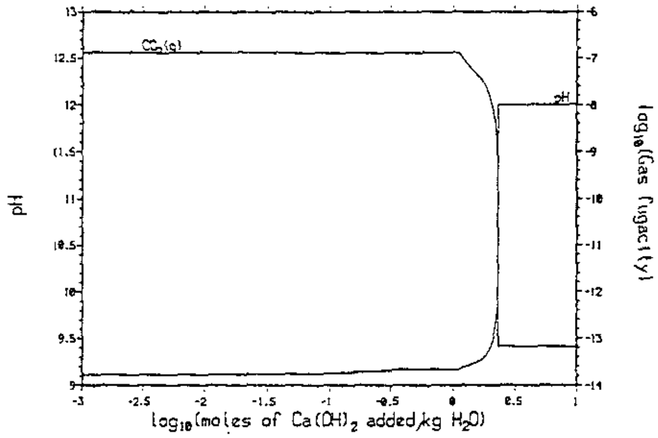

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WPO 35552

INFORMATION ONLY

REVISED INFORMAL MEMO

To: Joe Harvill, CTAC

March 20, 1996

From: Paul Drez, PD CTAC

Subject: FINAL PRELIMINARY ESTIMATE OF COMPLEXING AGENTS IN TRU SOLIDIFIED WASTE FORMS SCHEDULED FOR DISPOSAL IN WIPP

SUMMARY

This memo provides the best estimate of complexing agents, based on transuranic (TRU) waste generator/storage site input, in TRU waste expected to be shipped to the Waste Isolation Pilot Plant (WIPP) for disposal. The complexing agent inventories quoted in this memo are in response to a Sandia National Laboratory/New Mexico (SNL/NM) request for information to the U. S. Department of Energy (DOE) Carlsbad Area Office (CAO). The memo requesting the complexing agent information is contained in Appendix B of Revision 2 of the Transuranic Waste Baseline Inventory Report (TWBIR) (DOE, 1995). All waste inventory volumes quoted are derived from Rev. 2 of the TWBIR.

SNL/NM should use Table 3 as a summary of specific complexing agents that may be present in the TRU waste. Tables 1 and 2 provides a summary of Total Organic Carbon in the remote-handled (RH)-TRU sludges from Oak Ridge National Laboratory (ORNL) and a list of possible complexing agents that may contribute to the TOC in the sludges.

Estimates are provided in Table 4 of the volume of stored and projected TRU waste that contribute to the estimate of complexing agents in the waste. For contact handled (CH)-TRU waste, greater than 94% of TRU stored and projected final waste forms contribute to the complexing agent estimate and greater than 98% of the Solidified Organic final waste forms and greater than 92% of the Solidified Inorganic final waste forms. For RH-TRU waste, greater than 86% of TRU stored and projected final waste forms contribute to the complexing agent estimate and 100% of the Solidified Organic final waste forms and 100% of the Solidified Inorganic final waste forms.

BACKGROUND

Information has been received from all sites that were requested to provide data on potential complexing agents in their solidified waste forms: Rocky Flats Environmental Technology Site (RFETS), Los Alamos National Laboratory (LANL) and ORNL. In addition, several TRU waste sites which do not generate solidified waste forms (or small quantities) have also responded. A copy of the CAO memo requesting the complexing agent information is included as Attachment 1.

SWCF-A: 1.2.07.2.1; PA; PBWAC

The term "complexing agent" is being used in lieu of "chelating agents" in this memo, since chelating agents usually have a certain structure (chelating comes from the Greek work "chele" for claw, as in a crab), and are considered a subset of complexing agents. That is, acetate ion will "complex" with some metals and increase their solubility but does not have the structure that would label it as a chelating agent. A "commonly" known chelating agent is EDTA (ethylenediaminetetraacetic acid), which contains functional (acetate) anion groups arrange in parallel which resemble a "claw" like structure for complexing the cations. EDTA has two "claw" structures at either end of the molecule.

The original scope of this task was to ask the TRU waste generator/storage sites about "aqueous-soluble" complexing agents in their solidified waste forms. As this task was researched, the authors realized that the term "aqueous-soluble" is only a relative term, since everything is "aqueous-soluble" at some concentration level. Therefore, every potential chemical compound that has been reported from the TRU waste sites is included and the task of selecting aqueous soluble compounds is left to the SNL personnel in charge of performance assessment calculations.

TRU WASTE SITE RESPONSES

ORNL

ORNL has provided a list of organic compounds which contain some aqueous-soluble compounds that are apparent complexing agents. A copy of the list of all compounds reported by ORNL to the BIR team is attached for completeness (Table 1). The list in Table 1 is from an ORNL report on low-level waste (Kaiser, 1988), but the same compounds are anticipated to occur in the TRU waste based on process history (but not necessarily at the same concentrations). ORNL cannot quantify these compounds in their RH-TRU solidified wastes, but have provided an estimate of Total Organic Carbon (TOC) for each RH-TRU waste tank (Table 2). The sum of the TOC from all the RH-TRU tanks is approximately 3691 kg. It is anticipated that most of the TOC in the tanks is not associated with complexing agents, but that has not been verified at this time. As a conservatism, SNL/NM can assume that any complexing agents listed in Table 1 could form the bulk of the TOC in the ORNL RH-TRU tanks.

LANL

Los Alamos National Laboratory has provided estimates of four complexing agents that are anticipated to occur in their TRU solidified waste streams and as materials used in decontamination and spill clean-up operations (that would occur with the debris wastes) (Attachment 2). The quantities of these compounds are summarized in Table 3.

RFETS/INEL

The information provided by RFETS has been used to estimate the amount of complexing agents in the RFETS retrievable waste (post 1970) at Idaho National Engineering Laboratory (INEL). Attached is a listing of chemicals from RFETS that was provided to the BIR team as a basis for potential complexing agents in TRU waste scheduled for shipment to and disposal in WIPP (Table 3). This same list was originally put together as part of the documentation requested by the State of Nevada to document that less than 1% "complexing" agents occur in RFETS solidified low-level "saltcrete" waste that would be shipped to NTS for disposal (Attachment 3).

The list was provided as a yearly estimate of complexing agents used on site at RFETS. It is conservative to assume that all of these complexing agents would reside in the TRU waste. The inventory of complexing agents is the best estimate for all TRU waste generated across the entire RFETS site, which includes debris wastes. The mass of complexing agents reported in Table 3 for RFETS results from multiply the yearly estimates (in kilograms) by 20 years of production at RFETS (1970-1989), which includes RFETS waste in storage at INEL. The yearly estimates can be found in Attachment 3.

SRS

The Savannah River Site (SRS) has provided a letter in response to the DOE CAO request (Attachment 1) which is included as Attachment 4. SRS has provided information on three complexing agents used on site in connection with their operations, tributyl phosphate (TBP), tri-octyl phosphine oxide (TOPO) and tri-iso octylamine (TIOA). As discussed in the SRS letter, none of these compounds are expected to be found in SRS TRU waste.

Hanford

Hanford Operations has provided a listing from their database of potential chemicals in their TRU waste. The only chemical that appears on the list that might act as a chelating agent in aqueous solutions and has a reportable quantity associated with the waste is tributly phosphate (TBP). TBP is reported under three different spellings with a total of 92.5 kg. This value is summarized in Table 3. The entire list of chemicals reported by Hanford and quantities (in kg) are included in Attachment 5.

LLNL

Lawrence Livermore National Laboratory submitted the letter included as Attachment 6 documenting that no chelating agents occur in the LLNL TRU waste streams.

ESTIMATED VOLUME OF TRU WASTE INCLUDED IN COMPLEXING AGENT MEMO

Table 4 contains a listing of the total TRU waste destined for disposal in WIPP (stored plus projected to 2022), listed in Column 2. Column 3 estimates what volume of waste from each major site that has contributed to the estimate of complexing agents in TRU waste. Columns 4 and 5 provide the same data for Solidified Organics and Solidified Inorganics final waste forms. The two rows labelled "PERCENTAGE" provide an estimate of the percentage of waste that TRU waste generator/storage sites have provided data for estimating complexing agents in the waste.

REFERENCES

Kaiser, L. L., 1988, "ORNL Inactive Waste Tanks Sampling and Analysis Plan," ORNL/RAP/LTR-88/24, April 29, 1988, Oak Ridge National Laboratory, Oak Ridge, Tennessee

U. S. Department of Energy, 1995, "Transuranic Waste Baseline Inventory Report (Revision 2)," DOE/CAO-95-1121, December 1995, Carlsbad, New Mexico

cc: R. Bisping, DOE/CAO
M. Chu, SNL/NM
L. Storz, SNL/NM
L. Sanchez, SNL/NM

Table 1 Organic chemicals used regularly in the TPP (7920) and TURF (7930) and subsequently discharged to the ORNL LLLW system

Chemical	Approximate annual usage
Acetic acid	m^a
Acetone	100 L
Adogen-364-HP (~ triluarylamine)	100 L
Carbon tetrachloride	m
Deodotized mineral spirits (Amsco)	1000 L
2,5-di-tert-butylhydroquinone (DBHQ)	m
Deithylbenzene (DEB)	800 L
Diethylenetriaminepentaacetic acid (DPTA)	m
Di(2-ethylhexyl) phosphoric acid (HDEHP)	200 L
Di-isopropylbenzene (DIPB)	100 L
Ethanol	100 L
Ether	m
Ethylenediaminetetraacetic acid (EDTA)	m
2-ethyl-1-hexanol	m
α-hydroxyisobutyric acid (AHIB)	m
Isopropanol	m
Methanol	m
n-dodecane	m
n-paraffin (NPH)	m
Oxalic acid	m
Thenoyltrifluoroacetone (TTA)	m
Tributylphosphate (TBP)	m
Trichloroethylene (TCE)	m
Xylene	m

[a] m = minimal usage: ≤10 kg/year or ≤L/year.

TABLE 2. ORNL TOTAL ORGANIC CARBON ESTIMATES

TRU TANKS	TANK NO.	VOLUME (m3)	MASS (kg)	TOC (mg/kg)	TOC (kg)
INACTIVE TANKS					
North Tank Farm	W-03	5.3	5670	5300	30.05
	W-04	18.2	24527	200	4.91
South Tank Farm	W-07	37.5	45715	1300	59.43
	W-08	11.4	14080	8400	118.27
	W-09	0.8	833	2900	2.42
	W-10	28	31650	4900	155.09
Old Hydrofracture Facility	T-01	3	4845	18600	90.12
	T-02	4.6	7328	28000	205.18
	T-03	7.7	14829	9140	135.54
	T-04	5	6242	4620	28.84
	T-09	1.9	2967	7620	22.61
ACTIVE TANKS					
Evaporator Facility	C-2	45.6	63853	3281	209.50
	W-21	27.5	38524	6480	249.64
	W-22	43.5	60939	22.1	1.35
	W-23	64.2	89818	4120	370.05
MVSTs	W-24	52	72861	2940	214.21
	W-25	90.7	126911	2330	295.70
	W-26	59.2	82930	6220	515.82
	W-27	69.1	96707	3135	303.18
	W-28	16.5	23051	2500	57.63
	W-29	46.4	64913	3531	229.21
	W-30	46	64383	3531	227.34
	W-31	26.3	36828	4470	164.62
				Total TOC	3690.69

TABLE 3. RF/INEL AND LANL COMPLEXING CHEMICALS ESTIMATE

POTENTIAL COMPLEXING AGENTS IN ROCKY FLATS (INCLUDING STORED AT INEL), LANL, HANFORD TRU WASTE				
COMPOUND	RF MASS (kg)(1)	LANL MASS (kg)(2)	HANFORD MASS (kg)(3)	TOTAL MASS (kg)
Ascorbic Acid	90	7		97
Acetic Acid	132	10		142
Sodium Acetate	1110			1110
Citric Acid	90	1100.5		1190.5
Sodium Citrate	400			400
Oxalic Acid	90	13706		13796
EDTA	23			23
8-Hydroxyquinoline	46			46
Tributly Phosphate	74		92.5	166.5
1,10 Phenanthroline	0.24			0.24
Dihexyl-n,n-diethylcarbamoyl-methylphosphonate	72			72

(1) Letter from W.F. Weston to E.S. Goldberg, No. 89-RF-3055, dated September 1, 1989 (Attachment 3)

(2) Memorandum from C.L. Foxx to P. Drez dated March 12, 1996 (Attachment 2)

(3) Memorandum from F.M. Coony and M.R. Kerns to L.C. Sanchez thru S. Zott, dated January 25, 1996 (Attachment 5)

TABLE 4. CALCULATION OF AMOUNT OF WASTE COVERED IN COMPLEXING AGENT MEMO

Major Sites	Total TRU (m3)	Accounted For In Complexing Agent Estimate (m3)	Solidif. Org (m3)	Solidif. Inorg. (m3)
CH-TRU(1)				
RL (9)	45515.43	45515.43	0	23.39
INEL(2)	28606.74	28657.4	789.67	3349.6
LLNL(3)	941.13	941.13	0	20.18
LANL (4)	18405.15	18405.15	30.58	6922.02
NTS (5)	627.91	627.91	0	5.67
ORNL (6)	1560.42	0	0	0
RFETS (7)	5107.92	5107.92	140.93	1423.01
SRS (8)	9648.15	9648.15	0	1369.8
Total Major Sites	110[illegible]12.85	105903.09	961.[illegible]	13113.67
Total CH-TRU	111[illegible]21.43	111721.43	980[illegible]	14108.51
PERCENTAGE (10)		94.79%	98.0[illegible]%	92.95%
RH-TRU(1)				
RL (9)	21729.35	21729.35	0	0
INEL (2)	220.72	196.98	3.56	65.27
LANL (4)	193.13	1.93E+02	0	0
ORNL (6)	2915.64	1243.33	0	1243.33
Total Major Sites	25058.84	23[illegible]	3.56	1308.6[illegible]
Total RH-TRU	26930.88	2693[illegible]	3.56	1308.6[illegible]
PERCENTAGE (10)		86.75%	100.00%	100.00%

(1) Table 4-3 to 4-23, Rev 2 TWBIR

(2) Non RFETS Waste Subtracted

(3) Letter from K. Hainebach to J. Teak dated March 7, 1996 (Attachment 6)

(4) Memorandum from C.L. Foxx to P. Drez dated March 12, 1996 (Attachment 2)

(5) NTS waste is derived from LLNL only, see (4)

(6) ORNL was only asked to estimate complexing agents in solidified RH-TRU waste per DOE memorandum dated January 5, 1996 (Attachment 1)

(7) Letter from W.F. Weston to E.S. Goldberg, Letter No. 89-RF-3055, dated September 1, 1989 (Attachment 3)

(8) Letter from J. D'Amelio to J. Teak, SWE-SWE-96-0106, dated February 2[illegible], 1996 (Attachment 4)

(9) Memorandum from F.M. Coony and M.R. Kerns to L.C. Sanchez thru S. Lott, dated January 25, 1996 (Attachment 5)

(10) VOLUME PERCENTAGE OF TOTAL TRU WASTE, SOLIDIFIED ORGANICS AND SOLIDIFIED INORGANICS ACCOUNTED FOR IN COMPLEXING AGENT MEMO

ATTACHMENT 1

United States Government Department of Energy

memorandum

Carlsbad Area Office
Carlsbad, New Mexico 88221

DATE: JAN 5 1996

REPLY TO ATTN OF: CAO:NTP:RLB 96-0605

SUBJECT: Additional Transuranic (TRU) Waste Data Request for Sandia National Laboratories' Waste Isolation Pilot Plan (WIPP) Performance Assessment

TO: Distribution

We have been informed by representatives from Sandia National Laboratories (SNL) working on WIPP Performance Assessment (PA) that they require more information on certain TRU waste-related parameters in order to assess their influence on WIPP PA (see attached copy of relevant pages form SNL memo).

Data for most of these parameters have already been received from the sites either through responses to the Baseline Inventory Report (BIR), Revision 2, questionnaire or by discussions with site representatives. However, since the request from SNL for data on water soluble organic ligands (i.e., chelating agents) was not received in time for inclusion in the BIR Rev. 2 data call, WIPP PA still needs data for this parameter. As per the SNL memo, the data are needed by the end of February 1996, and therefore it is being addressed through this request separately from the upcoming BIR Rev. 3 data call.

As documented in the SNL memo, WIPP PA would like to have "best estimates" that are realistic and not overly conservative. Consequently, all sites that have existing data on chelating agents present in their waste are requested to submit the best available information to the BIR technical staff by February 26, 1996. The details on the nature of the information being requested by WIPP PA are being provided in Table 3 of the attachment.

A representative from SNL WIPP PA will be available at the upcoming BIR, Revision 3, Data Call Meeting to be held in Concord, California, on January 10, 1996. We anticipate that a brief presentation will be made at this meeting by WIPP PA staff explaining the importance of the data followed by any questions from site representatives. If you have any questions/clarifications regarding this matter, please be ready to discuss these at the upcoming meeting in Concord with the SNL WIPP PA representative.

Thank you for your continued cooperation.

Russ Bisping

Russ Bisping
Waste Certification Manager

Attachment

APPENDIX B

B) Special Request Non-PA Items

Also wanted at this time is additional information for several waste material characteristics. Although these characteristics have not been identified as waste material parameters to be used for WIPP PA, they are needed for non-PA scoping calculations to assess their influence on PA. Since these items are not currently PA parameters, inventory estimates of these characteristics as "additional information" in the TWBIR or supplied outside of the TWBIR via written correspondence. Below you will find an itemized list of these special request items.

1) Non-radioactive Materials

Additional information is needed on the five waste material characteristics (see Table 2): 1) vitrified wastes, 2) nitrates (NO_3^-), 3) sulfates (SO_4^{2-}), 4) phosphorus, and 5) cement. Of these waste parameters, the last four are needed for the gas generation modeling. The nitrates and the sulfates are involved in the denitrification and sulfate reduction processes which breakup the cellulosics, while the phosphorus is a nutrient for biodecay of cellulosics. The estimate of the mass quantities of cement in the waste inventory should include both the cement that is contained in the waste as cement itself (due to D&D activities, etc.) and the cement found in various sludges. Cement consumes CO_2 due to its content of $Ca(OH)_2$. The estimates for this non-radioactive waste constituent need only be "best estimates" at this present time so that non-PA scoping calculations can be made to determine their importance on overall repository performance. (Do not generate upper-bound estimates that are overly conservative.)

2) Residues

"Best estimates" are needed for residues, in addition to those already identified at the Rocky Flats Plant (RFP), that have the possibility of being changed from a resource category to a TRU waste category.

3) Organic Ligands (Chelating Agents)

"Best estimates", from currently available information, are needed for major water-soluble organic ligands which are under consideration for the actinide source term (see Table 3). If it is not possible to obtain data from major waste generating sites then supply guidance on how a first-order estimate may be made (from existing information such as process knowledge etc.) so that non-PA scoping calculations can be performed to identify if the presence of these ligands would have any significant impacts. (Do not generate estimates that are overly conservative.) Requested data is for final form "process-level" quantities used in production only for the key sites. If information on the "process-level" values does not exist at the key sites, then "laboratory-scale" values should be used in the requested assessment of the inventory. Should it be determined that more detailed information on organic ligands will be needed, you will be given a specific written request at a future time. This effort should be performed in parallel with the TWBIR. Technical data should be supplied in memorandum form by the end of February 1996 with supporting documentation by the end of March 1996.

Table 3. Justification of Special Request For Info On Organic Complexing Agents. (a)	
Ligand (b)	Discussion (c)
1) Total Complexants	The most valuable information at this time is a "best estimate" of the total amount of water soluble complexing agents (ligands) in the TRU waste matrix.
2) Citrate	Preliminary information indicates that citrate (citric acid) may be the largest used ligand at TRU waste generating sites. Hence, inventory quantities are very important.
3) Lactate	This is an important ligand that is produced by bacteria as part of its own metabolism. What is requested here is a "best estimate" of the quantity of lactate that actually exists in the TRU waste matrix (not just an initial amount supplied as part of a waste stream). However, if this information cannot be developed, then supply information on the initial amount.
4) Oxalate	This is an important ligand that is produced by bacteria as part of its own metabolism. What is requested here is a "best estimate" of the quantity of oxalate that actually exists in the TRU waste matrix (not just an initial amount supplied as part of a waste stream). However, if this information cannot be developed, then supply information on the initial amount.
5) EDTA	This ligand (ethylenediaminetetraacetic acid) is also of major importance due to its common use as a cleaning solvent.

(a) Information on these additional waste materials are needed for non-PA scoping calculations for assessment of their importance. The presence of these complexing agents are important for the actinide source term, with respect to increasing the solubility of radionuclides.
(b) These items are ranked in the order of their importance in the actinide source term.
(c) Also supply any available information that TRU waste generation sites may have on the degradation or decay rates of ligands in current (and expected) waste matrixes if possible. In cases where no information is available, supply guidance on estimating first-order quantities.

LCS:6741:lcs/(95-2082)

Copy to:
P.E. Drez [Drez Environmental Associates]
D. Bretzke [Science Applications International Corporation]
S. Chakraborti [Science Applications International Corporation]
MS-1320, C.F. Novak [Dept. 6119]
MS-1328, H. Jow [Dept. 6741]

JAN 5 1998

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Rudy Guercia, RL
Dale Ormond, SR
Jerry Wells, ID

ATTACHMENT 2

Los Alamos
NATIONAL LABORATORY
memorandum

Waste Management and
Environmental Compliance
NMT-7, MS E501

To/MS: Paul Drez, Drez Environ. Assoc.
Thru: James J. Balkey, NMT-7, MS E501

From/MS: C. L. Foxx, NMT-7, MS E501
Phone/FAX: 7-2328/ 7-9201
Symbol: NMT-7-WM/EC-96-035
Date: March 12, 1996

SUBJECT: CHELATING AGENTS IN LANL WASTE

I am certain that I have not captured all chelating agents, but I believe that I have identified and quantified roughly the important materials. The chelators are found in three waste streams:

1) Cemented evaporator bottoms from TA-55
2) Cemented sludge from the TA-50 Pretreatment Plant and dewatered sludge from the TA-50 Liquid Waste Treatment Plant
3) Combustible waste from TA-55

The three streams are summarized below.

It should be noted that waste generation data and analyses exist over the time frame of 1980 through 1995 or shorter intervals to support the estimated values. In some cases, quantitative data is almost nonexistent and the results are qualitative at best. Like Rocky Flats, plutonium processing at LANL attempts to avoid chelating agents which can interfere with recovery operations. From your list of compounds of interest, I am unaware of any significant usage of lactate or EDTA, so they have been eliminated from detailed consideration. I have added ascorbate which has been used as a reducing agent in HCl solutions, but not in nitric acid which attacks and decomposes ascorbate. One of the above streams is not an immobilized stream, but I believe that it is an important contributor of a soluble chelating agent in the form of citrate. If this information is extraneous to your purposes, just ignore it.

Cemented evaporator bottoms from TA-55. The evaporator bottoms are derived from nitric acid solutions some of which (27%) contain oxalate resulting from the precipitation of plutonium oxalate. Because of the pervasive usage of oxalate, it is contained at lower concentrations even in those solutions that do not arise from filtering an oxalate precipitate. Those numbers are based on analytical results. In addition the drums contain on the average, 3.2 liters of analytical solution residues. Those solutions contribute a negligible additional quantity of oxalate and small quantities of ascorbate, citrate and acetate. We have semi-quantitative values from the analytical organization for those chelators, based on the quantities used in the analytical processes that give rise to the residues. We know that 28 liters of solution went into a drum of cemented waste on the average from 1980 through June of 1988. Since that time, the average has been 43 liters of solution. In addition we have information regarding the number of drums generated from May, 1987 through April, 1995. The drum numbers and alternate cemented forms for the remaining years are estimated. The totals based on those data and estimates are shown here.

oxalate	1600 kg	90.04 / 88.04	= 1632
ascorbate	7 kg	176.14 / 175.14	= 7.04 ≈ 7
citrate	0.5 kg	192.14/191.14	= 0.5 ≈ 0.5
acetate	10 kg	60.05 / 59.05	≈ 10

Cemented sludge from the TA-50 Pretreatment Plant and dewatered sludge from the TA-50 Liquid Waste Treatment Plant. Based on experience at the liquid waste treatment plant with upsets in the treatment process due to the presence of chelators in the waste stream, it has been assumed that TA-55 is the only significant source of chelating agents in the sludge generated at that facility. Three waste lines carry liquids from TA-55 to TA-50. The industrial waste line is thought to be reasonably free of chelating agents. The evaporator distillate in the process acid waste line is unlikely to contain significant quantities of chelators because the distillation process creates a sharp reduction in the content of nonvolatile solution species.

The process caustic waste line solution is dominated by oxalate filtrates in hydrochloric acid that have been subjected to caustic treatment and filtration. Under the conditions of that treatment the oxalate and ascorbate (used historically) are soluble and follow the solution to TA-50 for a ferroflocculation treatment. The solution is used to neutralize the nitric acid distillate. Because there is an excess of nitric acid, the neutralization is completed with the addition of stock sodium hydroxide. I have assumed that the short term excess of nitric acid decomposes the ascorbate leaving only the oxalate. I have estimated the oxalate concentration in the hydroxide filtrate at 0.075 moles/liter. If this number drives the calculation then we should sample the solution in the caustic holding tank at TA-50 and get a representative value.

Volumes of caustic solution generated by TA-55 were available for the years 1983 and 1986 through 1992. Volumes for all other years were estimated. I am assuming that the oxalate will appear in the sludges due to the low solubility of calcium oxalate and because the floculations have relatively high concentrations of calcium. In addition magnesium and aluminum oxalates are insoluble in a caustic environment. The oxalate precipitates will be found in the cemented sludge, whenever generated, and in the dewatered sludge from the early and middle 80's. These oxalates will also be found in the cement-filled corrugated metal pipe (CMP) waste stream generated at DP site when plutonium operations were located there. The total of oxalate in those waste streams is 11,800 kg. ≈ 12070

Combustible waste from TA-55. The combustible waste stream contains rags that were used in decontamination and spill clean-up operations. In spill clean-up the rags from the first pass are nearly always TRU waste as measured on our MEGAS assay instrument. The rags are dampened with a solution labeled "versene". Versene is a name for EDTA. In the very early days of the laboratory versene solution may have contained EDTA, but it had been changed to sodium citrate solution by the time I arrived in 1969. Drums of combustible waste do not usually contain only decontamination rags and often contain no such rags. However our waste management personnel apparently used a unique identifier over about a four year period (1987 to 1991) for the decontamination rags. Each item also had a net disposal weight associated with it. Thus I was able to get a handle on the weight of decon rags generated in that time frame. The rags were discarded not dripping but distinctly damp. I dampened some cheesecloth, weighing before and after, to estimate the weight of solution contained in the rags. Knowing the weight of solution and the concentration of the citrate, I was able to calculate a weight of citrate in the discarded rags. In May, 1991 the usage of citrate for decontamination was restricted to certain matrices. I was able to locate records for versene solution preparation from 1989 into early 1991 and then again for the past year so I could understand usage before and after 1991. From that I have estimated the usage for the remaining years. With that information, I have estimated that the citrate contained in the combustible waste stream from 1971 to 2033 will be 1100 kg.

Cy: Andy Montoya, NMT-7, MS E501
NMT-7 File

ATTACHMENT 3

CORRES. CONTROL
OUTGOING LTR. NO.

89 RF 3055

DIST.	LTR	ENCL
ANCHINI, D.J.		
BAER, C.P.		
RFURDT, R.J.		
EINTZ, E.R.		
OOD, R.C.		
DEKER, E.H.		
INZER, J.E.		
IRBY, W.A.		
NETT, J.F.		
EYERS, G.W.		
DECKER, J.H.		
SHANNON, W.M.		
WESTON, W.F.	☒	
OZNIAK, B.D.		
OUNG, E.R.		
ETCHER, D.K.		
ARNIVAL, G.J.		
FERRERA, D.W.		
ARMAN, L.K.		
EBERT, J.L.		
OEY, J.B.		
OFFMAN, R.B.		
LAMANN, R.L.		
KRIEG, D.M.	☒	☒
URG, G.E.		
Y, K.B.	☒	
AIMON, E.R.	☒	☒
NEWBY, R.L.		
TURNER, H.L.		
VELASQUEZ, R.N.		
CORRES. CONTROL	X	X
CONTRACT ADMIN.		
Arnold PM	X	X
D'Amico EL	X	X
Jaskot GF	X	X
[illegible]	X	X
CLASSIFICATION		
UNCLASSIFIED	☒	☒
CONFIDENTIAL		
SECRET		

AUTH. CLASSIFIER SIG.

9/1/89
DATE

IN REPLY TO LTR. NO.
245RF89

REC #

VALS ECM

ORIG. & TYPIST INITIALS
ELD

A-46469 (Rev. 4/89)

Rocky Flats Plant
Aerospace Operations
Rockwell International Corporation
P.O. Box 464
Golden, Colorado 80402-0464
(303) 966-7000
Contractor to U.S. Department of Energy

SEP 0 1 1989

89-RF-3055

Edward S. Goldberg
Acting Area Manager, RFO

Attn: Mark Van Der Puy

APPLICATION TO SHIP SALTCRETE

Attached is a copy of the re-formatted Application to Ship Waste for saltcrete. This application addresses all the comments from the Nevada Operations Office document attached to your letter 1245-RF-89.

Please refer any questions regarding the attached application to E.L. D'Amico at (303) 966-5362 or P.M. Arnold at FTS 320-2056.

W.F. Weston, Director
Plutonium Operations

Orig. and 3 cc - E.S. Goldberg
Enc.

Table 8 (continued)
Reference Documents/Results Outlining Compliance
to the General Waste Form Criteria

		Boxes," specifies Waste Operations personnel to visually inspect for and remove any excessive particulate from each stored saltcrete box.
Gases	Not Applicable	Saltcrete is not a gaseous waste and does not contain radioactive gases.
Stabilization	WO-5004	As described in WO-5004, "Waste Treatment Spray Dryer and Saltcrete Process," cement is added to the salt waste stream to immobilize the particulate, solidify the liquids and moderate oxidizing characteristics.
Etiologic Agents	Not Applicable	Saltcrete does not contain pathogens, infectious wastes or other etiologic agents.
Chelating Agents	Quantity and type of complexing agents used per year at Rocky Flats: Ascorbic Acid: 4.5 kg Acetic Acid: 6.6 kg Sodium Acetate: 55.5 kg Citric Acid: 4.5 kg Sodium Citrate: 20.0 kg Oxalic Acid: 4.5 kg EDTA: 1.15 kg	Between 5/15/87 and 5/7/88, 917 triwall boxes of saltcrete were produced. The estimated saltcrete generation for any given year is between 1200 to 1600 triwalls. The average net weight of one triwall box of saltcrete is approximately 1600 pounds. Total weight of saltcrete produced between 5/15/87 and 5/7/88 is 917 boxes * 1600 pounds * 1 kg/2.2 pounds = 6.67*10^5 kg. As a worst case, if it is assumed that all 106.36 kg of complexing agents are

Table 8 (continued)
Reference Documents/Results Outlining Compliance to the General Waste Form Criteria

	8-Hydroxyquinoline: 2.3 kg Tributyl Phosphate: 3.7 kg 1,10 Phenanthroline: 0.012 kg dihexyl-n,n-diethylcarbamoyl methylphosphonate: 3.6 kg Total: 106.36 kg	disposed of with the saltcrete, then, $106.36/6.67*10^5=1.59*10^{-4}$ is the weight fraction of the complexing agents with respect to the saltcrete. Therefore, Rocky Flats' total yearly usage of complexing agents amounts to only 0.0159 weight percent of the total saltcrete production between 5/15/87 and 5/7/88. This extremely conservative estimate is well under the NTS limit of 1 weight percent.
GCD Waste	Not Applicable	Saltcrete does not meet any of the guidelines to be identified as a GCD waste.
Bulk LLW	Not Applicable	Saltcrete is not a bulk LLW.

4. Additional Mixed Waste Form Criteria

Table 9 references the documents (procedures, specifications, etc.) or test/analysis results that specify compliance to the Additional Mixed Waste Form Criteria outlined in Section 2.2.2 of NVO-325.

Table 9
Reference Documents/Results Outlining Compliance to the Additional Mixed Waste Form Criteria

Criterion	Compliance Documents or Results	Comments
Treated Waste	Not Applicable	Saltcrete is a treated waste that meets the land disposal restrictions and

ATTACHMENT 4

Westinghouse
Savannah River Company

P.O. Box 616
Aiken, SC 29802

February 28, 1996

SWE-SWE-96-0106
F/WSWE/XXX/ARNR
Response Required: N/A
Key Words: TRU Waste
Record Retention: Permanent

Jim Teak
Advanced Sciences, Incorporated
6739 Academy Road, N. E.
Albuquerque, New Mexico 87106-3345

Dear Mr. Teak:

FY96 TRANSURANIC WASTE BASELINE INVENTORY REPORT (TWBIR): RESPONSE TO THE TWBIR MEETING MINUTES REGARDING CHELATING AGENTS AND CONCRETE STABILIZATION (U)

The Savannah River Site (SRS) has reviewed its waste practices to determine whether chelating agents are present in retrievably stored TRU waste. SRS also has reviewed these practices to determine whether concrete has been used to solidify/stabilize TRU waste. These reviews revealed that SRS TRU waste steams do not currently contain chelating agents/complexants nor has SRS used concrete to solidify/stabilize TRU waste.

The Separations processes and the analytical/research laboratories at SRS have used chelating agents in the separation of plutonium from irradiated uranium and other materials. For example, tri-butyl phosphate (TBP) is the complexing agent used in SRS's PUREX process and many other laboratory processes. Also, agents such as tri-octyl phosphine oxide (TOPO) and tri-iso octylamine (TiOA) have been used or investigated through the years. However, none of these chelating agents/complexants has entered SRS TRU waste. The complexants are dissolved in organic solvents for use as liquid/liquid extractants in the separation process. These solvents are recycled until depleted and then discarded to SRS's solvent waste tanks in the Waste Disposal Facility. This means that SRS organic liquid streams have not entered the production lines (e.g., HB and FB-Lines) where most of SRS TRU waste is generated. Further, a small amount of liquid TBP containing TRU nuclides is generated by SRS laboratories. This laboratory waste is discarded to liquid waste streams, which are eventually disposed in SRS's High Level Waste Tanks. So, none of these liquid streams that contain complexants have entered SRS solid TRU waste streams.

SRS has not used concrete to solidify/stabilize TRU waste. The processes that generate slurries, which require stabilization, do not contain TRU radionuclides (e.g., plating of depleted uranium). For other processes that generate slurries, the waste is disposed in SRS's High Level Waste Tanks. Even the Low Level Waste (LLW) sludge generated by SRS's Effluent Treatment Facility (ETF) is disposed in the High Level Waste Tanks and is eventually fed to SRS's Saltstone Facility or the Defense Waste Processing Facility (DWPF). Finally, SRS does not expect to generate TRU waste containing chelating agents nor anticipate using concrete to solidify/stabilize TRU waste in the near-future.

Please direct your questions to L. Williams (803) 557-6759.

Sincerely,

Joseph A. D'Amelio
TRU Engineering Manager

JAD:lw

cc: A. Gibbs, 724-21E
W. T. Goldston, 705-3C
F. H. Gunnels, 705-3C
S. J. Mackmull, 703-A
S. J. Mentrup, 724-21E
D. Ormond, 703-A
L. Williams, 705-3C
Records Management, 705-3C
SWE Files, 705-3C

ATTACHMENT 5

To: L. C. Sanchez, SNL January 25, 1996

Thru: Sheila Lott, CTAC

From: F. M. Coony and M. R. Kerns, Hanford Site

RE: Additional TRU Waste Data Request for Sandia National Laboratories' Waste Isolation Pilot Plan Performance Assessment

References: 1) Memorandum, Russ Bisping, DOE/CAO to Distribution, same subject, dated January 5, 1996.

2) Trip Report, F. M. Coony to K. L. Hladek, January 15, 1996

The Reference 1 memo requests additional data on waste soluble organic ligands (i.e. chelating agents) from the generating sites by February 26, 1996.

Hanford's approach for responding to the additional data request is presented in the Reference 2 trip report. The first item of this approach is to provide SNL, through CTAC, a list of all hazardous constituents, and their quantities, that have been reported in solid TRU waste at Hanford since 1987, the date of the By-Product Rule.

The list of hazardous constituents and their quantities, from Hanford's record container tracking system, are presented in Table 2. The chemical names have been truncated to 30 characters. Hanford can provide complete names if needed. In some cases, the constituent is listed more than once because the constituent is spelled differently in the container tracking system. A quantity of 0.00 kg means typically that the constituent has been identified solely because it is a listed hazardous waste under RCRA. In these cases, the quantity is either absent or minimal.

Please evaluate the list of constituents, and indicate, in the space provided for each constituent, if the constituent is a soluble organic ligand. The suggested nomenclature is the following:

- N/A (meaning not soluble organic legand)
- C (meaning citrate)
- L (meaning lactate)
- OX (meaning oxalate)
- EDTA (meaning ethylenediaminetetraacadid acids

Please indicate any other relevant information by footnotes.

To meet the requested due date, please provide a response to me (by fax) no later than February 5, 1996. Please copy CTAC on the response.

If you have any questions, please contact Mike Coony at 509-376-8774 or Mark Kerns at 509-372-2383.

MASS
(KG)

Table 2. Quantities of Hanford Constituents

[illegible]	[illegible]	[illegible]
1,1,1-TRICHLOROETHANE	0.00	
2-BUTOXYETHANOL	0.02	
ACETONE	0.00	
ACID	0.14	
ALUMINUM NITRATE	0.10	
ALUMINUM NITRATE MONOHYDRATE	3.80	
AMERCOAT 234	0.05	
AMMONIUM CHLORIDE	0.01	
ARSENIC	0.02	
ASBESTOS	27.00	
BARIUM	1.86	
BERYLLIUM	0.17	
BIS(2-ETHYLHEXYL)PHTHALATE	0.82	
BISPHENOL A RESIN	0.54	
BUTYL ALCOHOL	0.41	
BUTYL GLYCIDYL ETHER	0.11	
CADMIUM	99.17	
CADMIUM HYDROXIDE	0.10	
CALCIUM CHLOROFLUOROPHOSPHATE	0.83	
CALCIUM HYDROXIDE	0.06	
CARBON TETRACHLORIDE	87.88	
CARBONTETRACHLORIDE	95.90	
CHLOROFORM	0.00	
CHROMIUM	14.52	
COPPER	0.00	
COPPER SULFATE	0.38	
CRESYLIC ACID	0.00	
CUPROUS CYANIDE	0.21	
CYANIDE SOLUTIONS	0.21	
CYCLOHEXANE	0.00	
DI(2-ETHYLHEXYL)PHTHALATE	0.06	
DI-OCTYL PHTHALATE	0.40	
DIOCTYL PHTHALATE	0.20	
DIOCTYL PHTHALATE (DOP)	8.47	
ETHANOL	0.20	
FERRIC NITRATE	4.38	
FORMIC ACID	0.21	
HEXONE	0.10	
HYDRAULIC FLUID	328.20	
HYDROCHLORIC ACID	0.07	

MASS
(KG)

[illegible]	MASS [illegible]	[illegible]
KEROSINE	0.00	
LEAD	8,915.59	
LEAD ACID	0.27	
LEAD CHROMATE	28.97	
LEAD CHROMATE OXIDE	1.54	
LEAD CHROMATE,CHLORIN.PARAFFIN	1.33	
LEAD CHROMATES	0.05	
LEAD SHIELDING	5,587.50	
LIGHT AROMATIC NAPHTHA	0.30	
MERCURY	1.51	
MERCURY METAL	0.00	
METHYL ETHYL KETONE	0.00	
METHYL ISOBUTYL KETONE	0.00	
METHYLENE CHLORIDE	8.03	
NICKEL HYDROXIDE	0.10	
NITRIC ACID	1.21	
OIL	0.00	
PCB	130.13	
PHOSPHORIC ACID	0.33	
PHTHALIC ACID BENZYL BUTYL EST	0.00	
PHTHALIC ACID BIS(2-ETHYLHEXYL	0.00	
PHTHALIC ACID, BIS(2-ETHYLHEXY	0.05	
POTASSIUM CYANIDE	0.21	
POTASSIUM FLUORIDE	0.00	
POTASSIUM HYDROXIDE	5.80	
RESIDUAL TANK FARM CORE SAMPLE	0.80	
SELENIUM	1.10	
SILVER	0.00	
SODIUM	0.13	
SODIUM CYANIDE	0.21	
SODIUM FLUORIDE	1.08	
SODIUM HYDROXIDE	24.37	
SODIUM NITRATE	173.00	
SODIUM SULFATE	3.92	
STRIPCOAT	34.09	
SULFAMIC ACID	0.04	
SULFURIC ACID	1.53	
THENOYL TRIFLUOROACETONE	0.00	
TRI BUTYL PHOSPHATE	49.30	
TRIBUTYL PHOSPHATE	43.13	
TRIBUTYLPHOSPHATE	0.07	

MASS
(KG)

[illegible]	[illegible]	[illegible]
TRICHLOROETHENE	3.28	
TRIISOOCTYLAMINE	0.00	
TRIMETHYLBENZENE	1.01	
TRIOCTYLPHOSPHINE OXIDE	0.00	
VANADIUM PENTOXIDE AQUEOUS SOL	0.21	
XYLENE	4.23	

ATTACHMENT 6

Lawrence Livermore National Laboratory

WASTE CERTIFICATION PROGRAM
WCP96-055

March 7, 1996

Jim Teak
Advanced Sciences Incorporated
6739 Academy Road NE
Albuquerque, NM 87109

Dear Jim,

This is in response to the CAO request concerning the presence of organic ligands (chelating agents) in TRU waste. I have consulted with Joe Magana, a chemist working in LLNL's Plutonium Facility. He tells me that there are no chelating agents in LLNL's TRU waste.

Sincerely yours,

Kem Hainebach

Kem Hainebach, Ph. D.
Waste Certification Engineer
Environmental Protection Department

KH:lh
c: Robert Fischer

Recycled

DEA Drez Environmental Associates

FAX COVER SHEET

DATE: March 20, 1996

TO:	COMPANY	FAX NO.	CONFIRMATION NO.
RUSS BISPING	CAO	505-887-0707	505-234-7446
MARGARET CHU	SNL/NM	505-848-0518	505-848-0778
JOE HARVILL	ASI/CTAC	505-887-5494	505-885-4218
LARRY SANCHEZ (GIVE TO JIM NOWAK)	SNL/NM	505-848-0705	505-848-0685
LENNY STORZ	SNL/NM	505-848-0881	505-848-0877
SAYAN CHAKRABORTI	SAIC	505-842-7798	505-842-7816
SHEILA LOTT	ASI/CTAC	505-823-6830	505-823-6873

FROM: PAUL DREZ

PAGES TO FOLLOW: 25

SUBJECT/PROJECT: FINAL PRELIMINARY COMPLEXING AGENT MEMO

COMMENTS:

THESE ARE THE FINAL NUMBERS FOR THE COMPLEXING AGENTS. SNL/NM SHOULD USE THESE NUMBERS IN THEIR CALCULATIONS. THE ONLY NUMBER THAT HAS CHANGED SINCE THE MARCH 13, 1996 REVISED MEMO IS THE TRIBUTYL PHOSPHATE (INCLUDES ESTIMATE FROM HANFORD). I AM SENDING THIS MEMO TO ALL TRU WASTE SITES THAT CONTRIBUTED DATA FOR THEIR REVIEW (A SEPARATE FAX SHEET). COMMENTS ARE DUE BACK COB THIS FRIDAY FROM EVERYONE TO ME. THIS REVIEW BY THE TRU WASTE SITES WAS PART OF THE AGREEMENT OF PROVIDING DATA TO THE BIR TEAM. ONLY DOE CAN ISSUE A "FINAL" MEMO AFTER RESOLUTION OF COMMENTS WITH THE TRU WASTE SITES.

PAUL

P.S. ATTACHMENT 3 HAS BEEN INCLUDED WITH ONLY A FEW PERTINENT PAGES TO CUT DOWN ON THE FAXING OF PAPER!!!!!!

If you do not receive all pages, please call:

Paul Drez
Drez Environmental Associates
8816 Cherry Hills Rd., NE
Albuquerque, NM 87111
Phone: (505) 828-9857 FAX: (505) 828-1342

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.12

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WPO 36163

NFORMATION ON

Sandia National Laboratories

Albuquerque, New Mexico 87185-

date: March 27, 1996

to: Craig F. Novak

RW

from: Ruth Weiner

Subject: Dissolved ligand concentrations

Ligand concentrations (acetate, citrate, oxalate, and EDTA) in the inundated repository were calculated from the "final preliminary" memo of Paul Drez to Joe Harvill of March 20, 1996 (scaled by a scaling factor of 2.05 as per BIR Rev. 2 Page 3-1) and the brine volume equal to 75% of the total repository area -- 29,841 m^3 -- as per the memo from Kurt Larsen to Vann Bynum of March 13, 1996. The table below summarizes the calculation:

	Inventory	Repositor	Molarity	Inventory
	grams	g/L		x 2.05
acetate	1252000	0.041956	0.000518	0.001062
citrate	1590500	0.053299	0.000227	0.000465
oxalate	13796000	0.462317	0.003612	0.007404
EDTA	23000	0.000771	2.03E-06	4.16E-06

The numbers in the second column -- "Repository g/L" -- were obtained by dividing the numbers in the first column by 29.841 x 10^6 liters. The molarities were obtained by dividing the numbers in the second column by the appropriate molecular weight.

cc:

E. J. Nowak

R. V. Bynum

C. C. Crafts

J. T. Holmes

M. S. Y. Chu

M. Siegel

SWCF-A: WBS 1.1.10.1.1:AST:NonQA: Actinide source term:chelators:ligands

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Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

WCA Attachment WCA.8.13

DOE F 1325.8

WPO 37064

United States Government

NFORMATIO

Department of Energy

memorandum

Carlsbad Area Office
Carlsbad, New Mexico 88221

DATE: April 4, 1996

REPLY TO ATTN OF: CAO:NTP:DW:96-1126

SUBJECT: Estimate of Cement Content in TRU Solidified Waste Forms Scheduled for Disposal in WIPP

TO: Les Shephard, Director, SNL

Attached is a summary of the best estimate of portland cement in stored and projected volumes of solidified waste streams listed in Revision 2 of the Transuranic (TRU) Waste Baseline Inventory Report (TWBIR). This information was requested from the TWBIR team in support of the Performance Assessment team.

These values have been scaled (similar to the methodology used for waste material parameters in the TWBIR) to the full volume of the Waste Isolation Pilot Plant (WIPP) repository. The total estimated weight of portland cement in these scaled solidified waste forms is 8.54E+06 kg. Dividing this value by 6.2E+06 ft^3 (~175,600 m^3), the maximum capacity of WIPP, yields a portland cement density in the overall combined contact-handled (CH) and remote-handled (RH) transuranic (TRU) waste of 48.6 kg/m^3. The portland cement reported is both reacted and unreacted cement in the waste. There are no data available to estimate the percentage of reacted versus unreacted cement.

The basic methodology was to perform a sort of the Revision 2 database that supports the TWBIR for all Solidified Inorganic and Solidified Organic waste streams. This sort resulted in 221 waste streams. Some waste streams were eliminated from further consideration for the following reasons:

- Data about most Rocky Flats waste streams (both residue and nonresidue waste streams) are for waste in current form only and not in final form. The item description code (IDC) for many particulate waste streams will change to final form because the waste is in a cemented final form. A total of 91 current-form RF TRU waste streams were eliminated because of this constraint, (the final form of these waste streams, however, is included in the portland cement estimate.)
- The Solidified Inorganic waste streams listed from Savannah River Site are all vitrified and therefore do not contain any portland cement. A total of 20 waste streams were eliminated because of this constraint.

If you have any questions concerning the attached information, please contact Mr. Russ Bisping of my staff at (505) 234-7446.

Don Watkins
Manager
National TRU Program

Attachment

cc w/attachment:
M. McFadden, CAO
K. Hunter, CAO
R. Bisping, CAO
P. Drez, CTAC
J. Harvill, CTAC
L. Sanchez, SNL
M. Chu, SNL
M. Marietta, SNL

Calculation Summary

At the bottom of Table 1 the total kilograms of portland cement is summarized for CH-TRU and RH-TRU waste for both stored plus projected waste (in "Total kg" column) and projected only waste (in "Projected kg" column). The TOTAL SCALED portland cement is calculated as follows:

CH-TRU "Total kg" + 2.05 * CH-TRU "Projected kg" + RH-TRU "Total Kg" = TOTAL SCALED kg of portland cement, or

$$5.28E+06 + 2.05(1.34E+06) + 5.05E+05 = 8.54E+06 \text{ kg portland cement}$$

The total density of portland cement is calculated as follows:

$$8.54E+06 \text{ kg}/175{,}600 \text{ m}^3 = 48.6 \text{ kg}/\text{ m}^3 \text{ portland cement}$$

Table 1. Estimate of Portland Cement in TRU Waste for Disposal in the WIPP

WIPP ID	Waste_Type	Handling	Final Waste Form	Solidification	Cement (kg/m^3)	Stored (m^3)	Projected (m^3)	Total kg	Projected kg	
W-W012.10	MTRU	RH	Solidified Inorganics	salt(1)	n/a					
W-W016.20	MTRU	RH	Solidified Inorganics	encapsulated metal(2)	n/a					
W-W020.13	MTRU	RH	Solidified Inorganics	evaporitic salt/sludge(3)	73.1	1.8	1.8	263.16	131.58	
W-W022.22	MTRU	RH	Solidified Inorganics	sludge/particulates(3)	73.1	0	0.9	65.79	65.79	
-W216.877	MTRU	RH	Solidified Inorganics	BIR	215.3	43.9	0	9451.67	0	
-W228.886	MTRU	RH	Solidified Inorganics	BIR	92.6	21.4	0	1981.64	0	
R-W042	MTRU	RH	Solidified Inorganics	BIR	396.6	175.3	0	69523.98	0	
R-W046	MTRU	RH	Solidified Inorganics	BIR	396.6	861.5	206.5	423568.8	81897.9	
-W317.1029	MTRU	RH	Solidified Organics	resins(3)	73.1	3.6	0	263.16	0	
E-W038	MTRU	CH	Solidified Inorganics	acid lab packs(3)	73.1	4.8	0	350.88	0	
E-W040	MTRU	CH	Solidified Inorganics	evaporitic salt/sludge(3)	73.1			0	0	
L-W005	MTRU	CH	Solidified Inorganics	nitric acid liquids(3)	73.1	0	0.4	29.24	29.24	
-W146.699	MTRU	CH	Solidified Inorganics	Assumed IN-W216.98	273.8	2.3	0	629.74	0	
-W159.1072	MTRU	CH	Solidified Inorganics	evaporitic salt/sludge	n/a					
-W163.1007	MTRU	CH	Solidified Inorganics	Ash(3)	73.1	0.7	0	51.17	0	
-W166.151	MTRU	CH	Solidified Inorganics	BIR	73.8	16	0	1180.8	0	
-W166.928	MTRU	CH	Solidified Inorganics	BIR	83.6	56.8	0	4748.48	0	
-W174.1082	MTRU	CH	Solidified Inorganics	Florco(4)	n/a					
-W174.154	MTRU	CH	Solidified Inorganics	Florco(4)	n/a					
-W177.1083	MTRU	CH	Solidified Inorganics	Florco(4)	n/a					
-W177.156	MTRU	CH	Solidified Inorganics	Florco(4)	n/a					
-W179.1084	MTRU	CH	Solidified Inorganics	BIR(5)	394.2	4.6	0	1813.32	0	
-W179.158	MTRU	CH	Solidified Inorganics	BIR(5)	325	1.5	0	487.5	0	
-W181.162	MTRU	CH	Solidified Inorganics	BIR	308.8	9.6	0	2964.48	0	
-W187.1094	MTRU	CH	Solidified Inorganics	Assumed IN-W222.116	102	0.7	0	71.4	0	
-W188.1093	MTRU	CH	Solidified Inorganics	BIR	308.8	1	0	308.8	0	
-W188.160	MTRU	CH	Solidified Inorganics	BIR	188.3	0	0.7	131.81	131.81	
-W216.875	MTRU	CH	Solidified Inorganics	BIR	308.8	1478.9	0	456684.32	0	
-W216.98	MTRU	CH	Solidified Inorganics	BIR	273.8	555.6	0	152123.28	0	
-W218.909	MTRU	CH	Solidified Inorganics	Assumed RF-MT0007	130.6	101.9	0	13308.14	0	
-W219.914	MTRU	CH	Solidified Inorganics	Grinding Sludge(3)	73.1	2.3	0	168.13	0	
-W220.114	MTRU	CH	Solidified Inorganics	BIR	27.6	122.8	0	3389.28	0	
-W220.925	MTRU	CH	Solidified Inorganics	BIR	308.8	443	0	136798.4	0	
-W221.113	MTRU	CH	Solidified Inorganics	BIR(6)	127.673	11.6	0	1481.0068	0	
-W221.927	MTRU	CH	Solidified Inorganics	BIR(6)	109.129	3.6	0	392.8644	0	
-W222.116	MTRU	CH	Solidified Inorganics	BIR	102	24.7	0	2519.4	0	
-W222.965	MTRU	CH	Solidified Inorganics	BIR	115.6	10.6	0	1225.36	0	
-W228.101	MTRU	CH	Solidified Inorganics	BIR	117.7	287.3	0	33815.21	0	
-W228.883	MTRU	CH	Solidified Inorganics	BIR	132.8	608.8	0	80848.64	0	
-W247.523	MTRU	CH	Solidified Inorganics	no solidification used	n/a					
-W257.947	MTRU	CH	Solidified Inorganics	Diatomaceous earth(7)	n/a					
-W263.520	MTRU	CH	Solidified Inorganics	no solidification used	n/a					
-W315.601	MTRU	CH	Solidified Inorganics	Wet Salt-Assumed INW216.875	308.8	0.4	0	123.52	0	
-W332.661	TRU	CH	Solidified Inorganics	Plaster(8)	n/a					
-W332.962	TRU	CH	Solidified Inorganics	Plaster(8)	n/a					
-W347.646	TRU	CH	Solidified Inorganics	Vermiculite(9)	n/a					
-W347.818	TRU	CH	Solidified Inorganics	Vermiculite(9)	n/a					
-W348.1012	TRU	CH	Solidified Inorganics	Particulates(3)	73.1	2.3	0	168.13	0	
-W353.859	TRU	CH	Solidified Inorganics	Liquid(3)	73.1	0.7	0	51.17	0	
-W353.917	TRU	CH	Solidified Inorganics	Liquid(3)	73.1	0.2	0	14.62	0	
-W375.1096	TRU	CH	Solidified Inorganics	Sludge- Assumed IN-W216.875	308.8	4.5	0	1389.6	0	
-M002	MTRU	CH	Solidified Inorganics	(10)	693	3053.5	553.3	2499512.4	383436.9	
-W003	MTRU	CH	Solidified Inorganics	(10)	645.9	1079.4875	559.1	1058363.666	361122.69	
-W006	MTRU	CH	Solidified Inorganics	(10)	508.1	301.7773	839.9	580086.2361	426753.19	
-T006	TRU	CH	Solidified Inorganics	(10)	514.4	4.225	81.5	44096.94	41923.6	
-T001	TRU	CH	Solidified Inorganics	(10)	100	14.4	5.8	2020	580	

Table 1. Estimate of Portland Cement in TRU Waste for Disposal in the WIPP

WIPP ID	Waste_Type	Handling	Final Waste Form	Solidification	Cement (kg/m^3)	Stored (m^3)	Projected (m^3)	Total kg	Projected kg	
ID-T001	TRU	CH	Solidified Inorganics	Sludge - Assumed IN-W179.1084	394.2	4.2	0	1655.64	0	
ID-W002	MTRU	CH	Solidified Inorganics	Florco(4)	n/a					
T-W021	TRU	CH	Solidified Inorganics	Mainly debris	n/a					
F-MT0001	MTRU	CH	Solidified Inorganics	BIR	187.6	3.7	0	694.12	0	
F-MT0007	MTRU	CH	Solidified Inorganics	BIR	130.6	0.8	0	104.48	0	
F-MT0800	MTRU	CH	Solidified Inorganics	BIR	193.8	65.5	38.9	20232.72	7538.82	
F-MT0803	MTRU	CH	Solidified Inorganics	BIR	55.6	2.9	2.1	278	116.76	
F-MT0807	MTRU	CH	Solidified Inorganics	BIR	71.7	73.4	41.6	8245.5	2982.72	
F-MT0377	MTRU	CH	Solidified Inorganics	Particulate(3)	73.1	3.5	0	255.85	0	
F-MT0806	MTRU	CH	Solidified Inorganics	BIR	73.1	0	1110.7	81192.17	81192.17	
F-TT0823	TRU	CH	Solidified Inorganics	BIR	17.5	7.1	23.1	528.5	404.25	
F-TT0806	TRU	CH	Solidified Inorganics	BIR	73.1	0	202.2	14780.82	14780.82	
F-T010	TRU	CH	Solidified Inorganics	BIR	140.2	0.6	0	84.12	0	
F-TT0802	TRU	CH	Solidified Inorganics	BIR(6)	68.32	7.5	26	2288.72	1776.32	
L-W281	MTRU	CH	Solidified Inorganics	Vermiculite(9)	n/a					
L-W383	TRU	CH	Solidified Inorganics	Vermiculite(9)	n/a					
L-W394	TRU	CH	Solidified Inorganics	Vermiculite(9)	n/a					
E-W039	MTRU	CH	Solidified Organics	resins(3)	73.1	0.2	0	14.62	0	
I-W157.144	MTRU	CH	Solidified Organics	BIR(6)	187.88	49.9	0	9375.212	0	
I-W157.906	MTRU	CH	Solidified Organics	BIR(6)	212.768	163.7	0	34830.1216	0	
I-W164.1060	MTRU	CH	Solidified Organics	Envirostone(11)	n/a					
I-W164.153	MTRU	CH	Solidified Organics	Envirostone(11)	n/a					
I-W167.149	MTRU	CH	Solidified Organics	calc-silicate(12)	n/a					
I-W167.926	MTRU	CH	Solidified Organics	calc-silicate(12)	n/a					
I-W309.610	MTRU	CH	Solidified Organics	calc-silicate(12)	n/a					
I-W317.757	MTRU	CH	Solidified Organics	resins(3)	73.1	39.1	0	2858.21	0	
I-W317.758	MTRU	CH	Solidified Organics	resins(3)	73.1	11.5	0	840.65	0	
I-W319.584	MTRU	CH	Solidified Organics	resins(3)	73.1	0.7	0	51.17	0	
I-W321.1023	MTRU	CH	Solidified Organics	resins(3)	73.1	1.3	0	95.03	0	
A-T002	TRU	CH	Solidified Organics	(10)	693	1.5	29.1	21205.8	20166.3	
-W019	MTRU	CH	Solidified Organics	Envirostone(11)	n/a					
F-MT0003	MTRU	CH	Solidified Organics	calc-silicate(12)	n/a					
F-MT0801	MTRU	CH	Solidified Organics	Envirostone(11)	n/a					
F-MT0375	MTRU	CH	Solidified Organics	Oil Dri(13)	n/a					
F-TT0809	TRU	CH	Solidified Organics	BIR	32	0	35.2	1126.4	1126.4	
L-W280	MTRU	CH	Solidified Organics	paint(14)	n/a					
L-W282	MTRU	CH	Solidified Organics	Mainly debris	n/a					
L-W285	MTRU	CH	Solidified Organics	Conweb pads(15)	n/a					
L-W286	MTRU	CH	Solidified Organics	Oil Dri(13)	n/a					
L-W326	MTRU	CH	Solidified Organics	Conweb pads(15)	n/a					
L-W329	MTRU	CH	Solidified Organics	PCB waste(16)	n/a					
L-W333	MTRU	CH	Solidified Organics	PCB waste(16)	n/a					
L-W338	MTRU	CH	Solidified Organics	Conweb pads(15)	n/a					
L-W344	MTRU	CH	Solidified Organics	Diatomaceous earth(7)	n/a					
L-W345	MTRU	CH	Solidified Organics	Conweb pads(15)	n/a					
L-W348	MTRU	CH	Solidified Organics	animal waste	n/a					
L-W361	TRU	CH	Solidified Organics	Vermiculite(9)	n/a					
L-W380	TRU	CH	Solidified Organics	Diatomaceous earth(7)	n/a					
						RH-TRU Total		505118.2	82095.27	kg
						CH-TRU Total		5282085.787	1344061.99	kg
otal Cement equals Stored + Projected plus 2.05 times Projected for CH TRU						TOTAL SCALED			8542531.067	kg
plus Stored + Projected for RH-TRU										

Table 1. Estimate of Portland Cement in TRU Waste for Disposal in the WIPP

WIPP_ID	Waste_Type	Handling	Final_Waste_Form	Solidification	Cement (kg/m³)	Stored (m³)	Projected (m³)	Total kg	Projected kg	
) Salt waste, does not contain any portland cement										
) Encapsulated metal waste, does not contain any portland cement										
) Assume RF-MT0806 for final form cement density										
) Florco (clay) is used as sorbent not portland cement										
) The portland cement for this waste stream in the BIR occurs in the "Other Inorganic Material"										
) Only 61% of the solidification agent reported as cement in the TWBIR is portland cement										
) Diatomaceous earth is used as the sorbent in this waste stream										
) Plaster of Paris used as solidification agent										
) Vermiculite used as sorbent in this waste stream										
0) Basis for portland cement are values reported in TWBIR supplemented with information provided by LANL										
for previous WIPP memo on nitrate, sulfate, and phosphate										
1) Solidification agent is Envirostone (a gypsum-based process) that does not contain portland cement										
2) Solidification agent is a calcium-silicate process that does not use portland cement										
3) Oil Dri is used as sorbent										
4) Solidified organics is paint, contains no portland cement										
5) Solidification agent/sorbent is conwed pads (plastic fiber absorbent) +/- vermiculite										
6) PCB containing waste, excluded from current WIPP inventory										

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.14

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WPO 31379

INFORMATION ONLY

CTAC MEMORANDUM

To: File

From: Paul E. Drez, CTAC PED

Subject: Preliminary Estimate for SNL/NM Performance Assessment Calculations of Nitrate, Sulfate, and Phosphate Content in Transuranic Solidified Wastes Destine for Disposal in WIPP

Date: January 26, 1996

SUMMARY

The density and mass of nitrate and sulfate in transuranic (TRU) waste destine for transport to and disposal in the Waste Isolation Pilot Plant (WIPP) has been estimated based on data from the TRU waste generator/storage sites. The average density scaled over the entire WIPP disposal inventory is 9.24 kg/m^3 for nitrate and 3.60 kg/m^3 for sulfate, and the total mass scaled over the entire WIPP disposal inventory is 1.62E+06 kg for nitrate and 6.33E+05 kg for sulfate. These densities and masses are for combined CH and RH TRU waste inventories. No value for phosphate has been proposed due to the lack of sufficient information. Trace quantities of inorganic phosphate might be expected in some of the sludges and solidification agents, but no supporting analytical data is available.

INTRODUCTION

Sandia National Laboratories/New Mexico (SNL/NM) has requested an estimate of the amount of nitrate, sulfate, and phosphate expected to be in the transuranic (TRU) inventory destined for transport to and disposal in the Waste Isolation Pilot Plant (WIPP)(Appendix B; DOE, 1995). The remainder of this memo describes the methodology and data used in order to calculate these preliminary estimates.

ASSUMPTIONS

This PRELIMINARY ESTIMATE is made based on the following assumptions:

- Values presented are those expected for final waste forms to be disposed of in the WIPP.
- Information has been requested from sites based on solidified inorganic and solidified organic waste forms only, and is the best available data from the TRU waste generator/storage sites:
    - The main source of nitrate is anticipated to be from the solidified inorganic

waste forms, which in most cases, are sludges produced from the neutralization/solidification of nitric acid-based solutions used at the TRU waste generator/storage sites. Nitrates are very soluble in aqueous solutions and generally do not produce precipitates in the sludges. The nitrates are generally thought to be present as ions sorbed on precipitates or as interstitial solution trapped in the precipitated sludges prior to solidification.

Minor amounts of nitrate, as evaporites, are anticipated in the debris waste forms that will be acceptable for WIPP disposal, but insufficient data is available to make any such estimates in the TRU waste at this time.

The main sources of sulfates are anticipated to be: 1) chemicals (e.g. iron sulfates) added to the inorganic solutions at the time of flocculation and precipitation of sludges and 2) the use of Envirostone [a gypsum ($CaSO_4$) based solidification material] for solidification of inorganic and/or organic solutions/sludges at some TRU waste generator/storage sites.

No quantifiable sources of phosphate have been identified in the inorganic solidified final waste forms at present. Trace quantities might be expected in some of the sludges and solidification agents, but no supporting analytical data is available. The quantities of inorganic phosphate are anticipated to be low in inorganic sludges based on process histories at TRU waste sites.

Analytical data in Attachment 2 provides only "less than 0.0025" weight percent values for phosphate, which are similar to the 0.001 weight percent estimate provided by LANL in Attachment 1. These values are too low to make any reliable estimate of phosphate in TRU waste, but indicate that the quantities will be very small, compared with the nitrate and sulfate values reported. The "40%" value reported on page A2-7 is an analytical error based on process knowledge and the lack of cations to support such a large value of phosphate in that particular analysis.

GENERAL VOLUME CALCULATIONS

Nitrate

The amount of nitrate is estimated on the basis of the volumes of Solidified Inorganics, which are calculated as explained below:

- Table 1 lists (in Column 2) the final waste form volumes of Solidified Inorganics for Contact-Handled (CH) TRU and Remote Handled (RH) TRU from Figures 3-9 and 3-16 of Revision 2 of the TWBIR (DOE, 1995) for the anticipated WIPP inventory (stored plus projected volumes until 2022).

- Footnotes in Columns 3 and 4 indicate why certain volumes of waste have been eliminated from further consideration in the calculations:
  - Footnote 1 eliminates those volumes of chemically precipitated solidified inorganics for which no nitrate estimates in the waste are available. An estimate of the nitrate contribution from these solidified inorganics will be accounted for in the scaling process.
  - Footnote 2 eliminates the volume of Solidified Inorganics from SRS from further consideration because it is a "vitrified" waste form which should not contain any significant amount of nitrates due to the thermal treatment proposed for that waste form.
  - Footnote 3 eliminates from further consideration those volumes of Solidified Inorganics which represent non-precipitated particulates (e.g., incinerator ash, graphite fines, etc.) which have been cemented to meet the WIPP WAC; nitrates are not expected to be present in these particulates.
- Rocky Flats Environmental Technology Site (RFETS) and Los Alamos National Laboratory (LANL) have provided analytical data/estimates for nitrate in Solidified Inorganics. The RFETS data has been used also for the RFETS waste stored at INEL.

Sulfate

- To determine the amount of solidified wastes that need to be considered for calculating the sulfate content of the WIPP inventory (Table 2), the volume of Solidified Organics must be added to the volume of Solidified Inorganics from Table 1:
  - The Solidified Organics from Figures 3-10 and 3-17 of Revision 2 of the TWBIR (DOE, 1995) have been added to Table 1 (above) to produce Table 2
  - LANL has used an Envirostone (gypsum-based) process for solidification of inorganic sludges in the past (approximately 9% of 4888 m^3 in storage at LANL) but plan to eliminate the process in the future and only use portland-based cement for solidification (as was used in the past prior to usage of the Envirostone)
  - Since the mid 1980's, RFETS has used an Envirostone solidification process for their organic sludges. Therefore, some of their waste in storage and projected contain large amounts of sulfate, as well as some Solidified Organics in storage at INEL.
  - LLNL is the only other TRU waste site known to be using Envirostone for the solidification of organic liquids/sludges (approximately 7 m^3 stored/projected).

NITRATE MASS CALCULATIONS

Table 3 contains in Column 1 a list of those waste streams that contain the volume of waste from each TRU waste generator/storage site listed in Column 4 of Table 1. The additional data provided are:

- Column 2 lists the Item Description Codes (IDCs) for waste streams produced at RFETS and/or stored at INEL. The RF111 designation is for Content Code 111 from RFETS, where the IDC is not specified.
- Column 3 lists the stored + projected volume for each waste stream.
- Column 4 lists the sum of the waste material parameters (WMP) for each waste stream from the individual Waste Stream Profiles in Revision 2 of the TWBIR. Exceptions to this rule are listed in footnotes in Table 3.
- Column 5 lists the mass of the waste for each waste stream which is the product of multiplying Columns 3 and 4.
- Column 6 lists the values of nitrate used for each waste stream. The sources of the these values are:
    - For RFETS, the nitrate values are from Appendix I of Revision 2 of the TWBIR. The 8% values for IDC 001 has also been applied to IDCs 002 and 007 at both RFETS and INEL. All these IDCs represent "older" methods of solidification where the sludges contain portland cement mainly as a sorbent interlayered with sludge which did not contain diatomaceous earth (see Clements, 1982 for drawings).

      The 4% value listed in Appendix I of the TWBIR for IDC 807 represents a "newer" method of solidification where diatomaceous earth is used as a vacuum filtration agent and portland cement is mixed with the resulting sludge to form a "monolithic" solidified final waste form. The dilution with diatomaceous earth and additional portland cement lowers the overall nitrate value of the final waste form.
    - For waste stream IN-W315.601, Clements (1982) indicates that the waste stream is made up of approximately 60% NaNO3 and 30% KNO3 (assumed weight percents). This calculates as 62% nitrate.
    - Attachment 1 represents a memo from LANL that provides estimates for nitrates in the waste streams. Note that the Envirostone process only accounts for a small percentage of stored volume for 3 of the waste streams. The values quoted in Column 6 are based on the small percentage of Envirostone

solidification agent in the overall waste streams.

- Column 7 represents the mass of nitrates in kg which is the product of multiplying Columns 5 and 6.

SULFATE MASS CALCULATIONS

The sulfate calculations presents in Table 4 follow the same format as the nitrate calculations in Table 3. The origin of the values used for sulfate in the RFETS, INEL, LLNL, and LANL waste streams are summarized below:

- RFETS/INEL
    - The 0.11% sulfate value is an average of the three analyses marked "7412 Sludge" in Attachment 2 which are applied to IDCs 001 and 002, and at half that value for IDCs 800 and 803 (as explained in the nitrate section).
    - The sulfate value of 0.02% is derived from the Attachment 2 analysis marked "374 Waste Sludge - Dried Sludge". This value is used for IDC 007 and at half value for IDC 807.
    - The sulfate value (25.1%) for the Envirostone solidification of organic sludges (IDC 801) is derived from an average value in Attachment 3, which represents guidelines for mixing constituents together for IDC 801 and IDC 700 (at INEL only in storage).
- LANL
    - The values for sulfate quoted in Column 7 are derived from data provided in Attachment 1. As with the nitrate calculations, the percentage of waste in each waste stream solidified by Envirostone versus portland cement is used to calculated the overall sulfate value for each waste stream.
- LLNL
    - No value for sulfate was requested from LLNL for their one Solidified Organic waste stream. The same value for Envirostone-solidified waste at RFETS (25.1%) was assumed for the LLNL waste stream.

SUMMARY CALCULATIONS

Table 5 presents the summary calculations for determining the density (kg/m^3) of nitrate and sulfate in the overall WIPP inventory and scaling of the density to take into account those chemically precipitated waste streams for which data was not available. SNL/NM should use the scaled densities for their calculations. The last column in Table 5 provides the estimated mass of nitrate and sulfate if the design capacity of WIPP for CH-TRU and RH-TRU are fully utilized based on the scaled densities for nitrate and sulfate.

REFERENCES

Clements, 1982, "Content Code Assessments for INEL Contact-Handled Stored Transuranic Wastes," WM-F1-82-021, Idaho Falls, Idaho.

U. S. Department of Energy, 1995, "Transuranic Waste Baseline Inventory Report (Revision 2)," DOE/CAO-95-1121, Carlsbad, New Mexico.

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TABLE 1. TRU VOLUMES FOR NITRATE CALCULATIONS (SOLIDIFIED INORGANICS ONLY)

TRU WASTE SITE	TOTAL VOLUME (STORED + PROJECTED) (m^3)	VOLUMES WITH NITRATE DATA OR WITH PARTICULATES (m^3)	VOLUMES OF SLUDGES WITH NITRATE DATA (m^3)
Hanford (CH)	23.39	(TO BE SCALED)[1]	(TO BE SCALED)[1]
ANL-E (CH)	5.20	(TO BE SCALED)[1]	(TO BE SCALED)[1]
NTS (CH)	5.67	(TO BE SCALED)[1]	(TO BE SCALED)[1]
SRS (CH)	1369.8	1369.8	[2]
RFETS (CH)	1423.01	1389.52	229.63[3]
INEL (CH)	4344.44	3900.39	3598.84[3]
Mound (CH)	6.03	(TO BE SCALED)[1]	(TO BE SCALED)[1]
LANL(CH)	6922.02	6922.02	6922.02
AL (CH)	0.42	(TO BE SCALED)[1]	(TO BE SCALED)[1]
LLNL (CH)	20.18	(TO BE SCALED)[1]	(TO BE SCALED)[1]
CH TOTAL	14120.15	13581.73	10750.49
ORNL (RH)	1243.33	(TO BE SCALED)[1]	(TO BE SCALED)[1]
INEL (RH)	65.27	65.27	65.27
ANL-E (RH)	30.26	(TO BE SCALED)[1]	(TO BE SCALED)[1]
RH TOTAL	1338.86	65.27	65.27
TRU TOTAL	15459.01	13647.0	10815.76

[1] Eliminates those volumes of chemically precipitated solidified inorganics for which no nitrate estimates in the waste are available. An estimate of the nitrate contribution from these solidified inorganics will be accounted for in the scaling process.

[2] Eliminates the volume of Solidified Inorganics from SRS from further consideration because it is a "vitrified" waste form which should not contain any significant amount of nitrates due to the thermal treatment proposed for that waste form.

[3] Eliminates from further consideration those volumes of Solidified Inorganics which represent non-precipitated particulates (e.g., incinerator ash, graphite fines, etc.) which have been cemented to meet the WIPP WAC and nitrates are not expected to be present in the particulates.

TABLE 2. TRU VOLUMES FOR SULFATE CALCULATIONS

TRU WASTE SITE	FINAL WASTE FORM	TOTAL VOLUME (m^3)	VOLUME WITH SULFATE DATA (m^3)
Hanford (CH)	Solidif. Inorg.	23.39	(TO BE SCALED)[1]
ANL-E (CH)	Solidif. Inorg.	5.20	(TO BE SCALED)[1]
NTS (CH)	Solidif. Inorg.	5.67	(TO BE SCALED)[1]
SRS (CH)	Solidif. Inorg.	1369.8	(TO BE SCALED)[1]
RFETS (CH)	Solidif. Inorg.	1423.01	229.63
INEL (CH)	Solidif. Inorg.	4344.44	3598.42
Mound (CH)	Solidif. Inorg.	6.03	(T BE SCALED)[1]
LANL (CH)	Solidif. Inorg.	6922.02	6922.02
AL (CH)	Solidif. Inorg.	0.42	(TO BE SCALED)[1]
LLNL (CH)	Solidif. Inorg.	20.18	(TO BE SCALED)[1]
RFETS (CH)	Solidif. Org.	140.93	108.99
Hanford (CH)	Solidif. Org.	76.13	(TO BE SCALED)[1]
LANL (CH)	Solidif. Org.	30.58	(TO BE SCALED)[1]
INEL (CH)	Solidif. Org.	789.67	2.55
ANL-E (CH)	Solidif. Org.	0.21	(TO BE SCALED)[1]
LLNL (CH)	Solidif. Org.	6.86	6.86
CH TOTAL		15164.53	10868.93
ORNL (RH)	Solidif. Inorg.	1243.33	(TO BE SCALED)[1]
INEL (RH)	Solidif. Inorg.	65.27	65.27
ANL-E (RH)	Solidif. Inorg.	30.26	(TO BE SCALED)[1]
INEL (RH)	Solidif. Org.	3.56	(TO BE SCALED)[1]
RH TOTAL		1342.42	65.27
TRU TOTAL		16506.95	10933.74

[1] No sulfate data available from these sites for any waste streams.

TABLE 3. NITRATE CALCULATION

Waste Stream	IDCs	Volume	Sum WMP	Mass Waste	% Nitrate	Nitrate
		(m3)	(kg/m3)	(kg)	(weight%)	(kg)
RF-MT0001	001	3.74	781.9	2924.31	8	233.94
RF-MT007	007	0.832	544.3	452.86	8	36.23
RF-MT0800	800	104.42	775.2	80946.38	4	3237.86
RF-MT0803	803	4.99	635.2	3169.65	4	126.79
RF-MT0807	807	115.02	819.6	94270.39	4	3770.82
RF-T010	800/803/807	0.62	796.1	493.58	4	19.74
TOTAL RFETS		229.622		182257.17		7425.37
IN-W216.875	001/002	1478.88	819.6	1212090.05	8	96967.20
IN-W216.877	001/002	43.91	571.4	25090.17	8	2007.21
IN-W216.98	001/002	555.65	726.6	403735.29	8	32298.82
IN-W218.909*	007	101.91	544.3	55469.61	8	4437.57
IN-W220.114	RF111	122.8	725.6	89103.68	4	3564.15
IN-W220.925	RF111	443.04	819.6	363115.58	4	14524.62
IN-W228.101	002	287.33	317.3	91169.81	8	7293.58
IN-W228.883	002	608.82	358	217957.56	8	17436.60
IN-W228.886	002	21.36	249.6	5331.46	8	426.52
IN-W315.601**	005	0.42	664	278.88	62	172.91
TOTAL INEL		3664.12		2463342.09		179129.19
LA-M002		3606.81	1296	4674425.76	8.8	411349.47
LA-T006		86.53	1004.8	86945.34	8.8	7651.19
LA-W003		1836.58	1339.3	2459731.59	8.7	213996.65
LA-W006		1392.1	1004.8	1398782.08	8.7	121694.04
TOTAL LANL		6922.02		8619884.78		754691.35
TOTAL TRU		10815.76		11265484		941245.91

* INEL did not report waste material parameters for this waste stream. The value for this IDC at RFETS was assumed.

** This waste stream was reported in Clements (1983) to be 60% $NaNO_3$ and 30% KNO_3. The weight of the waste for this IDC was used from Clements (1983), since no value was quoted in Revision 2 of the TWBIR.

TABLE 4. SULFATE CALCULATION

Waste Stream	IDCs	Waste Form	Volume (m3)	Sum WMP (kg/m3)	Mass Waste (kg)	% Sulfate (weight%)	Sulfate (kg)
RF-MT0001	001	Solidified Inorg	3.74	781.9	2924.31	0.11	3.22
RF-MT007	007	Solidified Inorg	0.832	544.3	452.86	0.02	0.09
RF-MT0800	800	Solidified Inorg	104.42	775.2	80946.38	0.055	44.52
RF-MT0801	801	Solidified Org.	108.99	877.1	95595.13	25.1	23994.38
RF-MT0803	803	Solidified Inorg	4.99	635.2	3169.65	0.055	1.74
RF-MT0807	807	Solidified Inorg	115.02	819.6	94270.39	0.01	9.43
RF-T010	800/803/807	Solidified Inorg	0.62	796.1	493.58	0.055	0.27
TOTAL RFETS			338.612		277852.30		24053.65
IN-W164.1060**	700	Solidified Org	1.66	877.1	1455.99	25.1	365.45
IN-W164.153**	700	Solidified Org	0.89	877.1	780.62	25.1	195.94
IN-W216.875	001/002	Solidified Inorg	1478.88	819.6	1212090.05	0.11	1333.30
IN-W216.877	001/002	Solidified Inorg	43.91	571.4	25090.17	0.11	27.60
IN-W216.98	001/002	Solidified Inorg	555.65	726.6	403735.29	0.11	444.11
IN-W218.909*	007	Solidified Inorg	101.91	544.3	55469.61	0.02	11.09
IN-W220.114	RF111	Solidified Inorg	122.8	725.6	89103.68	0.055	49.01
IN-W220.925	RF111	Solidified Inorg	443.04	819.6	363115.58	0.055	199.71
IN-W228.101	002	Solidified Inorg	287.33	317.3	91169.81	0.11	100.29
IN-W228.883	002	Solidified Inorg	608.82	358	217957.56	0.11	239.75
IN-W228.886	002	Solidified Inorg	21.36	249.6	5331.46	0.11	5.86
TOTAL INEL			3666.25		2465299.82		2972.11
LA-M002		Solidified Inorg	3606.81	1296	4674425.76	1.4	65441.96
LA-T006		Solidified Inorg	86.53	1004.8	86945.34	1.7	1478.07
LA-W003		Solidified Inorg	1836.58	1339.3	2459731.59	5.5	135285.24
LA-W006		Solidified Inorg	1392.1	1004.8	1398782.08	8.1	113301.35
TOTAL LANL			6922.02		8619884.78		315506.62
LL-W019***		Solidified Org	6.86	268	1838.48	25.1	461.46
TOTAL LLNL			6.86		1838.48		461.46
TOTAL TRU			10933.74		11364875.4		342993.8

* INEL did not report waste material parameters for this waste stream. The value for this IDC at RFETS was asumed

** INEL did not report waste material parameters for this waste stream. The value for this IDC at RFETS was asumed

*** Sulfate value for LLNL Solidified Organic waste orm assumed to be same as for RFETS Solidified Organics (IDC 801)

TABLE 5. NITRATE/SUL[illegible] DENSITY CALCULATIONS

Constituent	Volume Solidified Waste m3	Mass Solidified Waste kg	Mass Constituent kg	Anticipated Waste Volume m3	WIPP Average Density of Constituent kg/m3	% Sludge Used In Calculations %	WIPP Average Scaled Density of Constituent kg/m3	Total Mass of Consituent for WIPP Design Capacity kg
Footnotes	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
Nitrate	10815.76	11265484	941245.9	1.19E+05	7.91	85.6	9.24	1.62E+06
Sulfate	10933.74	11364875	342993.8	1.19E+05	2.88	80	3.60	6.33E+05

(1) "Total TRU" Volumes for Tables 3 and 4.

(2) "Total TRU" Mass from Tables 3 and 4.

(3) "Total TRU" Nitrate/Sulfate from Tables 3 and 4.

(4) Anticipated Volume of CH- and RH-TRU Waste (stored + projected to 2022) from Table 3-1 in Rev. 2 of TWBIR. RH-TRU anticipated volume is limited to 7080 m3; design capcaity of WIPP.

(5) "Mass of Constituent" Column divided by "Anticipated Waste Volume" Column.

(6) Calculated from Table 1 "Total TRU" data. Nitrate = subtract 10815.76 from 13647 to get amount of particulate waste (2831.24). Subtract 2831.24 from 15459.01 to get total chemically precipitated waste (12627.77). Divide 10815.76 by 12627.77 and multiply by 100%. Sulfate is calculated in similar manner.

(7) Divide "Density of Constituent" by "% Sludge Used in Calculations".

(8) Multiply "Scaled Density of Consituent" by 175,600 m3 (design capacity of WIPP).

ATTACHMENT 1

TELEPHONE CONFERENCE SUMMARY

Parties: Paul Drez, DEA/CTAC
Davis Christenson, LANL

For Solidified Inorganics waste stream LA-T006; LA-W003; LA-W006; and LA-M002 assume the following composition for final waste form:

Envirostone-based solidified waste forms:

Nitrate 8.2%
Sulfate 38.5%
Phosphate 0.001%

Portland Cement-based solidified waste forms:

Nitrate 8.8%
Sulfate 1.4%
Phosphate 0.001%

LA-M002 has only used portland cement; the other three have use portland cement until 1985 and then Envirostone:

	Stored Wasted		Projected Waste	
WS#	Portland	Envirostone	Portland	Envirostone
LA-T006	84.5%	15.5%	100%	0%
LA-W006	54.65%	45.35%	100%	0%
LA-W003	84.5%	15.5%	100%	0%
LA-M002	100%	0%	100%	0%

ATTACHMENT 2

```
D61472-01                 LABORATORY SAMPLE RESULTS                 DATE 04/10/80
                              7412 Sludge                                  PAGE  1

SAMPLE-ID             00-008395                DJC NUMBER        97038000
ENTRY DATE            11-01-79                 ACCOUNT CHARGED   8037
COMPLETION DATE       04-10-80                 BUILDING          559
                                               CLASS             SSPI
CUSTOMER              P. T. GODESAIBOIS
---------------------------------------------------------------------------------

                 ** ATOMIC ABSORPTION SPECTROMETRY RESULTS

    CA          86512.        PPM(W)        FE          61597.        PPM(W)
    GA    <        50.        PPM(W)        K            6162.        PPM(W)
    NA          65501.        PPM(W)        SI           3659.        PPM(W)

                 ** PLUTONIUM CHEMISTRY LABORATORY RESULTS

    CL(-)          0.16       %(W)          CO3=           0.36       %(W)
    F(-)          57.         PPM(W)        H2O           61.0        %(W)
    NO3            4.2        %(W)          PO4    <       0.0025     %(W)
    SO4            0.085      %(W)

                 ** SEMI-QUANTATIVE EMISSION SPEC RESULTS

    AG             50.        PPM(W)        AL          20000.        PPM(W)
    AS    <        50.        PPM(W)        B             100.        PPM(W)
    BA            100.        PPM(W)        BE             50.        PPM(W)
    BI    <        50.        PPM(W)        CA     >   200000.        PPM(W)
    CD    <      1000.        PPM(W)        CE     <      500.        PPM(W)
    CO    <        50.        PPM(W)        CR            500.        PPM(W)
    CS    <      1000.        PPM(W)        CU           4000.        PPM(W)
    FE          50000.        PPM(W)        GE     <       10.        PPM(W)
    HG    <        10.        PPM(W)        K           40000.        PPM(W)
    LI    <      1000.        PPM(W)        MG          10000.        PPM(W)
    MN            500.        PPM(W)        MO            500.        PPM(W)
    NA          50000.        PPM(W)        NB     <       50.        PPM(W)
    NI           2000.        PPM(W)        P      <     1000.        PPM(W)
    PB    <        50.        PPM(W)        RB     <      500.        PPM(W)
    SB    <        50.        PPM(W)        SI         100000.        PPM(W)
    SN    <        10.        PPM(W)        SR          10000.        PPM(W)
    TA    <        50.        PPM(W)        TE     <      100.        PPM(W)
    TH    <       500.        PPM(W)        TI            500.        PPM(W)
    TL    <       500.        PPM(W)        U      <      500.        PPM(W)
    V     <         5.        PPM(W)        W      <     1000.        PPM(W)
    ZN    <       500.        PPM(W)        ZR     <       50.        PPM(W)

                 ** RADIOCHEMISTRY LABORATORY RESULTS

    AM             0.0000317  G/G
```

ATTACHMENT 2

```
D61472-01                LABORATORY SAMPLE RESULTS                  DATE 04/10/80
                                                                          PAGE   2
SAMPLE-ID    00-008395
-------------------------------------------------------------------------------------

             ** RADIOCHEMISTRY LABORATORY RESULTS          (CONTINUED)

     PU                 0.0000223   G/G            U            0.0017     G/G

                                      AUTHORIZED SIGNATURE
```

Howell

ATTACHMENT 2

```
061472-01                 LABORATORY SAMPLE RESULTS                DATE 04/10/80
                                                                   PAGE    1

SAMPLE-ID              00-008396                DJO NUMBER       97038000
ENTRY DATE             11-01-79                 ACCOUNT CHARGED  8037
COMPLETION DATE        04-10-80                 BUILDING         559
                                                CLASS            SSP1
CUSTOMER               P. T. GODESAIBOIS
-------------------------------------------------------------------------------

                ** ATOMIC ABSORPTION SPECTROMETRY RESULTS

    CA          194587.        PPM(W)        FE          47915.          PPM(W)
    GA     <        50.        PPM(W)        MG           9581.          PPM(W)
    NA          105060.        PPM(W)        SI            158.          PPM(W)

                ** PLUTONIUM CHEMISTRY LABORATORY RESULTS

    CL(-)            0.15      %(W)          CO3=             0.74       %(W)
    F(-)           101.        PPM(W)        H2O             55.0        %(W)
    NO3              8.0       %(W)          PO4     <        0.0025     %(W)
    SO4              0.096     %(W)

                ** SEMI-QUANTATIVE EMISSION SPEC RESULTS

    AG                10.      PPM(W)        AL           10000.         PPM(W)
    AS     <          50.      PPM(W)        B              100.         PPM(W)
    BA               500.      PPM(W)        BE            1000.         PPM(W)
    BI     <          50.      PPM(W)        CA     >    200000.         PPM(W)
    CD     <        1000.      PPM(W)        CE     <       500.         PPM(W)
    CO     <          50.      PPM(W)        CR             500.         PPM(W)
    CS     <        1000.      PPM(W)        CU             500.         PPM(W)
    FE             50000.      PPM(W)        GE     <        10.         PPM(W)
    HG     <          10.      PPM(W)        K            40000.         PPM(W)
    LI     <        1000.      PPM(W)        MG           50000.         PPM(W)
    MN               500.      PPM(W)        MO             200.         PPM(W)
    NA             50000.      PPM(W)        NB     <        50.         PPM(W)
    NI              1000.      PPM(W)        P      <      1000.         PPM(W)
    PB                50.      PPM(W)        PU     <       100.         PPM(W)
    RB     <         500.      PPM(W)        SB     <        50.         PPM(W)
    SI            100000.      PPM(W)        SN     <        10.         PPM(W)
    SR             10000.      PPM(W)        TA     <        50.         PPM(W)
    TE     <         100.      PPM(W)        TH     <       500.         PPM(W)
    TI               500.      PPM(W)        TL     <       500.         PPM(W)
    U      <         500.      PPM(W)        V      <         5.         PPM(W)
    W      <        1000.      PPM(W)        ZN     <       500.         PPM(W)
    ZR     <          50.      PPM(W)
```

7412 Sludge

```
D61472-01                LABORATORY SAMPLE RESULTS                DATE 04/10/80
                                                                      PAGE   2
SAMPLE-ID    00-008396
---------------------------------------------------------------------------------

            ** RADIOCHEMISTRY LABORATORY RESULTS

   AM                0.00000546 G/G
   PU                0.0000389  G/G           U              0.000198   G/G

                                     AUTHORIZED SIGNATURE
```

Hawkes

ATTACHMENT 2

D61472-01 LABORATORY SAMPLE RESULTS DATE 04/10/80

7412 Sludge

PAGE 1

SAMPLE-ID	00-008397	DJO NUMBER	97038000
ENTRY DATE	11-01-79	ACCOUNT CHARGED	8037
COMPLETION DATE	04-10-80	BUILDING	559
		CLASS	SSPL
CUSTOMER	P. T. GODESAIBOIS		

** ATOMIC ABSORPTION SPECTROMETRY RESULTS

CA		121661.	PPM(W)	FE		49286.	PPM(W)
GA	<	50.	PPM(W)	MG		18377.	PPM(W)
NA		100179.	PPM(W)	SI		217.	PPM(W)

** PLUTONIUM CHEMISTRY LABORATORY RESULTS

CL(-)		1.5	%(W)	CO3=		0.59	%(W)
F(-)		143.	PPM(W)	H2O		60.2	%(W)
NO3		9.1	%(W)	PO4	<	0.0025	%(W)
SO4		0.14	%(W)				

** SEMI-QUANTATIVE EMISSION SPEC RESULTS

AG		40000.	PPM(W)	AL		10000.	PPM(W)
AS	<	50.	PPM(W)	B		100.	PPM(W)
BA		50.	PPM(W)	BE		1000.	PPM(W)
BI	<	50.	PPM(W)	CA		200000.	PPM(W)
CD	<	1000.	PPM(W)	CE	<	500.	PPM(W)
CO	<	50.	PPM(W)	CR		500.	PPM(W)
CS	<	1000.	PPM(W)	CU		1000.	PPM(W)
FE		50000.	PPM(W)	GE	<	10.	PPM(W)
HG	<	10.	PPM(W)	K		40000.	PPM(W)
LI	<	1000.	PPM(W)	MG		100000.	PPM(W)
MN		100.	PPM(W)	MO		200.	PPM(W)
NA		60000.	PPM(W)	NB	<	50.	PPM(W)
NI		500.	PPM(W)	P	<	1000.	PPM(W)
PB		50.	PPM(W)	PU	<	100.	PPM(W)
RB	<	500.	PPM(W)	SB	<	50.	PPM(W)
SI		100000.	PPM(W)	SN	<	10.	PPM(W)
SR		10000.	PPM(W)	TA	<	50.	PPM(W)
TE	<	100.	PPM(W)	TH	<	500.	PPM(W)
TI		300.	PPM(W)	TL	<	500.	PPM(W)
U	<	500.	PPM(W)	V	<	5.	PPM(W)
W	<	1000.	PPM(W)	ZN	<	500.	PPM(W)
ZR	<	50.	PPM(W)				

M

```
D61472-01              LABORATORY SAMPLE RESULTS               DATE 04/10/80
                                                                   PAGE    2
SAMPLE-ID    00-008397
------------------------------------------------------------------------------

               ** RADIOCHEMISTRY LABORATORY RESULTS

     AM            0.000628    MG/G
     PU            0.00000481  G/G           U              0.000561    G/G

                                  AUTHORIZED SIGNATURE
```

ATTACHMENT 2

Rockwell International

Energy Systems Group
Rocky Flats Plant
P.O. Box 464
Golden, Colorado 80401

ANALYTICAL REPORT

To C.T. Hewitt 374 ✓ File	Account No. 371	Date 7-24-81	Lab. No. M81-1109
		Reported by	
		Approved A.M. Miller A.M. Miller	

Sample Description

374 Waste Sludge — Dried sludge

Analysis Results

A characterization of the 374 waste sludge was requested. The analysis of a composited sample is given. All results are in %.

Ca	11
Mg	3.8
Si	5.8
Al	0.4
Cr	0.12
Fe	0.9
K	0.25
Na	0.8
C	13
S	0.36
SO_4	0.02
Cl	1.3
F	0.5
PO_4	40
NO_3	6.6
CO_3	0.04
HCO_3	0.33

The cations greater than 1% were determined by A^2 and those less than 1% by emission spectroscopy. The anions, except for HCO_3. CO_3, and NO_3 were determined on a nitric acid leach of the sludge. Eighteen percent of the sludge was soluble in water, and 36% soluble in nitric acid.

ATTACHMENT 3 WIPP-0104-0COR-0192

PAGE 1 OF 9 PAGES

CORRES. CONTROL
OUTGOING LTR NO

88 RF 1089

DIST.		
SANCHINI, D. J.		
BADER, C. P.		
CAMPBELL, G.W.		
HOOD, R. C.		
KINZER, J. E.		
KIRBY, W. A.		
McNETT, J.F.		
MEYERS, G.W.		
SHANNON, W.M.		
SMITH, R.E.		
WEIDNER, C.W.		
WESTON, W.F.	X	
WILSON, G.L.		
WOZNIAK, B.D.		
YOUNG, E.R.		
BETCHER, D.H.		
CARNIVAL, G.J.		
HARMAN, L.K.		
HEBERT, J.L.		
HOEY, J.B.		
HOFFMAN, R.B.		
KRIEG, D.M.	X	X
LIM, B.W.		
LOUDENBURG, G.E.		
NAIMON, E.R.	X	
NEWBY, R.L.		
ROECKER, J.H.		
VELASQUEZ, R.K.		
CORRES. CONTROL	x	x
BRETZKE, C.D.	X	
REINHART, W.D.	X	
PAYNTER, J.K.	X	X
HICKLE, E.L.	X	
CLASSIFICATION		
UNCLASSIFIED	X	X
CONFIDENTIAL		
SECRET		

AUTH. CLASSIFIER SIG.

4/6/88
DATE

IN REPLY TO LTR NO
0521-RF-88

DEC. WCPOY #32

LTR APPROVALS

JKP/jlc

Rocky Flats Plant
North American Space Operations
Rockwell International Corporation
P.O. Box 454
Golden, Colorado 80402-0464
(303) 966-7000
Contractor to U.S. Department of Energy

Rockwell International

April 4, 1988

88-RF-1089

Albert E. Whiteman
Area Manager
DOE, RFAO

ENGINEERING PARAMETERS FOR ROCKY FLATS WASTE FORMS

This information is for the attention of W. C. Rask.

Attached are the engineering parameters for Rocky Flats waste forms that were requested in the letter from J. B. Tollison to distribution, dated March 1, 1988. Information is included for all thirteen Rocky Flats waste forms, which will be transported in the TRUPACT-II container.

If you have questions regarding the enclosed information, contact Jim Alexander at (303) 966-7585 or Jeff Paynter at (303) 966-5252. With your approval please forward to DOE/AL, Waste Transportation.

E. R. Naimon, Manager
Waste Operations
Rocky Flats Plant
Aerospace Operations

Orig. and 3 cc - A. E. Whiteman
Enc.

ENGINEERING PARAMETERS FOR TRUPACT-II

Waste Stream - - TRU SOLIDIFIED ORGANIC WASTE (WF-112)

For data in Section 1, Secondary Container, and Section 2, Arrangement of Secondary Containers, see the General Engineering Parameters for TRUPACT II.

3 WASTE MATERIAL INFORMATION:

3.1 Structural:

3.1.1 Maximum and Minimum Weight - -

Drums: 750 lb max. / 530 lb avg. / 200 lb. min. (including the weight of the drum)

3.1.2 Acceptable Projectile Envelope - - NA, solid monolith cast in the liner inside the drum.

3.2 Thermal:

3.2.1 Quantity of Radionuclides - - Isotopic Composition (Mix Group 9, TRUPACT-II Spec.):

Isotope	Fraction
Pu-238	TRACE
Pu-239	0.930
Pu-240	0.058
Pu-241	0.004
Pu-242	TRACE
Am-241	TRACE
OTHER	0.007

Max. radionuclides (Weapons Grade Pu): 200 grams/drum

Maximum decay heat (Pu): 0.4 watts/drum
(Am): 0.3 watts/drum
Total: 0.7 watts/drum

3.2.2 Chemical Form - -	min.	max.	ave.
oils	10 %	30 %	
trichloroethane and trichlorotrifluoroethane	5 %	10 %	
carbon tetrachloride	2 %	5 %	
emulsifier (a polyethyl glycol ester)	5 %	10 %	
water	5 %	15 %	
gypsum cement	40 %	50 %	200 lb
total liquid (32 gallons)			250 lb

Title 40 CFR Part 191
Compliance Certification
Application
for the
Waste Isolation Pilot Plant

WCA Attachment WCA.8.15

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WPO 37743

Sandia National Laboratories

Albuquerque, New Mexico 87185-1341

INFORMATION ONLY

date: May 9, 1996

to: Distribution

from: Yifeng Wang (Org. 6748)

subject: Evaluation of the Thermal Effect of MgO Hydration for the Long-Term WIPP Performance Assessment

The hydration reaction of backfill MgO with inflow brines can potentially change repository temperatures, due to the exothermic nature of the reaction. This memorandum is to evaluate the thermal effect of MgO hydration on the long-term WIPP performance assessment.

To simplify the problem, we assume that MgO hydration can be described by the overall reaction:

$$MgO + H_2O \rightarrow Mg(OH)_2 \quad . \tag{1}$$

and that the reaction rate is much higher than the brine inflow rate and, therefore, the reaction will be limited by brine inflow. Considering the dimensions of the repository, we also assume that the heat released from the reaction will be dissipated away mainly from the ceiling and ground of the repository and the heat loss from the side walls is negligible. In addition, we assume that the hydration reaction will take place uniformly in a reaction region, which can be a panel or the whole repository.

Based on these assumptions, the thermal effect of MgO hydration can be modeled by a simplified system shown in Figure 1. The temperature distribution (T) can be described by the following equations:

$$C_p \rho \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial X^2} \tag{2}$$

$$T(X,0) = T_0 \tag{3}$$

$$\rho_W V \Delta H = -2Sk \left. \frac{\partial T}{\partial X} \right|_{X=0} \tag{4}$$

$$T(\infty,t) = T_0 \tag{5}$$

where C_p is the heat capacity of surrounding rocks; ρ is the molar density of surrounding rocks; t is time; X is the spatial coordinate; k is the thermal conductivity of surrounding rocks; T_0 is the background temperature; ρ_W is the molar density of water; V is the brine inflow rate; ΔH is the enthalpy change in Reaction (1); S is the horizontal area of the reaction region.

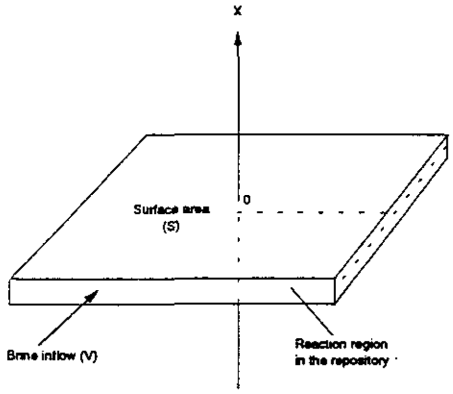

Figure 1. A modeling system for hydration heat production and heat conduction.

The above equations can be solved for T with a Laplace-transformation method:

$$T - T_0 = \frac{\rho_w V \Delta H}{2S\sqrt{C_p \rho k}} \left[2\sqrt{\frac{t}{\pi}}\, e^{-\frac{C_p \rho X^2}{4Kt}} - \sqrt{\frac{C_p \rho}{k}}\, X\, erfc\left(\frac{X}{2}\sqrt{\frac{Cp\rho}{kt}} \right) \right]. \qquad (6)$$

The temperature increase in the repository (ΔT) is obtained by setting $X = 0$ in equation (6):

$$\Delta T = T(0,t) - T_0 = \frac{\rho_w V \Delta H}{S}\sqrt{\frac{t}{\pi C_p \rho k}}. \qquad (7)$$

Equation (7) shows that the repository temperature will increase with t until all MgO becomes hydrated. Therefore, the maximum temperature increase (ΔT_{max}) in the repository can be calculated by

$$\Delta T_{max} = T(0,t) - T_0 = \frac{\Delta H}{S}\sqrt{\frac{\rho_w V M_{MgO}}{\pi C_p \rho k}} \qquad (8)$$

Where M_{MgO} is the inventory of MgO in the reaction region.

To be consistent with actinide solubility calculations, we assume that the reaction will occur uniformly in the whole repository, i.e., the reaction region shown in Figure 1 will extend to the whole repository. Then, $S = 1.1 \times 10^5$ m^2 and $M_{MgO} = 2 \times 10^9$ moles. The other parameters are estimated as follows:

$\rho_W = 5.56 \times 10^4$ moles/m^3;

maximum V = 1000 m^3/year (Joel Miller, personal communication);

$\Delta H = 3.89 \times 10^4$ J/mole (Drever, 1982);

$\rho = 3.7 \times 10^4$ moles/m^3 (Lide, 1994), assuming that the surrounding rocks can be represented by halite;

$C_p = 50$ J/mole/K (Lide, 1994), assuming that the surrounding rocks can be represented by halite;

$k = 6.3$ W/m/K $= 1.99 \times 10^8$ J/year/m/K (Lide, 1994), assuming the surrounding rocks can be represented by halite.

From these data, we estimate the maximum temperature increase in the repository due to MgO hydration to be 3.4 K. Therefore, the thermal effect of MgO hydration can be negligible.

References:

Drever J. I. (1982) The Geochemistry of Natural Water. Prentice-Hall.
Lide D. R. (1994) Handbook of Chemistry and Physics. CRC Press.

Distribution:

MS 1320 J. Nowak (Org. 6831)
MS 1320 R. V. Bynum (Org. 6831)
MS 1328 C. T. Stockman (Org. 6749)
MS 1335 M. S. Y. Chu (Org. 6801)
MS 1341 C. C. Crafts (Org. 6748)
MS 1341 J. T. Holmes (Org. 6748)
MS 1341 B. M. Butcher (Org. 6748)
MS 1341 L. H. Brush (Org. 6748)
MS 1341 Y. Wang (Org. 6748)
MS 1341 R. F. Weiner (Org. 6751)
MS 1343 A. S. Reiser (Org. 6751)
MS 1330 SWCF-A (Org. 6352), WBS 1.1.09.1.1(RC)

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Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

WCA Attachment WCA.8.16

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WPO 31165

INFORMATION ONLY

Sandia National Laboratories

Managed and Operated by Sandia Corporation
a Lockheed Martin Company
Albuquerque, New Mexico 87185-1328

date : January 17, 1996

to : T. Hicks, (Galson Science Ltd.)

from : L. C. Sanchez, Org 6741, MS-1328 (505)848-0685 Lawrence C. Sanchez
H. R. Trellue, Org 6741, MS-1328 (505)848-0820 Holly R Trellue

subject : **Estimation of Maximum RH-TRU Thermal Heat Load for WIPP**

[1] **Requested Information**

In previous communications [Ref. Hi-1], a request was made for an estimate of the upper bound for the expected thermal payload (internal heat generation) of a RH-TRU canister. This information can then be used to estimate the maximum temperature rise in the immediate vicinity of a RH-TRU canister with the largest expected thermal payload. Calculations presented in this memo correspond to two major analysis steps: 1) inverse internal shielding calculations, to identify the corresponding thermal payload for maximum allowable surface dose; and 2) heat conduction calculations for thermal payloads based on limited empirical data. The analysis steps are discussed below.

[2] **Inverse Internal Shielding Calculations**

These calculations yield first order "hand calculations" that are used to identify the radiation source term corresponding to the maximum allowable surface dose rate (1,000 *rem/hr*) for RH-TRU canisters [Ref. LWA-1]. The shielding calculations were performed only for gamma radiation because betas and alphas would not penetrate the waste matrix and/or the RH canister in any appreciable quantities (note: the internal heat generation of betas and alphas are incorporated when converting gamma activities to total (alpha, beta, and gamma) internal activities). Neutrons are not included because the dose equivalent rate from neutrons is about three orders of magnitude less than that for the maximum total allowable surface dose rate (i.e., the allowed neutron dose rate is 270 *mrem/hr* max [Ref. DOE-5]) and the corresponding neutron heating rate is insignificant. The computational steps used for gamma shielding are shown in Table 1.

Table 1. Calculation Steps For Inverse Shielding Calculations

Step	Calculation
1	For the identified dose equivalent rate (sometimes termed "biological dose" rate, formerly called "RBE dose" rate, or relative biological effectiveness, determine the corresponding absorbed dose rate for gamma-ray radiation.
2	For the identified absorbed dose rate determine the corresponding exposure rate for gamma-ray radiation.
3	Use the dose exposure rate equation for biological shielding to determine the gamma flux corresponding to the maximum allowed surface dose rate. Note: here we want a method for determining the activity load internal to the RH-TRU canister, not a kerma calculation for determining the gamma heating rate, because that heating rate value could not be used to identify the energy deposited internally in the canister.
4	Use the proper shielding equation with the point source isotropic exposure buildup factor for a self-shielding distributed source to identify the corresponding internally distributed gamma source strength (gamma activity).
5	Determine the total internal source strength (activity) from the gamma source strength.
6	Determine the total heat payload corresponding to the total internal source strength.

Step 1 requires use of Equation 1 [Ref. La-1], which incorporates the "quality factor" (see Table 2) which is a factor that takes into account the fact that equal absorbed doses of radiation of different qualities have, in general, different biological effects.

$$\dot{H} = Q\,\dot{D} \;, \quad \textit{rewritten as}:\; \dot{D} = \dot{H}/Q \qquad [1]$$

Likewise, Equation 2 [La-1b] relates the absorbed dose rate to the exposure rate through the parameter f (see Figure 1) and Equation 3 [La-1c], which describes the biological shielding (shielding to reduce radiation exposure to persons in the vicinity of radiation sources), relates the exposure rate to the gamma-ray flux density.

$$\dot{D} = f\,\dot{X} \;, \quad \textit{rewritten as}:\; \dot{X} = \dot{D}/f \qquad [2]$$

$$\dot{X} = C_d\,\phi \;, \quad \textit{rewritten as}:\; \phi = \dot{X}/C_d \qquad [3]$$

where:

$\dot{H}$ = *dose equivalent rate* [*rem/hr*]

$\dot{D}$ = *absorbed dose rate* [*rad/hr*]

Q = *quality factor* [*rem/rad*]

$\dot{X}$ = *exposure rate* [*R/hr*]

f = *exposure to absorbed dose conversion ratio* [*rad/R*]

$$= 0.874 \frac{(\mu_a/\rho)^{tissue}}{(\mu_a/\rho)^{air}} \qquad \text{[Ref. La–1b]} \qquad [3b]$$

ϕ = *gamma–ray flux density* [$\gamma/cm^2{-}s$]

C_d = *flux–to–dose conversion factor* [$(cm^2{-}sec/\gamma)\times(R/hr)$]

$$= 0.0659E{-}03\ E_\gamma(\mu_a/\rho)^{air} \qquad \text{[Ref. La–1c]} \qquad [3c]$$

E_γ = *gamma-ray energy* [*MeV*]

$(\mu_a/\rho)^{air}$ = *mass energy-absorption coefficient for air* [cm^2/g]

Table 2. Quality Factors for Various Types of Radiation *

Type of Radiation	Q
x–rays and γ–rays	1
β-rays, $E_{\max} > 0.03\,MeV$	1 †
β-rays, $E_{\max} < 0.03\,MeV$	1.7 †
Naturally occurring α-particles	10
Heavy recoil nuclei	20
Neutrons;	
Thermal to 1*keV*	2
10*keV*	2.5
100*keV*	7.5
500*keV*	11
1*MeV*	11
2.5*MeV*	9
5*MeV*	8
7*MeV*	7
10*MeV*	6.5
14*MeV*	7.5
20*MeV*	8
Energy not specified	10

* Taken from Lamarsh [Ref. La-1d], based on NCRP report 39 [Ref. Nc-1].

† Recommended in ICRP publication 9 [Ref. Ic-1].

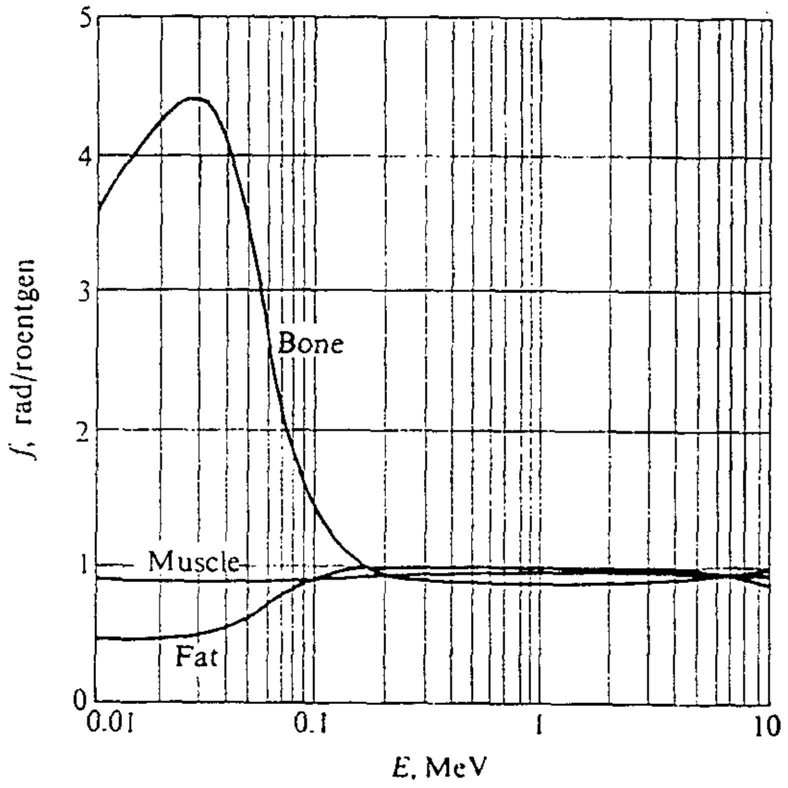


Figure 1 Parameter f as function of γ-ray energy.
(Taken from Ref. La-1b, originally from Mo-1.)

The mass energy-absorption coefficients (μ_a/ρ) for air and tissue for various gamma-ray energies are shown in Table 3. Performing Steps 1, 2 and 3 of Table 1 with the use of Equations 1, 2 and 3 yields Equation 4, which identifies the maximum allowable RH-TRU canister surface gamma flux density for a given maximum allowable surface dose (equivalent) rate.

$$\phi_s(max) = \frac{\dot{X}_S(max)}{C_d} = \frac{\dot{D}_s(max)}{C_d f} = \frac{\dot{H}_s(max)}{C_d f Q} \quad [4a]$$

$$= \frac{\dot{H}_s(max)}{0.0659E{-}03\, E_\gamma(\mu_a/\rho)^{air} f Q} = \frac{\dot{H}_s(max)}{5.75966E{-}05\, E_\gamma(\mu_a/\rho)^{tissue} Q} \quad [4b]$$

Table 3. Mass Energy-Absorption Coefficients for Air *

Gamma-ray Energy [MeV]	Mass Energy-Absorption Coefficient $(\mu_a/\rho)^x$ $[cm^2/g]$ Air	Tissue
0.1	0.0233	0.0271
0.15	0.0251	0.0282
0.2	0.0268	0.0293
0.3	0.0288	0.0312
0.4	0.0296	0.0317
0.5	0.0297	0.0320
0.6	0.0296	0.0319
0.8	0.0289	0.0311
1.0	**0.0280**	**0.0300**
1.25	0.0268	0.0288
1.50	0.0256	0.0276
2.0	0.0238	0.0256
3.0	0.0211	0.0220
4.0	0.0194	0.0206
5.0	0.0181	0.0192
6.0	0.0172	0.0182
8.0	0.0160	0.0168
10.0	0.0153	0.0160

* Data from Ref La-1f.
NOTE
are to be used for dose calculations. They are not attenuation coefficients which are used for shielding calculations.

If there is more than one radionuclide emitting gammas to be included in the gamma source term, then the total dose (equivalent) rate is composed of several components (see Equation 5) and, likewise, the gamma flux density will be composed of several components (not necessarily of the same gamma energy distribution).

$$\dot{H}_{total} = \sum_i \dot{H}_i \qquad [5]$$

Now the gamma flux density due to gamma-ray attenuation is needed. The equations for a point source are Equations 6 and 7.

$$\phi_o = \frac{S}{4\pi R^2} \qquad [\gamma/cm^2\text{–}sec] \qquad [6]$$

$$\phi_u = \phi_o e^{-\mu t} = \frac{S e^{-\mu t}}{4\pi R^2} \qquad [7]$$

where:

ϕ_o = *gamma-ray flux of an unshielded uncollided isotropic point source*

ϕ_u = *gamma-ray flux of a shielded uncollided isotropic point source*

S = *source strength* [γ/sec]

R = *distance from the point source* [*cm*]

t = *shielding thickness* [*cm*]

μ = *linear attenuation coefficient for shield* [*1/cm*]

= *mass attenuation coefficient* × *mass density* = $(\mu_s/\rho) \times \rho$ [7b]

Equation 6 corresponds to a bare isotropic point (gamma emitting) source and describes the direct-beam (uncollided) component of the unshielded source. Equation 7 includes the attenuation (the $e^{-\mu t}$ term) of an intervening absorbing material (ϕ_u corresponds only to the uncollided component of the gamma flux). ϕ_u does not include, however, important effects due to: 1) the Compton effect (scattering with loss of energy: this is very important since non-direct beams can be scattered to detector locations), 2) the photoelectric effect (producing x-rays), and 3) pair production (the incident photon in the vicinity of a nucleus produces a electron-positron pair and the annihilation of the positron with an electron generates gamma-ray radiation). The importance of these effects can be identified from Figures 2 and 3, which show qualitative effects on gamma energy spectra due to shielding material.

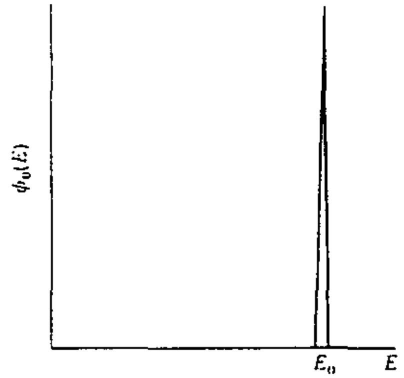


Figure 2 Energy spectrum of incident gamma-ray beam. (Taken from Ref. La-1g.)

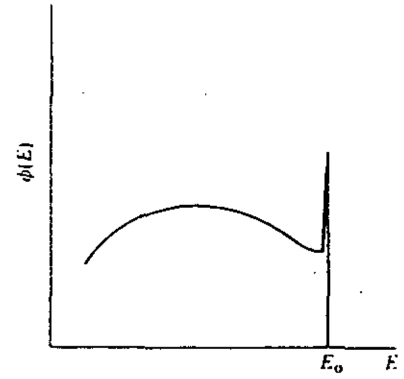


Figure 3 Energy spectrum of gamma-rays emerging from shield. (Taken from Ref. La-1g.)

The necessary correction factor for these effects is the gamma buildup factor ($B_p(\mu t)$ tabulated in many references and for many cases yielding acceptable estimates for calculated gamma fluxes) for the gamma-ray transport. The addition of this term yields Equation 8.

$$\phi_b = B_p(\mu t)\phi_u = B_p(\mu t)\phi_o e^{-\mu t} = S\, B_p(\mu t)\,\frac{e^{-\mu t}}{4\pi R^2} \qquad [8]$$

If more accurate gamma-ray transport calculations are needed, they should be performed with the Boltzmann transport equation which incorporates the complete treatment of the scattering component (this was not deemed necessary for this simple study). The time-independent transport theory (Boltzmann Equation) for photons is given by [Ref. Sc-1b]:

$$\nabla\cdot\Omega\phi(\mathbf{r},\Omega,E) + \Sigma_t(\mathbf{r},E)\phi(\mathbf{r},\Omega,E) = \qquad [9]$$

$$\int_{E'}\int_{\Omega'} \Sigma_s(\mathbf{r},E')p(E'\to E,\Omega'\to\Omega)\phi(\mathbf{r},\Omega',E')\,d\Omega' dE' + S(\mathbf{r},\Omega,E)$$

where:

$\mathbf{r}$ = *gamma-ray position vector*

E = *gamma-ray energy*

Ω = *solid angle*

ϕ = *gamma-ray flux*

p = *probability that a particle of energy E' and direction Ω' scatters into dE about E and $d\Omega$ about Ω*

S = *source term*

Σ_i = *macroscopic cross section ($i=t \to$ total, $i=s \to$ scattering)*

= *atom density × microscopic cross-section*

Equation 9 is a complex integral differential equation which has the extra dimensions of particle energy (E) and angular distribution (Ω), thus a one dimensional steady-state problem is actually a three dimensional problem. There are a significant number of available discrete ordinates and Monte Carlo codes for solving the Boltzmann equation, but this extra level of effort is not necessary for the problem at hand.

Proceeding with the simple shielding expressions, Equation 8 represents the total (direct and scattered) component with an intervening absorbing and scattering shield for a point source. The buildup factor is a function of the shielding thickness and the gamma-ray linear attenuation coefficient, which is dependent on gamma energy. Note; the buildup factors are problem specific; there is separate buildup factor for each source type -- mono-directional beam, isotropic, etc. There are various buildup factors for different specific geometries, such as a point source, line source, etc., see Refs. Sc-1 & Ja-1. Since real geometries correspond to distributed sources, it is necessary to integrate the collective fluxes from multipoint sources that are used to represent a distributed gamma source. Thus Equation 8 (which is for a point source) is integrated over all point source strengths convoluted with the attenuation kernel to yield Equation 10:

$$\phi(\mathbf{r}) = \int_{\text{all space}} S_V(\mathbf{r}')K(|\mathbf{r}'-\mathbf{r}|)\,d\mathbf{r}' \qquad [10]$$

$\mathbf{r}$ = *vector to the measuring point*

$\mathbf{r}'$ = *vector to any source-bearing point in space*

$S_V(\mathbf{r}')$ = *source strength per unit volume at $\mathbf{r}'$*

This equation for the "extended source term" (integrated volumetric source term) has the exponential point attenuation kernel given by:

$$K(R) = B(\mu r)\frac{e^{-\mu r}}{4\pi R^2} \quad [11]$$

The solution to Equation 10, for simple cases of uniformly distributed source geometries, is an exponential integral function [Gl-1], whose general form is given by Equation [12].

$$E_n(x) = x^{n-1}\int_x^{\infty}\frac{e^{-p}}{p^n}dp \quad [12]$$

Further description of the exponential point attenuation kernel can be found in Ref. Gl-1b.

For the problem at hand, the uncollided gamma flux at the source-shield interface (i.e., the interface between the RH-TRU waste matrix and the steel drum itself), from a right cylinder geometry, with a uniform source that is self-shielding, is given by Equation 13 [Ref. Ja-1].

$$\phi_u(upper\ limit) = \frac{S_V}{4\mu_s}\left[G(\mu_s h_1, b_5) + G(\mu_s h_2, b_5) + G(\mu_s h_1, b_6) + G(\mu_s h_2, b_6)\right] \quad [13a]$$

$$\phi_u(lower\ limit) = \frac{S_V}{4\mu_s}\left[G(\mu_s h_1, b_6) + G(\mu_s h_2, b_6) + G(\mu_s h_1, b_4) + G(\mu_s h_2, b_4)\right] \quad [13b]$$

where: ϕ_u = *uncollided gamma flux density within the RH-TRU waste matrix* $[\gamma/cm^2\text{–}s]$

S_V = *volumetric source term* $[\gamma/cm^3\text{–}s]$

G = *special exponential integral function*

μ_s = *linear attenuation coefficient of RH-TRU waste matrix* $[1/cm]$

$h_{½}$ = *half-height of the RH-TRU waste matrix* = $½H$ $[cm]$

h_1 = *height within RH-TRU waste matrix* $[cm]$

$h_2 = 2h_{½} - h_1$ $[cm]$

a = *radius of position under investigation* $[cm]$

R = *radius of the RH-TRU waste matrix* $[cm]$

$b_4 = \mu_s(R - a)$

$b_5 = \mu_s(R + a)$

$b_6 = \mu_s\sqrt{R^2 - a^2}$

Evaluating Equation 13 at the waste matrix-drum interface (i.e., $a = R$, $b_4 = b_6 = 0$) at center-plane (i.e., mid-height where $h_1 = h_2 = h_{½}$) yields Equation 14:

$$\phi_u(center\ plane) = \phi_u(cp) = \frac{S_V}{2\mu_s}\left[G(\mu_s h_{½}, 2\mu_s R)\right] \quad [14]$$

The values for G (for right cylinders) can be estimated from the graphical representation shown in Figures 4a and 4b [Ja-1]. From these figures, it should be noted that for significant values for $\mu_s h_{½}$ and $2\mu_s R$ that $G(\mu_s h_{½}, 2\mu_s R) \rightarrow 1.0$. This results because $\mu_s h_{½}$ and $2\mu_s R$ are the mean free path (mfp) lengths (also called the relaxation lengths) in the azimuthal and radial directions; for cylindrical sources with significant thickness and radii, the source looks like an infinite source (semi-infinite space volume source). For large waste matrix dimensions ($\mu_s h_{½} \geq 3$, $2\mu_s R \geq 3$), the surface flux can be approximated by:

$$\phi_u(cp) \approx \frac{S_V}{2\mu_s} \qquad [15]$$

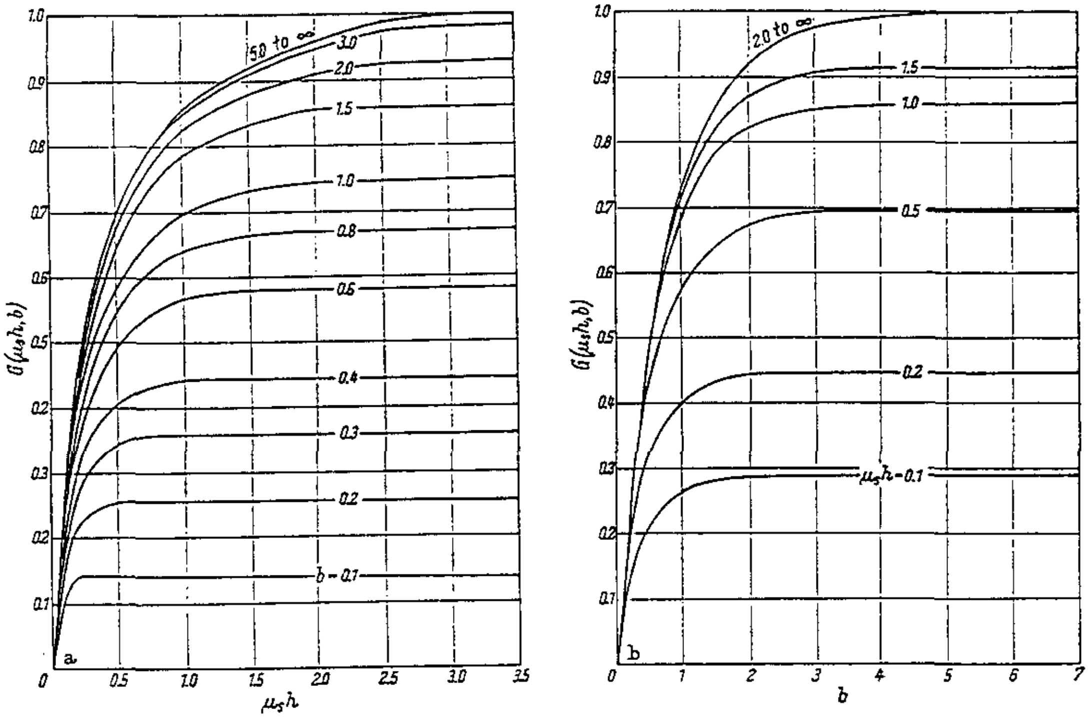


Figure 4 The function $G(\mu_s h, b)$ for G=0 to 1; (taken from Ja-1, originally from Ro-1). a) G vs. $\mu_s h$ for $\mu_s h$ = 0 to 3.5, b= 0.1 to ∞; b) G vs. b for $\mu_s h$ = 0.1 to ∞, b = 0, to 7.

To calculate the azimuthal and radial mean free path lengths requires the dimensions of the waste matrix within the RH-TRU canister. From Figure 5 [Ref. DOE-1] it can be identified that the inside dimensions of the RH-TRU canister is 25.5 in. for the diameter (not shown in Figure 5 is the thickness of the RH-TRU canister, which 0.25 in.), and a corresponding height slightly less that 120.5 in. In Ref. BIR-1f, the usable internal volume has been identified to be 0.89 cu.m.; thus, the active internal height can be calculated to be 270.12 cm. The 0.89 cu.m. volume, however, is inconsistent with the Ref. DOE-1b, which indicates that the RH-TRU canisters are to internally incorporate three standard (DOT-7C) CH-TRU waste drums (55-gal nominal volume), resulting in a waste matrix payload of 0.625 cu.m. for the RH-TRU canister. This inconsistency arises because there are actually two options for loading RH-TRU canisters: OPTION A -- place RH-TRU waste directly in the canisters (corresponding to a waste loading volume of 0.89 cu.m.) and OPTION B -- place RH-TRU waste directly into three 55-gallon DOT-7C drums, which would then in turn be placed into the RH-TRU canister (corresponding to a waste loading of 3x0.2082=0.6246 cu.m.) (see Ref. Sa-4 for more discussion). For OPTION B calculations, the drum dimension of a DOT-6M (the 6M uses a DOT 6C or 17C 55-gal metal outer drum, see Figures 6 and 7) were used because they were readily available in a previous report [Sa-1], and should be similar to DOT 7C specs. The internal waste matrix radius is 28.58 cm. and the internal individual drum height is 84.46 cm. Since the RH-TRU canister container contains three CH-TRU drums, the total internal waste matrix height is 253.38 cm, with a corresponding half-height (which is the parameter used in Equation 14) of 126.69 cm. Using 1) the waste matrix dimensions, 2) Equation 7b, and 3) a mass attenuation coefficient of 0.0595 cm^2/g (from Table 4 it can be seen that for gammas with energy of 1.0 MeV or less, that the mass attenuation coefficients are 0.0595 or greater, the 0.0595 number is used because it gives a conservative result for the final solution for the internal source term), a rough approximation for $G(\mu_s h_{½}, 2\mu_s R)$ can be approximated by Equation 16 (obtained by using singular value decomposition (SVD) [Ref. Sa-2], based on graphical data displayed in Figures 4a and 4b; note that there are noticeable errors in Figures 4a and 4b):

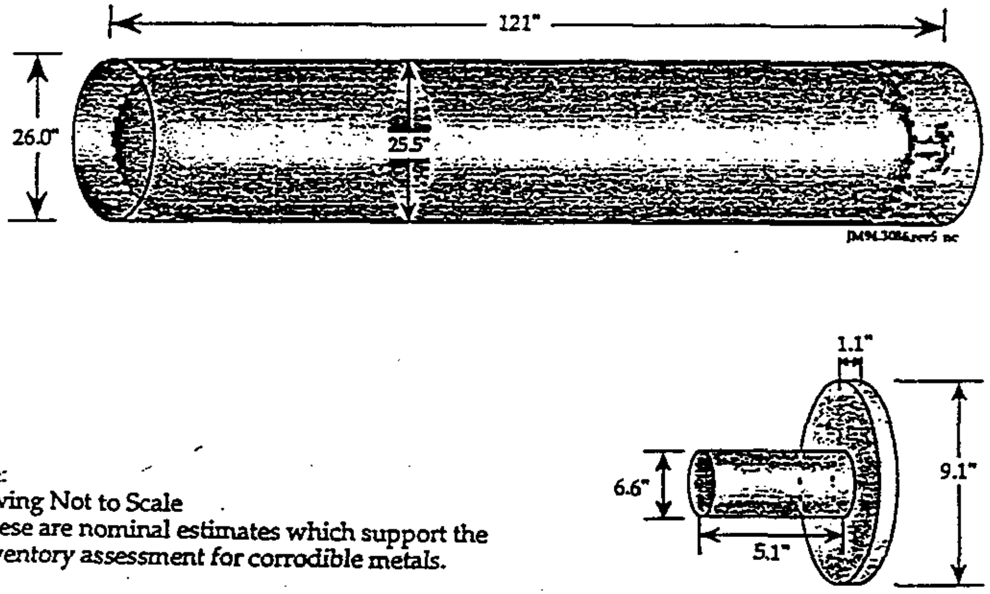
$$G(\mu_s h_{½}, 2\mu_s R) = \begin{cases} 1.0 & \text{if } sp.gr. > 2 \quad (\textit{good} \text{ for } 0.1\% \textit{ accuracy}) \\ 1 - e^{-(c_1 sp.gr. + c_2 sp.gr.^2)} & \text{if } 2 \geq sp.gr. \geq 0 \quad (\textit{good} \text{ for } 4\% \textit{ accuracy/OPTION } A) \\ 1 - e^{-(c_3 sp.gr. + c_4 sp.gr.^2)} & \text{if } 2 \geq sp.gr. \geq 0 \quad (\textit{good} \text{ for } 4\% \textit{ accuracy/OPTION } B) \end{cases} \qquad [16]$$

where

$c_1 = 5.4079558E{+}00$ $\quad c_2 = -9.7716046E{-}01$ *(for RH-TRU loading Option A)*

$c_3 = 4.8045511E{+}00$ $\quad c_4 = -6.7351092E{-}01$ *(for RH-TRU loading Option B)*

sp.gr. = the specific gravity of the RH-TRU waste matrix



Note:
Drawing Not to Scale
* These are nominal estimates which support the inventory assessment for corrodible metals.

Figure 5 General dimensions of the RH-TRU canister (Taken from Ref. DOE-1.)

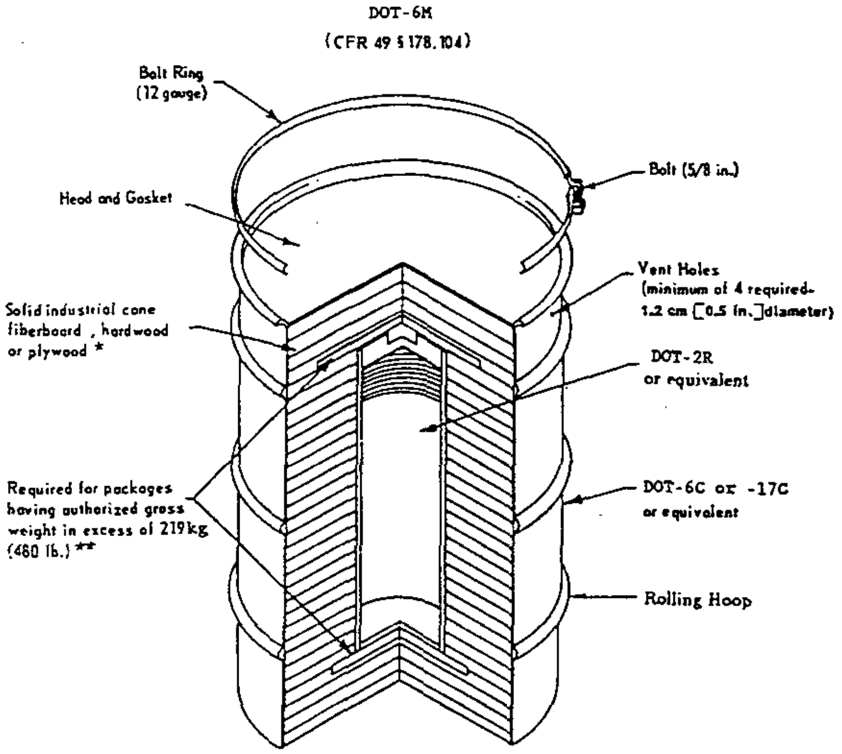


Figure 6 Geometry of 6M Containers (Taken from Sa-1, original Ref. Ed-1).

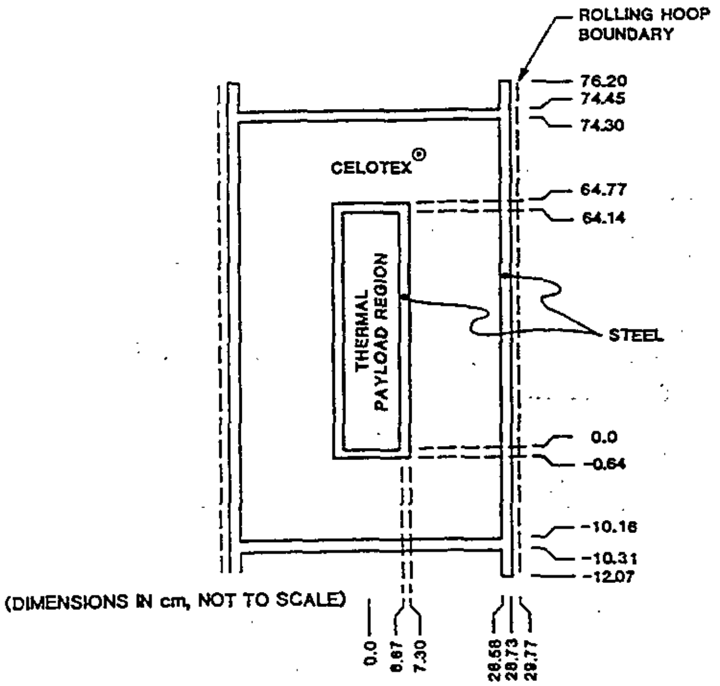


Figure 7 Schematic of the 55-Gallon 6M Container (taken from Sa-1).

Table 4. Mass Attenuation Coefficients *

Gamma Energy [MeV]	Mass Attenuation Coefficients, $(\mu_s/\rho)^x$ $[cm^2/g]$						
	Air	Concrete	Iron	Calcium	Silicon	Aluminum	Oxygen
0.1	0.151	0.169	0.344	0.238	0.172	0.161	0.151
0.3	0.106	0.107	0.106	0.109	0.107	0.103	0.107
0.5	0.0868	0.0870	0.0828	0.0876	0.0869	0.0840	0.0870
0.6	0.0804	0.0804	0.0762	0.0809	0.0802	0.0777	0.0806
0.8	0.0706	0.0706	0.0664	0.0708	0.0706	0.0683	0.0708
1.0	**0.0635**	**0.0635**	**0.0595**	**0.0634**	**0.0635**	**0.0614**	**0.0636**
1.5	0.0517	0.0517	0.0485	0.0518	0.0517	0.0500	0.0518
2.0	0.0445	0.0445	0.0424	0.0451	0.0447	0.0423	0.0445

* Data from Ref. Ra-1 (see Equation 7b for usage).

Equation 14 should now be modified to include the gamma flux buildup. The desired result is:

$$\phi_b(cp) = B_p^{waste}\,\frac{S_V}{2\mu_s}\left[G(\mu_s h_{1/2}, 2\mu_s R)\right] \qquad [17]$$

where

B_p^{waste} = *the buildup factor for the extended source*

We were not able to find a buildup factor for the extended source term. What is desired here is a buildup factor which has been properly integrated over the volumetric geometry of interest. As a first order approximation, a value of 1.31 was selected. From Table 5 it can be seen that this point source value was the minimum, hence conservative, of the values shown for gammas of energy of about 1.0 MeV. Equation 17 is only for the gamma flux at the waste matrix-drum interface. The buildup flux (uncollided plus collided) at the outer surface of the drum and RH-TRU canister can be estimated by using the expression for added linear shielding to a semi-infinite volume source term (see Ref. Ja-1b). Note; that this model does not include an inner liner for the RH-TRU canister, most likely made of polyethylene, which would have a linear attenuation coefficient (see Equation 7) that is an order of magnitude smaller than that of the RH-TRU canister itself. Using Equation 8, this yields Equation 18.

$$\begin{aligned}\phi_b(surface\ @\ cp) &= \phi_s \approx \phi_u\, B_p^{waste}\, B_p^{canister}\, E_2(\mu_{canister} t_{canister}) \qquad [18]\\ &= \frac{0.655\, S_V B_p^{canister}}{\mu_s} G(\mu_s h_{1/2}, 2\mu_s R)\, E_2(\mu_{canister} t_{canister})\end{aligned}$$

where:

$\mu_{canister}$ = *linear attenuation coefficient of RH canister and inner drum* $[1/cm]$

$t_{canister}$ = *combined thickness of RH canister and inner drum* $[cm]$

E_2 = *exponential integral function*

Table 5. Dose Buildup Factors for a Point Isotropic Source (a)

Material	Gamma Energy [MeV]	Relaxation Lengths, μx (b)				
		1	2	4	7	10
Water	0.5	2.52	5.14	14.3	38.8	77.6
	1.0	2.13	3.71	7.68	16.2	27.1
	2.0	1.83	2.77	4.88	8.46	12.4
Aluminum	0.5	2.37	4.24	9.47	21.5	38.9
	1.0	2.02	3.31	6.57	13.1	21.2
	2.0	1.75	2.61	4.62	8.05	11.9
Iron	0.5	1.98	3.09	5.98	11.7	19.2
	1.0	1.87	2.89	5.39	10.2	16.2
	2.0	1.76	2.43	4.13	7.25	10.9
Tin	0.5	1.56	2.08	3.09	4.57	6.04
	1.0	1.64	2.30	3.74	6.17	8.85
	2.0	1.57	2.17	3.53	5.87	8.53
Tungsten	0.5	1.28	1.50	1.84	2.24	2.61
	1.0	1.44	1.83	2.57	3.62	4.64
	2.0	1.42	1.85	2.72	4.09	5.27
Lead	0.5	1.24	1.42	1.69	2.00	2.27
	1.0	1.37	1.69	2.26	3.02	3.74
	2.0	1.39	1.76	2.51	3.66	4.84
Uranium	0.5	1.17	1.30	1.48	1.67	1.85
	1.0	1.31	1.56	1.98	2.50	2.97
	2.0	1.33	1.64	2.23	3.09	3.95

(a) Data from Ref. Ra-1b.

(b) μx = mass attenuation coefficient [cm^2/g] × shield thickness [cm] × shield density [g/cm^3].

Since the combined thickness of the metal drum (if OPTION B loading is used) and the RH-TRU canister is small, the gammas will be transported through less than one mean free path length; hence a conservative step is to set B_p^{waste} to unity. The solution for $E_2(b)$ is shown in Figure 8. A rough approximation for $E_2(b)$ can be given by Equation 19 (the fit for b values greater than 14 was based on data in Ref. Ab-1 and the fit for b values less than 14 (obtained by using singular value decomposition (SVD, Ref Sa-2)) was based on data in Ref. Ja-1b):

$$E_2(b) \approx \begin{cases} e^{-b}/(b+2) & \text{if } b > 14 \quad (\textit{good for } 1\% \textit{ accuracy}) \\ e^{-(c_5+c_6 b+c_7 b^2+c_8 b^3)} & \text{if } 14 \geq b \geq 1 \quad (\textit{good for } 7\% \textit{ accuracy}) \\ e^{-(c_9+c_{10} b+c_{11} b^2+c_{12} b^3)} & \text{if } 1 \geq b \geq 0 \quad (\textit{good for } 3\% \textit{ accuracy}) \end{cases} \qquad [19]$$

where

$c_5 = 5.5565607E{-}01$ $c_9 = 1.7837543E{-}02$

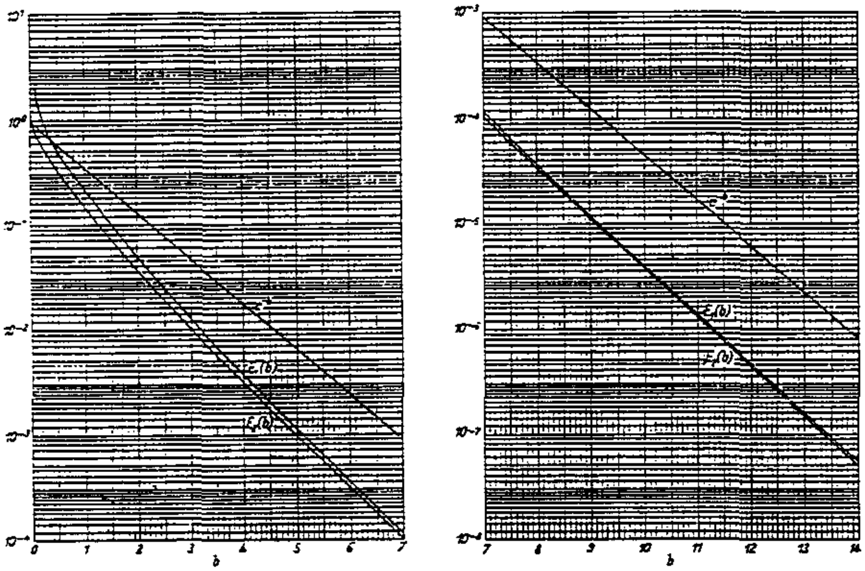
$c_6 = 1.4190903E{+}00$ $c_{10} = 3.0105850E{+}00$

$c_7 = -3.3941944E{-}02$ $c_{11} = -2.0438538E{+}00$

$c_8 = 1.1209473E{-}03$ $c_{12} = 9.3175783E{-}01$

Reformalizing Equation 18 to solve for S_V yields:

$$S_V = \frac{\phi_s \mu_s}{0.655\, G(\mu_s h_{½}, 2\mu_s R)\, E_2(\mu_{canister} t_{canister})} \qquad [20]$$



a

b

Figure 8 Solution for E_2. (Taken from Ja-1b.)

Assigning the maximum surface gamma flux density (from Equation 4) to ϕ_b nows gives us our final solution:

$$S_V(max) = \frac{\phi_s(max)\mu_s(max)}{0.655\, G(\mu_s h_{½}, 2\mu_s R)\, E_2(\mu_{canister} t_{canister})} \qquad [21a]$$

$$= \frac{\phi_s(max)(\mu_a/\rho)^{waste}\, \rho^{waste}(max)}{0.655\, G(\mu_s h_{½}, 2\mu_s R)\, E_2(\mu_{canister} t_{canister})} \qquad [21b]$$

$$= \frac{\dot{H}_s(max)\mu_s(max)}{C_d\, f\, Q\, 0.655\, G(\mu_s h_{½}, 2\mu_s R)\, E_2(\mu_{canister} t_{canister})} \qquad [21c]$$

$$= \frac{\dot{H}_s(max)(\mu_a/\rho)^{waste}\, \rho^{waste}(max)}{3.77258E{-}05\, E_\gamma (\mu_a/\rho)^{tissue}\, Q\, G(\mu_s h_{½}, 2\mu_s R)\, E_2(\mu_{canister} t_{canister})} \qquad [21d]$$

The key information that is needed to use Equation 21 is the linear attenuation coefficient for the RH-TRU waste matrix and the geometric dimensions for the RH-TRU canister. Several mass attenuation coefficients are presented in Table 4. As can be seen from this table, the mass attenuation coefficient is fairly similar for a wide variety of materials. Since the linear attenuation coefficient is comprised of the product of the mass attenuation coefficient (not the mass energy-absorption coefficient) and the total mass density (see Equation 7b), Table 4 indicates that the driving component of the linear attenuation coefficient is the total mass density. For this study it was assumed that the gamma energy of interest is about 1.0 MeV. For this energy, the mass attenuation coefficient for most waste matrix materials would be expected to be on the order of 0.0595 $[cm^2/g]$ (see Table 4 for coefficients and note that the 0.0595 number corresponds to the minimum value of the various materials at 1.0 MeV). Also, as can be noted from Figures 5 and 7, the combined thickness of carbon steel (due to the drum wall and the RH-TRU canister wall) is $0.15 + 0.6350 = 0.7850$ *cm (this is for* OPTION B loading of RH-TRU waste, for OPTION A loading the combined thickness is 0.6350 cm.). With a specific gravity of 7.86 for carbon steel [Ref. CRC-1d] for which $\mu_{canister} t_{canister} = 0.3671$ mean free path lengths (this value is for OPTION B assuming $(\mu/\rho)^{steel} = 0.0595$ cm^2/g -- the value for OPTION A loading is 0.2970) we get a value of 0.4091296 for $E_2(\mu_{canister} t_{canister})$ (this value is for OPTION B -- the value for OPTION A loading is 0.46951977). Using the above information and the value of $\phi_s(max)$, Equation 21b can be simplified to the form in Equation 22 which only depends upon the total specific gravity (or density) of the RH-TRU waste matrix and correctly indicates that the internal gamma source term increases with increasing waste matrix density.

$$S_V(max)\ [dis/(s-cm^3] = \frac{(5.787E{+}08)(0.0595)\,sp.gr.^{waste}(max)}{(0.655)\,E_2(\mu_{canister} t_{canister})\,G(\mu_s h_{1/2}, 2\mu_s R)} \qquad [22a]$$

$$\approx \begin{cases} 1.1196E{+}08\,\dfrac{sp.gr.^{waste}(max)}{G(\mu_s h_{1/2}, 2\mu_s R)} & (\textit{for RH-TRU loading Option A}) \\[2ex] 1.2849E{+}08\,\dfrac{sp.gr.^{waste}(max)}{G(\mu_s h_{1/2}, 2\mu_s R)} & (\textit{for RH-TRU loading Option B}) \end{cases}$$

$$\approx \begin{cases} 1.1196E{+}08\,sp.gr.(max) & (if\ \ sp.gr.^{waste} \geq 2) \qquad \textit{Option A} \\ \left[\dfrac{1.1196E{+}08\,sp.gr.(max)}{1-e^{-(c_1 sp.gr.(max)+c_2 sp.gr.^2(max))}}\right] & (if\ \ 2 \geq sp.gr.^{waste} \geq 0) \end{cases} \qquad [22b]$$

$$\approx \begin{cases} 1.2849E{+}08\,sp.gr.(max) & (if\ \ sp.gr.^{waste} \geq 2) \qquad \textit{Option B} \\ \left[\dfrac{1.2849E{+}08\,sp.gr.(max)}{1-e^{-(c_3 sp.gr.(max)+c_4 sp.gr.^2(max))}}\right] & (if\ \ 2 \geq sp.gr.^{waste} \geq 0) \end{cases}$$

The above equations yields the total gamma source term in units of (*disintegration/sec*); to convert this to curies, one must remember that 3.7E+10 (*dis/s*) is equal to 1 curie of activity. Rewriting Equation 22b in units of curies yields:

$$S_V(max)\,[\gamma curies/cm^3] = S_V(max)/3.7E{+}10 \qquad [22c]$$

$$\approx \begin{cases} 3.0260E{-}03\,sp.gr.(max) & (if\ \ sp.gr.^{waste} \geq 2) \qquad \textit{Option A} \\ \left[\dfrac{3.0260E{-}03\,sp.gr.(max)}{1-e^{-(c_1 sp.gr.(max)+c_2 sp.gr.^2(max))}}\right] & (if\ \ 2 \geq sp.gr.^{waste} \geq 0) \end{cases}$$

$$\approx \begin{cases} 3.4727E{-}03\,sp.gr.(max) & (if\ \ sp.gr.^{waste} \geq 2) \qquad \textit{Option B} \\ \left[\dfrac{3.4727E{-}03\,sp.gr.(max)}{1-e^{-(c_3 sp.gr.(max)+c_4 sp.gr.^2(max))}}\right] & (if\ \ 2 \geq sp.gr.^{waste} \geq 0) \end{cases}$$

$$S_V(max)\,[\gamma curies/canister] = S_V(max) \times Volume/3.7E{+}10 \qquad [22d]$$

$$\simeq \begin{cases} 2.6932E{+}03\, sp.gr.(max) & (if\ \ sp.gr.^{waste} \geq 2) \qquad Option\ A \\ \left[\dfrac{2.6932E{+}03\, sp.gr.(max)}{1-e^{-(c_1 sp.gr.(max)+c_2 sp.gr.^2(max))}} \right] & (if\ \ 2 \geq sp.gr.^{waste} \geq 0) \end{cases}$$

$$\simeq \begin{cases} 2.1704E{+}03\, sp.gr.(max) & (if\ \ sp.gr.^{waste} \geq 2) \qquad Option\ B \\ \left[\dfrac{2.1704E{+}03\, sp.gr.(max)}{1-e^{-(c_3 sp.gr.(max)+c_4 sp.gr.^2(max))}} \right] & (if\ \ 2 \geq sp.gr.^{waste} \geq 0) \end{cases}$$

The identification of the appropriate total mass density for the RH-TRU waste matrix requires an interrogation of the data in the WIPP Transuranic Waste Baseline Inventory Report (WTWBIR) Rev. 1 [Ref. BIR-1]. As can be seen in Table 6, the majority (79%) of the RH-TRU waste volume is in the "heterogeneous" waste form, of which 80% will come from the Hanford site. In Table 7 the heterogeneous waste form, along with the other waste forms, is further broken down according to its material composition. Unfortunately, the data reported in the WTWBIR is presented for partial densities (not total density as is needed). To further complicate the matter, there was not enough data presented to identify the statistical nature of the reported data (i.e., statistical variances are not presented). Only presented was the minimum, average (assumed to be the arithmetic *sampled* mean), and the maximum of the partial density of each material component. At this point, an "engineering" judgement is required. One's first inclination to determining a maximum total density would be to sum all the maximum partial densities of the RH-TRU waste matrix materials (i.e., sum-up the maximum values identified in column two of Table 7). However, it is not possible to have all maximum partial densities occur in the same waste matrix [Ref. Br-1]. Thus the plan-of-attack is to determine a statistically-based maximum total density. Not enough data is presented to allow one to identify the probability distribution function (pdf) (i.e., identify if the pdf is a "normal", "log-normal", or some other type of distribution) or calculate the statistical variance. Enough data is present, however, to identify an upper bound on the cumulative distribution function (cdf). This is done by applying the "maximum entropy formalism" which yields a distribution that maximizes the uncertainty [Refs. Ti-1 and Ti-2]. The maximizing distribution identified for this problem is the truncated exponential distribution function with a pdf given by Equation 23.

$$f(x) = \frac{\lambda e^{-\lambda x}}{e^{-\lambda a} - e^{-\lambda b}} \qquad [23]$$

where:

$\int f(x)\,dx$ = *probability that uncertain parameter X lies in interval [x,x+dx]*

λ = *a yet to be determined constant*

a = *minimum value of uncertain parameter X*

b = *maximum value of uncertain parameter X*

The corresponding cdf is given by:

$$F(x) = Pr\{X \leq x\} = \int_a^x f(s)\,ds \qquad [24]$$

$$= probability\ that\ uncertain\ parameter\ X \leq x$$

$$= \int_a^x \frac{\lambda e^{-\lambda x}}{e^{-\lambda a} - e^{-\lambda b}}\,dx = \frac{\lambda}{e^{-\lambda a} - e^{-\lambda b}} \int_a^x e^{-\lambda x}\,dx$$

Using Ref. CRC-1 yields:

$$F(x) = \frac{e^{-\lambda a} - e^{-\lambda x}}{e^{-\lambda a} - e^{-\lambda b}} = P = \mathit{Percentile\ with\ range}\ (0 \le P \le 1) \qquad [25]$$

It's Equation 25 that we need to use to identify the percentiles of $F(x)$ (i.e., we can use Equation 25 to identify x_P for a given percentile, see Equation 26).

$$x_P = F^{-1}(P) = -\frac{1}{\lambda}\ln\left[e^{-\lambda a} - P(e^{-\lambda a} - e^{-\lambda b})\right] \qquad [26]$$

Unfortunately, Equation 25 has the unknown constant λ. The trick to solving for this constant [Ref. Ti-1] is to determine the expression for the "population" mean value (also called the "expectation" value or more simply, *mean*, denoted by $[x]$) of the distribution in Equation 23 and equate it to the *sample mean* (denoted by $\hat{x}$) that is identified in the WTWBIR. The population mean, $[x]$, is defined by Equation 27.

$$[x] = \hat{x} = \int_a^b x\, f(x)\, dx \quad \mathit{for\ a\ continuous\ distribution} \qquad [27]$$

$$= \int_a^b \frac{\lambda x e^{-\lambda x}}{e^{-\lambda a} - e^{-\lambda b}}\, dx = \frac{\lambda}{e^{-\lambda a} - e^{-\lambda b}} \int_a^b x\, e^{-\lambda x}\, dx$$

Using Ref. CRC-1b, Equation 27 can be integrated to yield:

$$[x] = \frac{1}{\lambda} + \frac{a\, e^{-\lambda a} - b\, e^{-\lambda b}}{e^{-\lambda a} - e^{-\lambda b}} \qquad [28]$$

The value of λ can now be solved for by finding the roots of the function $h(\lambda)$ given by:

$$h(\lambda) = \hat{x} - \frac{1}{\lambda} - \frac{a\, e^{-\lambda a} - b\, e^{-\lambda b}}{e^{-\lambda a} - e^{-\lambda b}} \qquad [29]$$

Using standard iteration techniques, the values of λ for most of the RH-TRU waste matrix materials (those identified with $a \neq \hat{x}$) were determined to five significant digits and are displayed in column three of Table 7. Also identified in columns 4 thru 6 in Table 7 are the values of the 68.26%, 95.44% and 99.74% percentiles [Ref. CRC-1c] (i.e., the x values corresponding to $F(x) = .6826$, .9544 and .9974), which correspond to the normal benchmarks of 1σ, 2σ, and 3σ. All of the statistical results calculated up to now correspond only to partial densities and not the maximum total density that is needed for determining the linear attenuation coefficient (remember Equation 21?). The engineering judgement made at this time is to sum-up partial densities in the following manner: 1) the maximum partial material density is identified for each waste matrix material, 2) percentile values for the non-maximum values are identified (for cases where minimum and average partial densities are equal it is not possible to calculate λ, in which case the maximum partial density is used for the percentile values), and 3) the total density is comprised of the sum of the non-maximum percentile values with the maximum value (see Equation 30).

$$\mathit{total\ density\ (for\ F(68.26\%))} = \rho_{maximum} + \sum_{i \neq \max} \rho_i \qquad [30]$$

In Table 7 we have thus determined the following five total densities for each RH-TRU waste matrix: 1) the "average" total density, 2) the "F(68%.26)" total density (this corresponds to a 1σ value for the partial densities, with the exception of the maximum value which is added at full value), 3) the "F(95.44%)" total density (corresponding to a 2σ value), 4) the "F(99.74%)" total density (corresponding to a 3σ value), and 5) the "worst-case" total density (even though we previously identified that this case is not possible, it is included to provide an absolute upper-bound case). The maximum of each of the above described cases is displayed in Table 7 in bold, which shows that "heterogeneous" waste has the largest statistical values and the largest "worst-case" value and "solidified inorganics" waste has the largest "average" value.

Now there is enough data to identify the internal source term of the RH-TRU waste matrix. Table 8 displays the dose rate and gamma density flux at the surface of the RH-TRU canister. In order to use Table 8 data to calculate the internal heat load, additional data is needed (i.e., the RH-TRU total heat-to-total curie load ratio and the RH-TRU total *curie-to-total gamma curie ratio). The total heat-to-total curie load ratio is 0.003668* watts/curie and was obtained by calculating the heat load for each radionuclide, summing up these values, and then comparing to the sum of the total curie load from data reported in the WTWBIR [BIR-1d] (see footnote 1 of Table 9). The total curie-to-total gamma curie ratio is 1.01 and was obtained by comparing the total curie load to the sum of the calculated total gamma curie inventory load for each of the radionuclides (see footnote 1 of Table 10). There was a lot of work involved in generating Tables 9 and 10, and the major *findings (such as average waste container heat loads, etc.,) can be found in the many foot*notes at the end of the tables. With the conversion ratios calculated in Tables 9 and 10, the internal volumetric heat generation rates (source terms) can be calculated and are presented in Table 11. In this table, many various source terms (i.e., RH-TRU waste average value, 300 watt LWA limit, etc.,) were calculated and will be used as input for heat transfer calculations. As will be identified in the next section (heat transfer section), these case studies do not present a problem.

Table 6. Site RH-TRU Waste Anticipated Volumes *

Final Waste From	Site RH-TRU Anticipated Waste Volumes [m^3]					
	Site Name					
	ANL-W	BCLDP	BT	HAN	INEL	KAPL
Combustible						
Filter	2.98					
Graphite						
Heterogeneous	0.67	71.	1.557	**3,006.873**	16.434	36.46
Inorganic Non-metal						
Salt Waste					2.8	
Solidified Inorganics					2.1	
Solidified Organics						
Uncategorized Metals	8.532				9.71	
Unknown	23.736				11.13	
Lead/Cadmium Metal Waste	0.36				5.6	
Site Total	36.278	71.00	1.557	3006.873	47.774	36.46

	Site Name					
	LANL	ORNL	SRS		WIPP Total	WIPP %
Combustible	18.				18.	0.38
Filter					2.98	0.06
Graphite						
Heterogeneous		565.51	63.92		3,762.424	**78.57**
Inorganic Non-metal						
Salt Waste					2.8	0.06
Solidified Inorganics		785.00			787.1	16.44
Solidified Organics						
Uncategorized Metals	155.96				174.202	3.64
Unknown					34.866	0.73
Lead/Cadmium Metal Waste					5.96	0.12
Site Total	173.96	**1,350.51**	63.92		4,788.332	100.00 %

* Data from Ref. BIR-1b.

Table 7. Statistics for RH-TRU Waste Densities (a)

Materials		Waste Density [Kg/m^3]				
		Heterogeneous (78.6 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ [m^3/Kg]	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	0.0/108.5/1716.4	9.21657-1	1.2451+2	3.3503+2	6.4581+2
	Aluminum Based	0.0/23.0/263.0	4.34728-2	2.6397+1	7.1024+1	1.3682+2
	Other Metals	0.0/0.2/500.0	4.99999+0	2.2952-1	6.1757-1	1.1905+0
	Other Inorganics	0.0/38.6/**2000.0**	NC (c)	**2000.0**(d)	**2000.0**(d)	**2000.0**(d)
Organics	Cellulose	0.0/34.3/961.5	2.91545-2	3.9362+1	1.0591+2	2.0416+2
	Rubber	0.0/5.9/163.5	1.69491-1	6.7708+0	1.8218+1	3.5118+1
	Plastics	0.0/30.7/550.0	3.25732-2	3.5231+1	9.4797+1	1.8273+2
Solidified	Inorganic	0.0/0.1/15.0	9.99999+0	1.1476-1	3.0879-1	5.9522-1
Materials	Organic	0.0/0.0/3.0	NP	3.0(d)	3.0(d)	3.0(d)
Soils		0.0/2.3/193.0	4.34783-1	2.6395+0	7.1021+0	1.3690+1
	Total(ave) Total(max)	243.6 **6,365.4**		**2,238.3**	**2,636.0**	**3,223.1**
		Solidified Inorganics (16.4 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ [m^3/Kg]	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Aluminum Based	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Other Metals	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Other Inorganics	0.0/1.1/528.8	9.09090-1	1.2624+0	3.3966+0	6.5475+0
Organics	Cellulose	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Rubber	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Plastics	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Solidified	Inorganic	173.1/792.2/1057.7	NC (c)	1057.7(d)	1057.7(d)	1057.7(d)
Materials	Organic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Soils		0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Total(ave) Total(max)	793.3 1,586.5		1,059.0	1,061.1	1,064.2

(a) Data from Ref. BIR-1c (ranked by volume percentages to be sent to WIPP).
(b) Statistical analysis perform with use of Equations 22 → 27.
(c) Maximum material partial density for final waste form.
(d) Value assign is material maximum, not calculated value.
NC Not computed because parameter is maximum partial density of material.
NP Not possible to compute because $a=\hat{x}$ (i.e., data does not correspond to a truncated exponential function).

Table 7 Continued. Statistics for RH-TRU Waste Densities (a)

Materials		Waste Density $[Kg/m^3]$				
		Uncategorized Metal (3.6 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ $[m^3/Kg]$	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	0.0/226.8/380.3	2.9133-19	3.8030+2	3.803+2	3.803+2
	Aluminum Based	0.0/2.2/141.4	4.54545-1	2.5247+0	6.7933+0	1.3095+1
	Other Metals	0.0/279.0/913.5	NC (c)	913.5(d)	913.5(d)	913.5(d)
	Other Inorganics	0.0/7.7/34.6	1.21617-1	9.1771+0	2.3161+1	3.3294+1
Organics	Cellulose	0.0/1.8/68.7	5.55555-1	2.0657+0	5.5581+0	1.0714+1
	Rubber	0.0/0.1/18.0	9.99999+0	1.1476-1	3.0878-1	5.9522-1
	Plastics	0.0/1.6/82.1	6.24999-1	1.8362+0	4.9406+0	9.5236+0
Solidified	Inorganic	0.0/0.0/3.7	NP	3.7(d)	3.7(d)	3.7(d)
Materials	Organic	0.0/0.0/3.7	NP	3.7(d)	3.7(d)	3.7(d)
Soils		0.0/0.0/2.9	NP	2.9(d)	2.9(d)	2.9(d)
	Total(ave)	519.2				
	Total(max)	1,648.9		1,318.8	1,344.9	1,371.3

		Unknown (0.73 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ $[m^3/Kg]$	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Aluminum Based	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Other Metals	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Other Inorganics	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Organics	Cellulose	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Rubber	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Plastics	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Solidified	Inorganic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Materials	Organic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Soils		0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Total(ave)	0.0				
	Total(max)	0.0		0.0	0.0	0.0

(a) Data from Ref. BIR-1c (ranked by volume percentages to be sent to WIPP).
(b) Statistical analyses performed with use of Equations 22 → 27.
(c) Maximum material partial density for final waste form.
(d) Value assign is material maximum, not calculated value.
NC Not computed because parameter is maximum partial density of material.
NP Not possible to compute because $a = \hat{x}$ (i.e., data does not correspond to a truncated exponential function).

Table 7 Continued. Statistics for RH-TRU Waste Densities (a)

Materials		Waste Density $[Kg/m^3]$				
		Combustible (0.38 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ $[m^3/Kg]$	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	254.0/257.7/265.2	NC (c)	265.2	265.2	265.2
	Aluminum Based	0.4/0.4/0.4	NP	0.4(d)	0.4(d)	0.4(d)
	Other Metals	18.8/18.8/89.7	NP	89.7(d)	89.7(d)	89.7(d)
	Other Inorganics	6.8/6.8/6.8	NP	6.8(d)	6.8(d)	6.8(d)
Organics	Cellulose	59.2/64.0/68.7	1.40200-9	6.5685+1	6.8267+1	6.8675+1
	Rubber	1.0/1.1/1.2	1.01000-7	1.1365+0	1.1909+0	1.1995+0
	Plastics	4.9/5.3/5.7	1.02010-8	5.4461+0	5.6635+0	5.6979+0
Solidified	Inorganic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Materials	Organic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Soils		0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Total(ave) Total(max)	354.1 437.7		434.4	437.2	437.7
		Lead/Cadmium Metal Waste (0.12 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ $[m^3/Kg]$	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	0.0/12.0/256.1	8.33333-2	1.3771+1	3.7054+1	7.1427+1
	Aluminum Based	0.0/1.3/27.8	7.69230-1	1.4919+0	4.0142+0	7.7379+0
	Other Metals	0.0/43.6/109.6	1.14806-2	5.8419+1	1.0013+2	1.0903+2
	Other Inorganics	1.2/165.7/754.8	NC (c)	754.8(d)	754.8(d)	754.8(d)
Organics	Cellulose	0.0/7.7/45.3	1.27539-1	8.9459+0	2.3719+1	4.0531+1
	Rubber	0.0/92.3/190.4	9.60477-4	1.2611+2	1.8092+2	1.8986+2
	Plastics	0.0/15.1/67.6	6.19505-2	1.8006+1	4.5391+1	6.5084+1
Solidified	Inorganic	0.0/5.9/619.2	1.69491-1	6.7708+0	1.8218+1	3.5118+1
Materials	Organic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Soils		0.0/0.4/1.2	1.79093+0	5.1586-1	1.0343+0	1.1891+0
	Total(ave) Total(max)	344.0 2,072.0		988.8	1,165.3	1,274.8

(a) Data from Ref. BIR-1c (ranked by volume percentages to be sent to WIPP).
(b) Statistical analysis perform with use of Equations 22 → 27.
(c) Maximum material partial density for final waste form.
(d) Value assign is material maximum, not calculated value.
NC Not computed because parameter is maximum partial density of material.
NP Not possible to compute because $a=\hat{x}$ (i.e., data does not correspond to a truncated exponential function).

Table 7 Continued. Statistics for RH-TRU Waste Densities (a)

Materials		Waste Density [Kg/m^3]				
		Filter (0.06 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ [m^3/Kg]	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Aluminum Based	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Other Metals	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Other Inorganics	214.9/232.5/241.2	NC (c)	241.2(d)	241.2(d)	241.2(d)
Organics	Cellulose	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Rubber	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Plastics	8.8/8.8/8.8	NP	8.8(d)	8.8(d)	8.8(d)
Solidified	Inorganic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Materials	Organic	0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
Soils		0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Total(ave) Total(max)	241.3 250.0		250.0	250.0	250.0

		Salt Waste (0.06 vol%) a / $\hat{x}$ / b [min/ave/max]	Truncated Exponential Distribution (b)			
			λ [m^3/Kg]	Statistical Results		
				F(68.26%)	F(95.44%)	F(99.74%)
Inorganic	Iron Based	3.7/20.1/28.6	1.30100-12	2.0697+1	2.7465+1	2.8535+1
	Aluminum Based	0.0/0.2/3.1	4.99998+0	2.2952-1	6.1757-1	1.1904+0
	Other Metals	1.6/8.4/16.9	4.38995-2	1.0855+1	1.5927+1	1.6843+1
	Other Inorganics	106.3/239.2/591.1	NC (c)	591.1(d)	591.1(d)	591.1(d)
Organics	Cellulose	0.0/1.0/3.8	8.7642-1	1.2248+0	2.8855+0	3.7227+0
	Rubber	0.0/0.0/0.8	NP	0.8(d)	0.8(d)	0.8(d)
	Plastics	1.1/1.9/5.2	1.20560+0	2.0393+0	3.5458+0	4.9438+0
Solidified	Inorganic	0.0/0.0/0.4	NP	0.4(d)	0.4(d)	0.4(d)
Materials	Organic	0.0/0.0/0.4	NP	0.4(d)	0.4(d)	0.4(d)
Soils		0.0/0.0/0.0	NP	0.0(d)	0.0(d)	0.0(d)
	Total(ave) Total(max)	270.8 650.3		627.7	643.1	647.9

(a) Data from Ref. BIR-1c (ranked by volume percentages to be sent to WIPP).
(b) Statistical analysis perform with use of Equations 22 → 27.
(c) Maximum material partial density for final waste form.
(d) Value assign is material maximum, not calculated value.
NC Not computed because parameter is maximum partial density of material.
NP Not possible to compute because $a = \hat{x}$ (i.e., data does not correspond to a truncated exponential function).

Table 8. RH-TRU Surface Dose and Gamma Flux Rates

Variable	Corresponding Result (a)	
	Conventional Units	SI Units
$\dot{H}$ (b)	1000.0 [rem/hr]	10. [Sv/hr]
Q (c)	1.0	1.0
$\dot{D}$ (d)	1000.0 [rad/hr]	10. [Gy/hr]
f (e)	0.93643	0.93643
$\dot{X}$ (f)	$\sim$ 1067.9 [R/hr]	$\sim$ 0.276 [$coul/kg-hr$] (i)
C_p (g)	$1.8452E-6$	$1.8452E-6$
ϕ_s (h)	$\sim 5.787E+08$ [γ/cm^2-sec] (j)	$\sim 5.787E+08$ [γ/cm^2-sec]

(a) Results in this table correspond to steps 1 → 4 of Table 1.
(b) Maximum RH-TRU canister surface dose rate allowed by Ref. LWA-1.
(c) Value from Table 2.
(d) Calculated via Equation 1.
(e) Calculated via Equation 3b using Table 3, assuming $E_\gamma = 1.0\,MeV$.
(f) Calculated via Equation 2.
(g) Calculated via Equation 3c using Table 3, assuming $E_\gamma = 1.0\,MeV$.
(h) Calculated via Equation 4.
(i) There isn't a SI conversion for Roentgen, mks equivalent is given.
(j) Note, this is a very large gamma flux, very dangerous radiation field.

Table 9. Disposal Radionuclide Inventory

Nuclide		WIPP TRU Waste					
ID	Energy [*MeV/dis*] (a)	Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
		CH	RH	CH	RH	CH	RH
Ac225	5.893E+00	2.030E+00	3.280E-01	7.09E-02	1.15E-02	8.39E-05	1.48E-04
Ac227	8.169E-02	6.550E-01	1.520E-02	3.17E-04	7.36E-06	3.75E-07	9.51E-08
Ac228	1.458E+00	5.270E-01	4.080E-03	4.55E-03	3.53E-05	5.39E-06	4.56E-07
Ag109m	8.696E-02	4.850E+01	NR	2.50E-02	--	2.96E-05	--
Ag110	1.212E+00	5.610E-06	1.070E-05	4.03E-08	7.69E-08	4.77E-11	9.93E-10
Ag110m	2.817E+00	4.210E-04	8.060E-04	7.03E-06	1.35E-05	8.32E-09	1.74E-07
Am241	5.604E+00	2.230E+05	5.300E+02	7.41E+03	1.76E+01	8.76E+00	2.28E-01
Am242	1.915E-01	4.930E-02	NR	5.60E-05	--	6.62E-08	--
Am242m	6.664E-02	4.960E-02	NR	1.96E-05	--	2.32E-08	--
Am243	5.423E+00	2.940E+01	1.220E-02	9.45E-01	3.92E-04	1.12E-03	5.07E-06
Am245	3.130E-01	9.070E-09	2.520E-14	1.68E-11	4.68E-17	1.99E-14	6.04E-19
At217	7.199E+00	2.030E+00	3.280E-01	8.66E-02	1.40E-02	1.02E-04	1.81E-04
Ba137m	6.624E-01	5.030E+03	3.100E+05	1.98E+01	1.22E+03	2.34E-02	1.57E+01
Bi210	3.890E-01	1.010E+00	4.090E-11	2.33E-03	9.43E-14	2.75E-06	1.22E-15
Bi211	6.729E+00	6.570E-01	1.460E-02	2.62E-02	5.82E-04	3.10E-05	7.53E-06
Bi212	2.869E+00	2.770E+01	9.030E+00	4.71E-01	1.54E-01	5.57E-04	1.98E-03
Bi213	7.092E-01	2.030E+00	3.280E-01	8.53E-03	1.38E-03	1.01E-05	1.78E-05
Bi214	2.162E+00	5.840E+00	7.230E-10	7.48E-02	9.27E-12	8.85E-05	1.20E-13
Bk249	1.250E-01	6.250E-04	1.740E-09	4.63E-07	1.29E-12	5.48E-10	1.67E-14
Bk250	1.172E+00	2.350E-06	NR	1.63E-08	--	1.93E-11	--
C14	4.947E-02	1.830E+01	1.510E+02	5.37E-03	4.43E-02	6.35E-06	5.72E-04
Cd109	1.960E-02	4.850E+01	NR	5.64E-03	--	6.66E-06	--
Cd113m	2.840E-01	4.650E-05	2.360E-05	7.83E-08	3.97E-08	9.26E-11	5.13E-10
Ce144	1.119E-01	8.220E+01	5.580E+02	5.45E-02	3.70E-01	6.45E-05	4.78E-03
Cf249	7.806E+00	1.560E+00	8.110E-02	7.22E-02	3.75E-03	8.54E-05	4.85E-05
Cf250	6.267E+00	3.540E-01	NR	1.32E-02	--	1.56E-05	--
Cf251	6.027E+00	3.930E-03	NR	1.40E-04	--	1.66E-07	--
Cf252	1.204E+01	1.850E+02	5.110E+01	1.32E+01	3.65E+00	1.56E-02	4.71E-02
Cm242	6.216E+00	1.480E-02	NR	5.45E-04	--	6.45E-07	--
Cm243	6.189E+00	1.330E+00	2.010E+03	4.88E-02	7.37E+01	5.77E-05	9.53E-01
Cm244	5.901E+00	5.400E+03	1.070E+04	1.89E+02	3.74E+02	2.23E-01	4.84E+00
Cm245	5.598E+00	5.160E+01	1.320E-05	1.71E+00	4.38E-07	2.03E-03	5.66E-09
Cm246	5.523E+00	1.100E-01	NR	3.60E-03	--	4.26E-06	--
Cm247	2.390E+00	2.980E-09	NR	4.22E-11	--	4.99E-14	--
Cm248	2.100E+01	5.060E-02	2.340E-03	6.30E-03	2.91E-04	7.45E-06	3.76E-06
Co58	1.009E+00	5.500E-05	7.920E-07	3.29E-07	4.74E-09	3.89E-10	6.12E-11
Co60	2.601E+00	1.530E+02	1.080E+04	2.36E+00	1.67E+02	2.79E-03	2.15E+00
Cr51	3.620E-02	NR	2.540E-31	--	5.45E-35	--	7.04E-37
Cs134	1.717E+00	5.880E+00	2.150E+03	5.98E-02	2.19E+01	7.08E-05	2.83E-01
Cs135	5.630E-02	7.900E-03	4.580E-03	2.64E-06	1.53E-06	3.12E-09	1.98E-08

Table 9 Continued. Disposal Radionuclide Inventory

Nuclide		WIPP TRU Waste					
ID	Energy *[MeV/dis]* (a)	Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
		CH	RH	CH	RH	CH	RH
Cs137	1.866E-01	5.320E+03	3.280E+05	5.88E+00	3.63E+02	6.96E-03	4.69E+00
Es254	6.623E+00	2.350E-06	NR	9.23E-08	--	1.09E-10	--
Eu150	1.540E+00	3.650E-05	NR	3.33E-07	--	3.94E-10	--
Eu152	1.276E+00	7.410E+00	5.280E+04	5.61E-02	3.99E+02	6.63E-05	5.16E+00
Eu154	1.509E+00	3.050E+01	2.760E+04	2.73E-01	2.47E+02	3.23E-04	3.19E+00
Eu155	1.227E-01	4.140E+01	6.780E+03	3.01E-02	4.93E+00	3.56E-05	6.37E-02
Fe55	5.700E-03	3.296E-05	1.440E+01	1.11E-09	4.87E-04	1.32E-12	6.29E-06
Fe59	1.306E+00	1.960E-02	4.040E-19	1.52E-04	3.13E-21	1.79E-07	4.04E-23
Fr221	6.511E+00	2.030E+00	3.280E-01	7.84E-02	1.27E-02	9.27E-05	1.64E-04
Fr223	4.381E-01	9.040E-03	2.100E-04	2.35E-05	5.45E-07	2.78E-08	7.05E-09
H3	5.608E-03	9.640E-01	8.230E+01	3.20E-05	2.74E-03	3.79E-08	3.54E-05
I129	7.804E-02	1.280E-09	NR	5.92E-13	--	7.00E-16	--
Kr85	2.527E-01	2.240E-01	9.580E+01	3.36E-04	1.44E-01	3.97E-07	1.85E-03
Mn54	8.398E-01	1.120E-02	2.760E+00	5.58E-05	1.37E-02	6.59E-08	1.78E-04
Nb95	8.092E-01	4.960E-01	9.900E+00	2.38E-03	4.75E-02	2.81E-06	6.14E-04
Nb95m	2.344E-01	1.660E-03	3.410E-02	2.31E-06	4.74E-05	2.73E-09	6.12E-07
Ni59	6.700E-03	3.380E-03	NR	1.34E-07	--	1.59E-10	--
Ni63	1.700E-02	4.190E-01	5.030E+01	4.22E-05	5.07E-03	4.99E-08	6.55E-05
Np237	5.156E+00	8.820E+01	1.180E-02	2.70E+00	3.61E-04	3.19E-03	4.66E-06
Np238	8.080E-01	2.480E-04	NR	1.19E-06	--	1.40E-09	--
Np239	4.078E-01	2.940E+01	1.220E-02	7.11E-02	2.95E-05	8.41E-05	3.81E-07
Np240	1.788E+00	1.100E-09	1.780E-13	1.17E-11	1.89E-15	1.38E-14	2.44E-17
Np240m	9.776E-01	1.000E-06	1.620E-10	5.80E-09	9.39E-13	6.85E-12	1.21E-14
Pa231	5.083E+00	4.080E-03	1.780E-01	1.23E-04	5.36E-03	1.45E-07	6.93E-05
Pa233	3.829E-01	3.320E+01	1.180E-02	7.54E-02	2.68E-05	8.91E-05	3.46E-07
Pa234	2.423E+00	2.440E-02	1.700E-02	3.50E-04	2.44E-04	4.15E-07	3.16E-06
Pa234m	8.337E-01	1.880E+01	1.310E+01	9.29E-02	6.47E-02	1.10E-04	8.37E-04
Pb209	1.940E-01	2.030E+00	3.280E-01	2.33E-03	3.77E-04	2.76E-06	4.87E-06
Pb210	3.908E-02	1.010E+00	4.090E-11	2.34E-04	9.48E-15	2.77E-07	1.22E-16
Pb211	5.055E-01	6.570E-01	1.460E-02	1.97E-03	4.38E-05	2.33E-06	5.65E-07
Pb212	3.212E-01	2.770E+01	9.030E+00	5.27E-02	1.72E-02	6.24E-05	2.22E-04
Pb214	5.380E-01	5.840E+00	7.230E-10	1.86E-02	2.31E-12	2.20E-05	2.98E-14
Pd107	1.000E-02	1.170E-03	6.770E-04	6.94E-08	4.01E-08	8.20E-11	5.19E-10
Pm147	6.051E-02	1.260E+03	4.100E+03	4.52E-01	1.47E+00	5.35E-04	1.90E-02
Po210	5.408E+00	8.920E-01	3.050E-11	2.86E-02	9.78E-13	3.38E-05	1.26E-14
Po211	7.592E+00	1.790E-03	3.980E-05	8.06E-05	1.79E-06	9.53E-08	2.31E-08
Po212	8.940E+00	1.780E+01	5.780E+00	9.43E-01	3.06E-01	1.12E-03	3.96E-03
Po213	8.537E+00	1.990E+00	3.210E-01	1.01E-01	1.62E-02	1.19E-04	2.10E-04

Table 9 Continued. Disposal Radionuclide Inventory

Nuclide		WIPP TRU Waste					
ID	Energy [*MeV/dis*] (a)	Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
		CH	RH	CH	RH	CH	RH
Po214	7.833E+00	5.840E+00	7.230E-10	2.71E-01	3.36E-11	3.21E-04	4.34E-13
Po215	7.531E+00	6.570E-01	1.460E-02	2.93E-02	6.52E-04	3.47E-05	8.42E-06
Po216	6.906E+00	2.770E+01	9.030E+00	1.13E+00	3.70E-01	1.34E-03	4.78E-03
Po218	6.113E+00	5.840E+00	7.230E-10	2.12E-01	2.62E-11	2.50E-04	3.39E-13
Pr144	*1.240E+00*	*8.220E+01*	*5.580E+02*	*6.04E-01*	*4.10E+00*	*7.15E-04*	*5.30E-02*
Pu236	5.871E+00	1.690E-02	NR	5.88E-04	–	6.96E-07	–
Pu238	5.591E+00	**1.890E+06** (e)	3.530E+03	6.26E+04	1.17E+02	**7.41E+01** (g)	1.51E+00
Pu239	5.199E+00	3.850E+05	6.410E+03	1.19E+04	1.98E+02	1.40E+01	2.55E+00
Pu240	5.253E+00	7.220E+04	1.740E+02	2.25E+03	5.42E+00	2.66E+00	7.00E-02
Pu241	5.230E-03	1.010E+06	9.060E+02	3.13E+01	2.81E-02	3.70E-02	3.63E-04
Pu242	4.982E+00	1.270E+03	1.480E-02	3.75E+01	4.37E-04	4.44E-02	5.65E-06
Pu243	1.947E-01	2.980E-09	NR	3.44E-12	–	4.07E-15	–
Pu244	4.892E+00	1.000E-06	1.620E-10	2.90E-08	4.70E-12	3.43E-11	6.07E-14
Ra223	6.007E+00	6.570E-01	1.460E-02	2.34E-02	5.20E-04	2.77E-05	6.72E-06
Ra224	5.790E+00	2.770E+01	9.030E+00	9.51E-01	3.10E-01	1.12E-03	4.00E-03
Ra225	1.183E-01	2.040E+00	3.310E-01	1.43E-03	2.32E-04	1.69E-06	3.00E-06
Ra226	4.871E+00	5.840E+00	7.230E-10	1.69E-01	2.09E-11	1.99E-04	2.70E-13
Ra228	1.300E-02	5.270E-01	4.080E-03	4.06E-05	3.14E-07	4.80E-08	4.06E-09
Rh106	1.618E+00	4.020E+01	8.420E+02	3.86E-01	8.08E+00	4.56E-04	1.04E-01
Rn219	7.000E+00	6.570E-01	1.460E-02	2.73E-02	6.06E-04	3.22E-05	7.83E-06
Rn220	6.405E+00	2.770E+01	9.030E+00	1.05E+00	3.43E-01	1.24E-03	4.43E-03
Rn222	5.590E+00	5.840E+00	7.230E-10	1.94E-01	2.40E-11	2.29E-04	3.10E-13
Ru106	1.003E-02	4.020E+01	8.420E+02	2.39E-03	5.01E-02	2.83E-06	6.47E-04
Sb125	5.274E-01	1.580E+01	2.460E+03	4.94E-02	7.69E+00	5.84E-05	9.94E-02
Sb126	3.117E+00	2.130E-03	1.230E-03	3.94E-05	2.27E-05	4.65E-08	2.94E-07
Sb126m	2.148E+00	1.520E-02	8.850E-03	1.94E-04	1.13E-04	2.29E-07	1.46E-06
Se79	*4.200E-02*	*6.860E-03*	*3.970E-03*	*1.71E-06*	*9.88E-07*	2.02E-09	*1.28E-08*
Sm151	1.978E-02	2.500E+01	1.420E+01	2.93E-03	1.67E-03	3.47E-06	2.15E-05
Sn119m	8.720E-02	6.800E-03	1.370E-02	3.52E-06	7.08E-06	4.16E-09	9.15E-08
Sn121m	3.380E-01	4.820E-01	2.690E-01	9.66E-04	5.39E-04	1.14E-06	6.96E-06
Sn126	*2.104E-01*	*1.520E-02*	*8.800E-03*	*1.90E-05*	*1.10E-05*	2.24E-08	*1.42E-07*
Sr90	1.958E-01	4.070E+03	**6.680E+05** (f)	4.72E+00	7.75E+02	5.59E-03	1.00E+01
Ta182	5.000E-01	NR	1.720E-04	–	5.10E-07	–	6.59E-09
Tc99	8.460E-02	2.460E+01	2.280E-01	1.23E-02	1.14E-04	1.46E-05	1.48E-06
Te125m	1.418E-01	6.550E-04	1.010E+03	5.51E-07	8.49E-01	6.51E-10	1.10E-02
Te127	2.278E-01	3.070E-02	1.130E-01	4.15E-05	1.53E-04	4.90E-08	1.97E-06
Te127m	9.074E-02	3.150E-02	1.150E-01	1.69E-05	6.19E-05	2.00E-08	7.99E-07

Table 9 Continued. Disposal Radionuclide Inventory

Nuclide		WIPP TRU Waste					
ID	Energy [*MeV/dis*] (a)	Total Inventory [Curies] (b)		Heat Load [Watts] (c)		% Heat Load [%]	
		CH	RH	CH	RH	CH	RH
Th227	6.157E+00	6.560E-01	1.480E-02	2.39E-02	5.40E-04	2.83E-05	6.98E-06
Th228	5.517E+00	2.770E+01	9.040E+00	9.06E-01	2.96E-01	1.07E-03	3.82E-03
Th229	5.161E+00	2.050E+00	3.360E-01	6.27E-02	1.03E-02	7.42E-05	1.33E-04
Th230	4.774E+00	4.900E-02	8.790E-07	1.39E-03	2.49E-08	1.64E-06	3.21E-10
Th231	9.466E-02	2.880E+00	2.210E+03	1.62E-03	1.24E+00	1.91E-06	1.60E-02
Th232	4.084E+00	6.070E-01	7.090E-03	1.47E-02	1.72E-04	1.74E-05	2.22E-06
Th234	6.840E-02	1.880E+01	1.310E+01	7.62E-03	5.31E-03	9.02E-06	6.86E-05
Tl207	4.954E-01	6.560E-01	1.450E-02	1.93E-03	4.26E-05	2.28E-06	5.50E-07
Tl208	3.970E+00	9.960E+00	3.240E+00	2.34E-01	7.63E-02	2.77E-04	9.85E-04
Tl209	2.803E+00	4.390E-02	7.080E-03	7.29E-04	1.18E-04	8.63E-07	1.52E-06
Tl210	--(d)	1.230E-03	1.520E-13	--	--	--	--
U232	5.416E+00	2.630E+01	1.160E+01	8.44E-01	3.72E-01	9.99E-04	4.81E-03
U233	4.904E+00	1.380E+03	8.570E+02	4.01E+01	2.49E+01	4.74E-02	3.22E-01
U234	4.859E+00	2.500E+02	4.180E-02	7.20E+00	1.20E-03	8.52E-03	1.56E-05
U235	4.418E+00	2.880E+00	5.660E+00	7.54E-02	1.48E-01	8.92E-05	1.92E-03
U236	4.570E+00	1.340E-01	4.110E-05	3.63E-03	1.11E-06	4.29E-06	1.44E-08
U237	3.192E-01	2.470E+01	2.220E-02	4.67E-02	4.20E-05	5.53E-05	5.43E-07
U238	4.279E+00	1.880E+01	1.310E+01	4.77E-01	3.32E-01	5.64E-04	4.29E-03
U240	1.384E-01	1.000E-06	1.620E-10	8.20E-10	1.33E-13	9.70E-13	1.72E-15
Y90	9.350E-01	4.070E+03	**6.680E+05** (f)	2.26E+01	3.70E+03	2.67E-02	**4.78E+01** **(h)**
Zn65	5.904E-01	1.210E-08	NR	4.23E-11	--	5.01E-14	--
Zr93	1.960E-02	8.870E-02	5.140E-02	1.03E-05	5.97E-06	1.22E-08	7.72E-08
Zr95	8.545E-01	2.240E-01	4.600E+00	1.13E-03	2.33E-02	1.34E-06	3.01E-04
Sum =		**3.61E+06** (i)	**2.11E+06** (j)	**8.46E+04** (k)	**7.74E+03** (l)	1.00E+02	1.00E+02

-- Not calculated.

NR Not Reported by sites (see Ref. BIR-1d).

(a) Data from Ref Or-1.

(b) Data from Ref BIR-1d.

(c) Data calculated from the equation;

$$\text{Heat Load} = TOTAL\ ACTIVITY(Ci)\frac{3.7E+10(dis/sec)}{Ci}\ ENERGY(MeV/dis)\ \frac{E+06\,eV}{MeV}\ \frac{1.60219E-19\,J}{eV}\ \frac{watt-sec}{J}$$

$$\text{Heat Load (watts)} = 0.005928103 \times TOTAL\ ACTIVITY(Ci) \times ENERGY(MeV/dis)$$

(d) Disintegration energy not available in Ref. Or-1.

(e) Max total curie load for CH-TRU wastes.

(f) Max total curie load for RH-TRU wastes.

(g) Max heat load for CH-TRU wastes.

(h) Max heat load for RH-TRU wastes.

(i) Note, the total CH-TRU curie load is only 3.61 MCi (also, 63.1 % of the total curie load in WIPP). The average CH-TRU volumetric total curie load is 3.61E+06/5.95E+06 = 0.607 (Ci/cu. ft.) = 21.43 (Ci/cu. m.). [See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume.

The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values applicable to expected waste at WIPP (See Ref. BIR-1e).]

(j) Note, the total RH-TRU curie load is only 2.11 MCi (also, 36.9 % of the total curie load in WIPP).
This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1].
The average RH-TRU volumetric total curie load is 2.11E+06/0.25E+06 = 8.440 (Ci/cu. ft.) = **298.1 (Ci/cu. m.)**.
[See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft.]

(k) Note, the total CH-TRU heat load is only **84.6 kW** (also, 91.6 % of the total heat load in WIPP).
The ratio for CH-TRU of total heat load to total curie load is 84.6E+03/3.61E+06 = **0.02343**.
The average CH-TRU volumetric heat load is 84.6E+03/5.95E+06 = 0.0142 (W/cu. ft.) = 0.502 (W/cu. m.).
The average CH-TRU drum heat load is 0.502 (W/cu. m.)x 0.2082 (cu. m.) = **0.1045 W**.
[The volume of a CH-TRU drum was set equal to the nominal volume of a 55-gal drum.]

(l) Note, the total RH-TRU heat load is only **7.74 kW** (also, 8.4 % of the total heat load in WIPP).
The ratio for RH-TRU of total heat load to total curie load is 7.74E+03/2.11E+06 = **0.003668**.
The average RH-TRU volumetric heat load is 7.74E+03/0.25E+06 = 0.0310 (W/cu. ft.) = 1.09 (W/cu. m.).
The average RH-TRU canister heat load is 1.09 (W/cu. m.)x 0.6246 (cu. m.) = **0.6808 W** (this is about ten times that of an average CH-TRU drum). [The volume of a RH-TRU canister was set equal to three times the nominal volume of a 55-gal drum. Even though the reported volume of a RH-TRU canister is 0.89 cu. m. [Ref. BIR-1f], these canisters are loaded with three 55-gal drums internally. Ref. Lo-1.]

Table 10. RH-TRU Waste Radionuclide Gamma Activity Ratios

Nuclide		WIPP TRU Waste					
ID	Gamma Activity Fraction (a)	Total Inventory [Curies] (b)		Gamma Inventory [Curies] (c)		% Gamma Inventory [%]	
		CH	RH	CH	RH	CH	RH
Ac225	0.000E+00	2.030E+00	3.280E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ac227	9.862E-01	6.550E-01	1.520E-02	6.46E-01	1.50E-02	6.27E-05	7.18E-07
Ac228	1.000E+00	5.270E-01	4.080E-03	5.27E-01	4.08E-03	5.11E-05	1.95E-07
Ag109m	1.000E+00	4.850E+01	NR	4.85E+01	–	4.70E-03	--
Ag110	1.000E+00	5.610E-06	1.070E-05	5.61E-06	1.07E-05	5.44E-10	5.13E-10
Ag110m	1.000E+00	4.210E-04	8.060E-04	4.21E-04	8.06E-04	4.08E-08	3.86E-08
Am241	0.000E+00	2.230E+05	5.300E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Am242	1.000E+00	4.930E-02	NR	4.93E-02	--	4.78E-06	--
Am242m	9.950E-01	4.960E-02	NR	4.94E-02	--	4.79E-06	--
Am243	0.000E+00	2.940E+01	1.220E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Am245	1.000E+00	9.070E-09	2.520E-14	9.07E-09	2.52E-14	8.80E-13	1.21E-18
At217	0.000E+00	2.030E+00	3.280E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ba137m	1.000E+00	5.030E+03	3.100E+05	5.03E+03	3.10E+05	4.88E-01	1.49E+01
Bi210	1.000E+00	1.010E+00	4.090E-11	1.01E+00	4.09E-11	9.80E-05	1.96E-15
Bi211	2.800E-03	6.570E-01	1.460E-02	1.84E-03	4.09E-05	1.79E-07	1.96E-09
Bi212	6.407E-01	2.770E+01	9.030E+00	1.78E+01	5.79E+00	1.72E-03	2.77E-04
Bi213	9.784E-01	2.030E+00	3.280E-01	1.99E+00	3.21E-01	1.93E-04	1.54E-05
Bi214	9.998E-01	5.840E+00	7.230E-10	5.84E+00	7.23E-10	5.66E-04	3.46E-14
Bk249	1.000E+00	6.250E-04	1.740E-09	6.25E-04	1.74E-09	6.06E-08	8.33E-14
Bk250	1.000E+00	2.350E-06	NR	2.35E-06	–	2.28E-10	--
C14	1.000E+00	1.830E+01	1.510E+02	1.83E+01	1.51E+02	1.78E-03	7.23E-03
Cd109	1.000E+00	4.850E+01	NR	4.85E+01	–	4.70E-03	--
Cd113m	1.000E+00	4.650E-05	2.360E-05	4.65E-05	2.36E-05	4.51E-09	1.13E-09
Ce144	1.000E+00	8.220E+01	5.580E+02	8.22E+01	5.58E+02	7.97E-03	2.67E-02
Cf249	0.000E+00	1.560E+00	8.110E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cf250	8.000E-04	3.540E-01	NR	2.83E-04	–	2.75E-08	–
Cf251	0.000E+00	3.930E-03	NR	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cf252	3.090E-02	1.850E+02	5.110E+01	5.72E+00	1.58E+00	5.55E-04	7.56E-05
Cm242	0.000E+00	1.480E-02	NR	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cm243	2.400E-03	1.330E+00	2.010E+03	3.19E-03	4.82E+00	3.10E-07	2.31E-04
Cm244	0.000E+00	5.400E+03	1.070E+04	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cm245	0.000E+00	5.160E+01	1.320E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cm246	3.000E-04	1.100E-01	NR	3.30E-05	–	3.20E-09	--
Cm247	0.000E+00	2.980E-09	NR	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Cm248	8.260E-02	5.060E-02	2.340E-03	4.18E-03	1.93E-04	4.05E-07	9.26E-09
Co58	1.000E+00	5.500E-05	7.920E-07	5.50E-05	7.92E-07	5.34E-09	3.79E-11
Co60	1.000E+00	1.530E+02	1.080E+04	1.53E+02	1.08E+04	1.48E-02	5.17E-01
Cr51	1.000E+00	NR	2.540E-31	--	2.54E-31	–	1.22E-35
Cs134	1.000E+00	5.880E+00	2.150E+03	5.88E+00	2.15E+03	5.70E-04	1.03E-01
Cs135	1.000E+00	7.900E-03	4.580E-03	7.90E-03	4.58E-03	7.66E-07	2.19E-07

Table 10 Continued. RH-TRU Waste Radionuclide Gamma Activity Ratios

Nuclide		WIPP TRU Waste					
ID	Gamma Activity Fraction (a)	Total Inventory [Curies] (b)		Gamma Inventory [Curies] (c)		% Gamma Inventory [%]	
		CH	RH	CH	RH	CH	RH
Cs137	1.000E+00	5.320E+03	3.280E+05	5.32E+03	3.28E+05	5.16E-01	1.57E+01
Es254	0.000E+00	2.350E-06	NR	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Eu150	1.000E+00	3.650E-05	NR	3.65E-05	–	3.54E-09	–
Eu152	1.000E+00	7.410E+00	5.280E+04	7.41E+00	5.28E+04	7.19E-04	2.53E+00
Eu154	1.000E+00	3.050E+01	2.760E+04	3.05E+01	2.76E+04	2.96E-03	1.32E+00
Eu155	1.000E+00	4.140E+01	6.780E+03	4.14E+01	6.78E+03	4.02E-03	3.25E-01
Fe55	1.000E+00	3.296E-05	1.440E+01	3.30E-05	1.44E+01	3.20E-09	6.90E-04
Fe59	1.000E+00	1.960E-02	4.040E-19	1.96E-02	4.04E-19	1.90E-06	1.94E-23
Fr221	0.000E+00	2.030E+00	3.280E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Fr223	9.999E-01	9.040E-03	2.100E-04	9.04E-03	2.10E-04	8.77E-07	1.01E-08
H3	1.000E+00	9.640E-01	8.230E+01	9.64E-01	8.23E+01	9.35E-05	3.94E-03
I129	1.000E+00	1.280E-09	NR	1.28E-09	--	1.24E-13	–
Kr85	1.000E+00	2.240E-01	9.580E+01	2.24E-01	9.58E+01	2.17E-05	4.59E-03
Mn54	1.000E+00	1.120E-02	2.760E+00	1.12E-02	2.76E+00	1.09E-06	1.32E-04
Nb95	1.000E+00	4.960E-01	9.900E+00	4.96E-01	9.90E+00	4.81E-05	4.74E-04
Nb95m	1.000E+00	1.660E-03	3.410E-02	1.66E-03	3.41E-02	1.61E-07	1.63E-06
Ni59	1.000E+00	3.380E-03	NR	3.38E-03	–	3.28E-07	–
Ni63	1.000E+00	4.190E-01	5.030E+01	4.19E-01	5.03E+01	4.06E-05	2.41E-03
Np237	0.000E+00	8.820E+01	1.180E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Np238	1.000E+00	2.480E-04	NR	2.48E-04	–	2.41E-08	–
Np239	1.000E+00	2.940E+01	1.220E-02	2.94E+01	1.22E-02	2.85E-03	5.84E-07
Np240	1.000E+00	1.100E-09	1.780E-13	1.10E-09	1.78E-13	1.07E-13	8.53E-18
Np240m	1.000E+00	1.000E-06	1.620E-10	1.00E-06	1.62E-10	9.70E-11	7.76E-15
Pa231	0.000E+00	4.080E-03	1.780E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pa233	1.000E+00	3.320E+01	1.180E-02	3.32E+01	1.18E-02	3.22E-03	5.65E-07
Pa234	1.000E+00	2.440E-02	1.700E-02	2.44E-02	1.70E-02	2.37E-06	8.14E-07
Pa234m	1.000E+00	1.880E+01	1.310E+01	1.88E+01	1.31E+01	1.82E-03	6.27E-04
Pb209	1.000E+00	2.030E+00	3.280E-01	2.03E+00	3.28E-01	1.97E-04	1.57E-05
Pb210	1.000E+00	1.010E+00	4.090E-11	1.01E+00	4.09E-11	9.80E-05	1.96E-15
Pb211	1.000E+00	6.570E-01	1.460E-02	6.57E-01	1.46E-02	6.37E-05	6.99E-07
Pb212	1.000E+00	2.770E+01	9.030E+00	2.77E+01	9.03E+00	2.69E-03	4.33E-04
Pb214	1.000E+00	5.840E+00	7.230E-10	5.84E+00	7.23E-10	5.66E-04	3.46E-14
Pd107	1.000E+00	1.170E-03	6.770E-04	1.17E-03	6.77E-04	1.14E-07	3.24E-08
Pm147	1.000E+00	1.260E+03	4.100E+03	1.26E+03	4.10E+03	1.22E-01	1.96E-01
Po210	0.000E+00	8.920E-01	3.050E-11	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Po211	0.000E+00	1.790E-03	3.980E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Po212	0.000E+00	1.780E+01	5.780E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Po213	0.000E+00	1.990E+00	3.210E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table 10 Continued. RH-TRU Waste Radionuclide Gamma Activity Ratios

Nuclide		WIPP TRU Waste					
ID	Gamma Activity Fraction (a)	Total Inventory [Curies] (b)		Gamma Inventory [Curies] (c)		% Gamma Inventory [%]	
		CH	RH	CH	RH	CH	RH
Po214	0.000E+00	5.840E+00	7.230E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Po215	0.000E+00	6.570E-01	1.460E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Po216	0.000E+00	2.770E+01	9.030E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Po218	2.000E-04	5.840E+00	7.230E-10	1.17E-03	1.45E-13	1.13E-07	6.93E-18
Pr144	1.000E+00	8.220E+01	5.580E+02	8.22E+01	5.58E+02	7.97E-03	2.67E-02
Pu236	0.000E+00	1.690E-02	NR	0.00E+00	–	0.00E+00	--
Pu238	0.000E+00	**1.890E+06** (e)	3.530E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu239	0.000E+00	3.850E+05	6.410E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu240	0.000E+00	7.220E+04	1.740E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu241	1.000E+00	1.010E+06	9.060E+02	1.01E+06	9.06E+02	**9.80E+01** (g)	4.34E-02
Pu242	0.000E+00	1.270E+03	1.480E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pu243	1.000E+00	2.980E-09	NR	2.98E-09	–	2.89E-13	--
Pu244	1.300E-03	1.000E-06	1.620E-10	1.30E-09	2.11E-13	1.26E-13	1.01E-17
Ra223	0.000E+00	6.570E-01	1.460E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ra224	0.000E+00	2.770E+01	9.030E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ra225	1.000E+00	2.040E+00	3.310E-01	2.04E+00	3.31E-01	1.98E-04	1.59E-05
Ra226	0.000E+00	5.840E+00	7.230E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ra228	1.000E+00	5.270E-01	4.080E-03	5.27E-01	4.08E-03	5.11E-05	1.95E-07
Rh106	1.000E+00	4.020E+01	8.420E+02	4.02E+01	8.42E+02	3.90E-03	4.03E-02
Rn219	0.000E+00	6.570E-01	1.460E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rn220	0.000E+00	2.770E+01	9.030E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rn222	0.000E+00	5.840E+00	7.230E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ru106	1.000E+00	4.020E+01	8.420E+02	4.02E+01	8.42E+02	3.90E-03	4.03E-02
Sb125	1.000E+00	1.580E+01	2.460E+03	1.58E+01	2.46E+03	1.53E-03	1.18E-01
Sb126	1.000E+00	2.130E-03	1.230E-03	2.13E-03	1.23E-03	2.07E-07	5.89E-08
Sb126m	1.000E+00	1.520E-02	8.850E-03	1.52E-02	8.85E-03	1.47E-06	4.24E-07
Se79	1.000E+00	6.860E-03	3.970E-03	6.86E-03	3.97E-03	6.65E-07	1.90E-07
Sm151	1.000E+00	2.500E+01	1.420E+01	2.50E+01	1.42E+01	2.43E-03	6.80E-04
Sn119m	1.000E+00	6.800E-03	1.370E-02	6.80E-03	1.37E-02	6.60E-07	6.56E-07
Sn121m	1.000E+00	4.820E-01	2.690E-01	4.82E-01	2.69E-01	4.68E-05	1.29E-05
Sn126	1.000E+00	1.520E-02	8.800E-03	1.52E-02	8.80E-03	1.47E-06	4.22E-07
Sr90	1.000E+00	4.070E+03	6.680E+05	4.07E+03	6.68E+05	3.95E-01	**3.20E+01** (h)
Ta182	1.000E+00	NR	1.720E-04	--	1.72E-04	–	8.24E-09
Tc99	1.000E+00	2.460E+01	2.280E-01	2.46E+01	2.28E-01	2.39E-03	1.09E-05
Te125m	1.000E+00	6.550E-04	1.010E+03	6.55E-04	1.01E+03	6.35E-08	4.84E-02
Te127	1.000E+00	3.070E-02	1.130E-01	3.07E-02	1.13E-01	2.98E-06	5.41E-06
Te127m	1.000E+00	3.150E-02	1.150E-01	3.15E-02	1.15E-01	3.06E-06	5.51E-06

Table 10 Continued. RH-TRU Waste Radionuclide Gamma Activity Ratios

Nuclide		WIPP TRU Waste					
ID	Gamma Activity Fraction (a)	Total Inventory [Curies] (b)		Gamma Inventory [Curies] (c)		% Gamma Inventory [%]	
		CH	RH	CH	RH	CH	RH
Th227	0.000E+00	6.560E-01	1.480E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Th228	0.000E+00	2.770E+01	9.040E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Th229	0.000E+00	2.050E+00	3.360E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Th230	0.000E+00	4.900E-02	8.790E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Th231	1.000E+00	2.880E+00	2.210E+03	2.88E+00	2.21E+03	2.79E-04	1.06E-01
Th232	0.000E+00	6.070E-01	7.090E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Th234	1.000E+00	1.880E+01	1.310E+01	1.88E+01	1.31E+01	1.82E-03	6.27E-04
Tl207	1.000E+00	6.560E-01	1.450E-02	6.56E-01	1.45E-02	6.36E-05	6.94E-07
Tl208	1.000E+00	9.960E+00	3.240E+00	9.96E+00	3.24E+00	9.66E-04	1.55E-04
Tl209	1.000E+00	4.390E-02	7.080E-03	4.39E-02	7.08E-03	4.25E-06	3.39E-07
Tl210	--(d)	1.230E-03	1.520E-13	--	--	--	--
U232	0.000E+00	2.630E+01	1.160E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U233	0.000E+00	1.380E+03	8.570E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U234	0.000E+00	2.500E+02	4.180E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U235	0.000E+00	2.880E+00	5.660E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U236	0.000E+00	1.340E-01	4.110E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U237	1.000E+00	2.470E+01	2.220E-02	2.47E+01	2.22E-02	2.40E-03	1.06E-06
U238	0.000E+00	1.880E+01	1.310E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
U240	1.000E+00	1.000E-06	1.620E-10	1.00E-06	1.62E-10	9.70E-11	7.76E-15
Y90	1.000E+00	4.070E+03	**6.680E+05** (f)	4.07E+03	6.68E+05	3.95E-01	**3.20E+01** (h)
Zn65	1.000E+00	1.210E-08	NR	1.21E-08	--	1.17E-12	--
Zr93	1.000E+00	8.870E-02	5.140E-02	8.87E-02	5.14E-02	8.60E-06	2.46E-06
Zr95	1.000E+00	2.240E-01	4.600E+00	2.24E-01	4.60E+00	2.17E-05	2.20E-04
Sum =		**3.610E+06** (i)	**2.112E+06** (j)	**1.03E+06** (k)	**2.09E+06** (l)	1.00E+02	1.00E+02
% =				**28.551 %** (m)	**98.848 %** (n)		

-- Not calculated.
NR Not Reported by sites (see Ref. BIR-1d).
(a) Fraction of radionuclide disintegrations due to gammas only.
(γ fraction = 1 - (α, β, & n fractions).
α, β, and n fraction values from Ref Or-1.
(b) Data from Ref BIR-1d.
(c) Data calculated from the equation;
Gamma inventory$(Ci) = ACTIVITY(Ci) \times GAMMA\ FRACTION$
(d) Fraction values not available in Ref. Or-1.
(e) Max total curie load for CH-TRU wastes.
(f) Max total curie load for RH-TRU wastes.
(g) Max total gamma load for CH-TRU wastes.

(h) Max total gamma load for RH-TRU wastes.

(i) Note, the total CH-TRU curie load is only 3.61 MCi (also, 63.1 % of the total curie load in WIPP).
The average CH-TRU volumetric curie load is 3.61E+06/5.95E+06 = 0.607 (Ci/cu. ft.) = **21.43 (Ci/cu. m.)**.
[See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft.]

(j) Note, the total RH-TRU curie load is only 2.11 MCi (also, 36.9 % of the total curie load in WIPP).
This curie load is much less than the RH-TRU limit of 5.1 MCi [Ref. LWA-1].
The average RH-TRU volumetric curie load is 2.11E+06/0.25E+06 = 8.440 (Ci/cu. ft.) = **298.1 (Ci/cu. m.)**.
[See discussion note on Ref. LWA-1 for volumes -- RH→0.25E+06 cu. ft. Also note that the 5.95E+06 volume number is a volume limit, stored waste and projected waste volumes sum up to a volume less than this volume. The summed up volume is then "scaled" to yield a total volume of 5.95E+06, likewise the curie loads are also "scaled" by the same factor. Thus ratios of curie loads (or heat loads) to volume yield values applicable to expected waste at WIPP (see Ref. BIR-1e).]

(k) Note, the total CH-TRU gamma curie load is 1.031MCi (28.550912 % of the total curie load).
The ratio for CH-TRU of total curie load to gamma curie load is 3.61/1.031 = **3.50**.
The majority of the curie load of the CH-TRU is due to alpha and beta emitters.
The average CH-TRU volumetric gamma curie load is 1.03E+06/5.95E+06 = 0.173 (Ci/cu. ft.) = **6.113 (Ci/cu. m.)**.
[See discussion note on Ref. LWA-1 for volumes -- CH→5.95E+06 cu. ft.]
The average CH-TRU drum gamma curie load is 6.113 (Ci/cu. m.)x 0.2082 (cu. m.) = **1.273 Ci**.
[The volume of a CH-TRU drum was set equal to the nominal volume of a 55-gal drum.]

(l) Note, the total RH-TRU gamma curie load is 2.088MCi (98.848088 % of the total curie load).
The ratio for RH-TRU of total curie load to gamma curie load is 2.11/2.088 = **1.01**.
The vast majority of the curie load of the RH-TRU is due to gamma emitters.
Since gamma emitters tend to be short lived this means that the RH-TRU waste curie load should rapidly (within several hundred years) decay to low levels.
The average RH-TRU volumetric gamma curie load is 2.09E+06/0.25E+06 = 8.360 (Ci/cu. ft.) = **295.2 (Ci/cu. m.)**.
The average RH-TRU drum canister curie load is 295.2 (Ci/cu. m.)x 0.6246 (cu. m.) = **184.4 Ci**.
[The volume of a RH-TRU canister was set equal to three times the nominal volume of a 55-gal drum. Even though the reported volume of a RH-TRU canister is 0.89 cu. m. [Ref. BIR-1f], these canisters are loaded with three 55-gal drums internally. Ref. Lo-1.]

(m) Percent of total CH-TRU waste curie load due to gammas.

(n) Percent of total RH-TRU waste curie load due to gammas.

Table 11. Results of Shielding Calculations (RH-TRU Waste Matrix Only)

Case (a) Study	Total (b) Density [kg/m^3]	$S_v(\gamma)$ (c) [Ci(γ)/cm^3]		$S_v(total)$ (d) [Ci(total)/cm^3]	
		Option A	Option B	Option A	Option B
1) Maximum Ave (e)	793.3	2.463E-03	2.851E-03	2.489E-03	2.881E-03
2) F(68.26%) (e)	2,238.3	6.773E-03	7.773E-03	6.844E-03	7.855E-03
3) F(95.44%) (e)	2,636.0	7.977E-03	9.154E-03	8.061E-03	9.250E-03
4) F(99.74%) (e)	3,223.1	9.783E-03	1.123E-02	9.886E-03	1.135E-02
5) Worst Case (e)	6,365.4	1.926E-02	2.211E-02	1.946E-02	2.234E-02
6) 300 Watt Limit (f)	--	--	--	--	--
7) WIPP Ave	--	--	--	2.981E-04(g)	2.981E-04(g)
7b) WIPP Ave +/- 10%	--	--	--	3.279E-04(g)	3.279E-04(g)
7c) WIPP Ave +/- 100%	--	--	--	5.962E-04(g)	5.962E-04(g)
7d) WIPP Ave +/- 200%	--	--	--	8.943E-04(g)	8.943E-04(g)

(a) Results in this table correspond to steps 1 → 5 of Table 1.
(b) Values obtained from Table 7.
(c) Calculated using Equation 22c.
(d) $S_v(total) = 1.01\ S_v(\gamma)$
The total curie-to-total gamma curies ratio of 1.01 was calculated in footnote 1 of Table 10.
(e) See Table 7.
(f) 300 Watt limit from Ref. LWA-1.
(g) Calculated using footnote j in Table 10.

[3] Heat Conduction Calculations

The purpose of the heat transfer calculations is to identify if there is any significant temperature rise near the "worst-case" RH-TRU canister. Should there be a meaningful temperature increase rise, this could significantly affect thermally dependent properties. For instance, the solubility of actinides in WIPP brine could increase by about an order of magnitude for a temperature rise of ten degrees centigrade (assuming that solubility acts like many thermal-chemical properties that can be described by classical collision theory, where the collision frequency increases exponentially with increasing temperature and generally increases by an order of magnitude for each ten degree increase in temperature). The heat transfer problem was addressed by solving a simple steady-state solution. This approach would be realistic if the heat source term was constant for all time. However, the true heat source decreases with time (in fact the heat and curie loads of RH-TRU waste eventually decay to values less than that of CH-TRU waste -- see Ref. DOE-1) and performing steady-state calculations yield very conservative results. Since the volumetric heat loads identified in Table 11 were very low, using very conservative steady-state heat transfer calculations will still show low (insignificant) thermal results. The problem was solved for a two region geometry (see Figure 9).

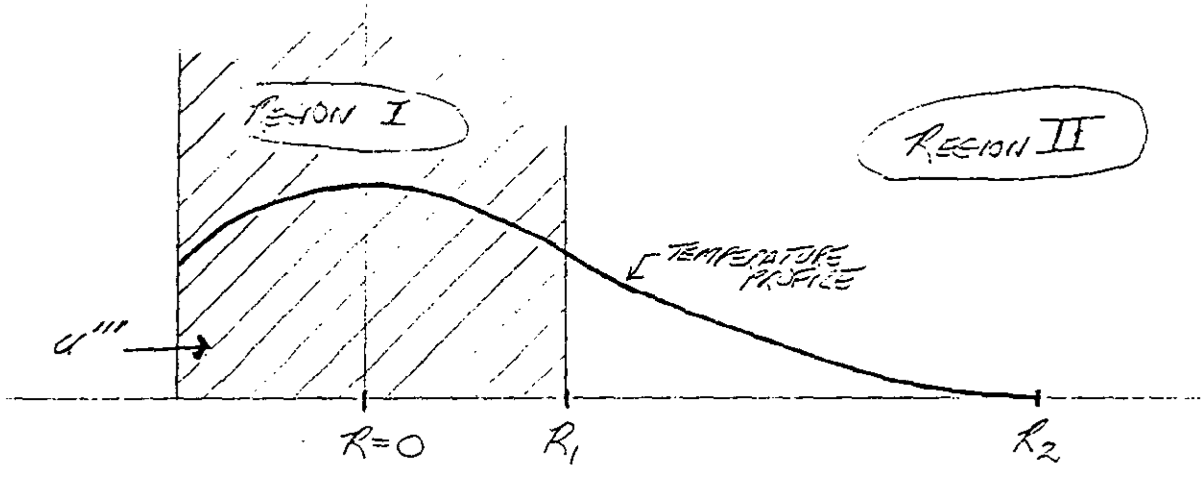


Figure 9 Geometry for two region heat conduction analyses.

The first region corresponds to a pure conduction region with a uniform heat generation source term. The second region corresponds to a pure conduction region without a heat generation source term. In both regions, the thermal conductivity is assumed to be a constant. The differential equations were derived from Equation 31 (a general form of the heat conduction equation). For the assumptions made above, this equation then becomes Equations 32 and 33.

$$\rho\, c_p \frac{dT}{d\tau} = \nabla \cdot \left\{ k\, \nabla T \right\} + u''' \qquad [31]$$

where

$u''' = heat\ source\ load\quad [W/m^3]$
$k = thermal\ conductivity\quad [W/m-K]$
$\rho = material\ density\quad [kg/m^3]$
$c_p = material\ specific\ heat\quad [J/kg-K]$
$T = temperature\quad [K]$
$\tau = time\quad [\text{sec}]$

$$\frac{d}{dr}\left\{ r\,\frac{dT^I}{dr} \right\} + r\,\frac{u'''}{k_I} = 0 \qquad [for\ Region\ I,\quad steady-state] \qquad [32]$$

$$\frac{d}{dr}\left\{ r\,\frac{dT^{II}}{dr} \right\} = 0 \qquad [for\ Region\ II,\quad steady-state] \qquad [33]$$

Performing a change of variable, changing to a ΔT via Equation 34, yields Equations 35 and 36.

$$\Theta = \Delta T = T - T_\infty \qquad (d\Theta = dT) \qquad [34]$$

$$\frac{d}{dr}\left\{ r\,\frac{d\Theta^I}{dr} \right\} + r\,\frac{u'''}{k_I} = 0 \qquad [for\ Region\ I] \qquad [35]$$

$$\frac{d}{dr}\left\{ r\,\frac{d\Theta^{II}}{dr} \right\} = 0 \qquad [for\ Region\ II] \qquad [36]$$

The general solutions to these equations are given by Equations 37 and 38.

$$\Theta^I = -\frac{r^2}{4}\,\frac{u'''}{k_I} + C_1 ln(r) + C_2 \qquad [37]$$

$$\Theta^{II} = C_3 ln(r) + C_4 \qquad [38]$$

The necessary boundary conditions are given by Equations 39 → 42 (note, boundary condition # 4 corresponds to the sphere of influence for this boundary value problem).

$$B.C.\#1 \qquad \frac{d\Theta^I}{dr}\,\Big|_{r=0} = 0 \qquad [39]$$

$$B.C.\#2 \qquad k_I\,\frac{d\Theta^I}{dr}\,\Big|_{r=R_1} = k_{II}\,\frac{d\Theta^{II}}{dr}\,\Big|_{r=R_1} \qquad [40]$$

$$B.C.\#3 \qquad \Theta^I\,\Big|_{r=R_1} = \Theta^{II}\,\Big|_{r=R_1} \qquad [41]$$

$$B.C.\#4 \qquad \Theta^I\,\Big|_{r=R_2} = 0 \qquad [42]$$

Applying boundary conditions is shown in Equations 43 → 46 which yield the particular solutions shown in Equations 47 and 48.

$$Applying\quad B.C.\ \#1 \qquad \frac{d\Theta^I}{dr}\,\Big|_{r=0} = 0 = \frac{C_1}{r}\,\Big|_{r\to 0} \quad ☞ \quad C_1 = 0 \qquad [43]$$

Applying B.C. #4 $$\Theta^{II}\,|_{r=R_2} = 0 = C_3\,ln(R_2) + C_4 \quad \text{☞} \quad C_4 = -C_3 ln(R_2) \qquad [44]$$

Applying B.C. #2 $$k_I \frac{d\Theta^I}{dr}\,|_{r=R_1} = k_{II}\frac{d\Theta^{II}}{dr}\,|_{r=R_1} = \frac{-R_1 u'''}{2} \qquad [45]$$

$$= \frac{C_3 k_{II}}{R_1} \quad \text{☞} \quad C_3 = -\frac{R_1^2 u'''}{2k_{II}}$$

Applying B.C. #3 $$\Theta^I\,|_{r=R_1} = \Theta^{II}\,|_{r=R_1} = C_2 - \frac{R_1^2 u'''}{4k_I} = C_3 \ln\left(\frac{R_1}{R_2}\right) \qquad [46]$$

$$= -\frac{R_1^2 u'''}{2k_{II}}\ln\left(\frac{R_1}{R_2}\right)$$

$$\text{☞} \quad C_2 = \frac{R_1^2 u'''}{4}\left(\frac{1}{k_I} - \frac{2}{k_{II}}\ln\left(\frac{R_1}{R_2}\right)\right)$$

$$\Theta^I = \frac{R_1^2 u'''}{4}\left(\frac{1}{k_I} - \frac{2}{k_{II}}\ln\left(\frac{R_1}{R_2}\right)\right) - \frac{r^2}{4}\frac{u'''}{k_I} \qquad [47]$$

$$\Theta^{II} = \frac{R_1^2 u'''}{2k_{II}}\ln\left(\frac{R_2}{r}\right) \qquad [48]$$

Since the Δ temperature of interest is that which occurs at $r = R_1$, evaluating either Equation 47 or 48 will yield the desired result (given by Equation 49).

$$\Theta(R_1) = \Theta^I(R_1) = \Theta^{II}(R_1) = \frac{R_1^2 u'''}{2k_{II}}\ln\left(\frac{R_2}{R_1}\right) \qquad [49]$$

Using the assumptions in Equation 50 yields the final result shown in Equation 51.

assume $$R_2 = 100\,R_1 \qquad [50]$$

$$k_{II} = k_{salt} = k_{salt\,@\,300K}$$

$$= \lambda_{300} \quad (1992\ \mathit{WIPP\ PA\ Vol}\ 3, \mathit{pg.}\ A{-}117 \quad [\mathit{Ref.WPA}{-}1]$$

$$= 5.40\ \frac{W}{mK}$$

$$R_1 = \begin{cases} 0.32385\,m. & \mathit{Option\ A} \\ 0.28580\,m & \mathit{Option\ B} \end{cases}$$

$$\Theta(R_1)\ \ [K(={}^{\circ}C)] = \Delta T(\mathit{due\ to\ max\ RH\text{-}TRU\ canister}) \qquad [51]$$

$$= \begin{cases} 0.044720817 \times u''' & \mathit{Option\ A} \\ 0.034829431 \times u''' & \mathit{Option\ B} \end{cases}$$

where

u''' *is in units of* $[W/m^3]$

Computational results using Equation 51 are shown in Table 12.

Table 12. Results of Heat Transfer Calculations

Case (a) Study	u''' (b) [$Watt/m^3$]		ΔT (c) [K]	
	Option A	Option B	Option A	Option B
1) Maximum Ave (d)	9.121E+00	1.056E+01	4.079E-01	3.678E-01
2) F(68.26%) (d)	2.508E+01	2.879E+01	1.122E+00	1.003E+00
3) F(95.44%) (d)	2.954E+01	3.390E+01	1.321E+00	1.181E+00
4) F(99.74%) (d)	3.623E+01	4.158E+01	1.620E+00	1.448E+00
5) Worst Case (d)	7.133E+01	8.186E+01	3.190E+00	2.851E+00
6) 300 Watt limit (e)	3.371E+02	4.800E+02	1.507E+01	1.672E+01
7) WIPP Ave	1.093E+00	1.093E+00	4.885E-02	3.805E-02
7b) WIPP Ave +/- 10%	1.202E+00	1.202E+00	5.374E-02	4.185E-02
7c) WIPP Ave +/- 100%	2.185E+00	2.185E+00	9.771E-02	7.610E-02
7d) WIPP Ave +/- 200%	3.277E+00	3.277E+00	1.466E-01	1.142E-01

(a) Results in this table correspond to step 6 of Table 1.
(b) Values calculated from values in Table 11, using footnote 1 of Table 9.
(d) $u''' = 0.003668E+06\ S_v(total)$
The total heat load-to-total curies ratio of 0.003668E+06 was calculated in footnote 1 of Table 10.
(c) Calculated using Equation 51.
(d) See Table 7.
(e) 300 Watt limit from Ref. LWA-1.

[4] Overall Results

The results obtained in this study (see Table 12) indicate that a negligible thermal increase is expected in the immediate vicinity of an RH-TRU canister such as those expected at the WIPP (based on Rev.1 data from the WTWBIR). The only calculated temperature difference of any significance found in this study was that associated with the 300 Watt limit. That value was computed using a simple thermal analysis that yields a conservative value (i.e., an overestimated value for the temperature difference). The other computed values have additional conservatism because the "maximum" values (see Table 7) from Rev.1 of the WTWBIR are the maximum of values of both "Stored" (legacy) and "Projected" (future) wastes, and for most cases, the maximum values estimated for projected wastes are overpredicted. In this study, the worst-case RH waste form was "Heterogeneous" waste as identified in Table 7. Unfortunately, the maximum estimated material density was extreme, namely, fifty times the average value. The extreme value for the "maximum" waste density was identified as coming from a "Projected" RH-TRU heterogeneous waste from the Battelle Columbus Laboratory (BCLDP). This waste stream may never be generated, because the funding for the project that would generate this waste stream is questionable. Moreover, the total volume from this projected waste stream is small (Table 6 indicates that the total amount of waste overall originating at BCLDP is only 71. cu.m.) and the BCLDP may have grossly overestimated the expected density of the waste stream (BCLDP does not currently have RH-TRU waste on site and they may not have a lot of experience with RH-TRU waste).

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CH-TRU plus RH-TRU. The WIPP LWA seems to be patterned after the WIPP C&C agreement [DOE-4]. It is in the WIPP C&C that a misquote was made to the WIPP ROD. The WIPP C&C quotes the WIPP ROD as applying the 6.2 million cubic meters to (all) transuranic waste. Even though the WIPP LWA is technically incorrect, the volumes identified there are to be used for WIPP calculations. More thorough discussion can be found in Ref. Sa-3.]

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Application
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INFORMATION ONLY

date: January 26, 1996

to: Martin S. Tierney (6741)

Larry Brush

from: Yifeng Wang & Larry Brush (Org. 6748)

subject: Estimates of Gas-Generation Parameters for The Long-Term WIPP Performance Assessment

Introduction

Steel corrosion and organic-material biodegradation have been identified as major gas-generation processes in the WIPP repository (Brush, 1995). Gas production will affect room closure and chemistry (Butcher, 1990; Brush, 1990). This memorandum provides the current estimates of gas-generation parameters for the long-term WIPP performance assessment. The parameters provided here include the rates of gas generation under inundated and humid conditions, the stoichiometric factors of gas generation reactions, and the probability of the occurrence of organic material biodegradation (Table 1). To satisfy the quality assurance (QA) requirement (QAP 9-5), we summarize all hand calculations for estimating these parameters in Appendices I and II.

Biodegradation of Organic Materials

Cellulosics, plastics, and rubbers have been identified as the major organic materials to be emplaced in the WIPP repository (DOE/CAO, 1996) and could be degraded by microbes in 10,000 years. Cellulosics has been demonstrated experimentally to be the most biodegradable among these materials (Francis et al., 1995). The occurrence of significant microbial gas generation in the repository will depend on: (1) whether microbes capable of consuming the emplaced organic materials will be present and active; (2) whether sufficient electron acceptors will be present and available; (3) whether enough nutrients will be present and available. Considering uncertainties in evaluation of these factors and also in order to bracket all possible effect of gas generation on the WIPP performance assessment, we assign a 50% probability to the occurrence of significant microbial gas generation.

• *Microbial Reactions*

Microorganism will consume cellulosics mainly via the following reaction pathways in the repository (Brush, 1995):

$$C_6H_{10}O_5 + 4.8\ H^+ + 4.8\ NO_3^- \rightarrow 7.4\ H_2O + 6\ CO_2 + 2.4\ N_2 \qquad (1)$$

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

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$$C_6H_{10}O_5 \rightarrow 3\ CH_4 + 3\ CO_2. \qquad (3)$$

We assume that Reactions 1 to 3 will proceed sequentially according to the energy yield of each reaction. Here we ignore the reaction pathways of aerobic respiration, Mn(IV) and Fe(III) dissimilatory reduction, since the quantities of O_2, Mn(IV) and Fe(III) initially present in the repository will be negligible relative to the other electron acceptors. In Reactions 1 to 3, biomass accumulation is also not taken into account. This is because significant biomass accumulation seems unlikely in the WIPP repository and the accumulated biomass, if any, will be recycled by microbes after all biodegradable cellulosics is consumed.

In addition to Reaction (3), methanogenesis may proceed via:

$$4\ H_2 + CO_2 \rightarrow CH_4 + 2\ H_2O. \qquad (4)$$

However, this reaction will be ignored in our calculations, because (1) no experimental data are available to evaluate the rate of this reaction and (2) the net effect of this reaction is to reduce the total gas generation and the amount of CO_2 in the repository and, therefore, it is conservative to ignore this reaction in respect of repository pressurization and actinide solubility.

- *Rates of Cellulosics Biodegradation*

The rate of cellulosics biodegradtion was measured by incubating representative cellulose materials (filter paper, paper towels, and tissue) in WIPP brine with microbes enriched from various WIPP environments (Francis & Gillow, 1994; Francis et al., 1995). The incubation experiments were conducted under various conditions: aerobic or anaerobic, inundated or humid, with or without bentonite, amended or unamended with nutrients or NO_3^-. Because the repository is expected to become anoxic shortly after waste emplacement and also because bentonite will not be added as a backfill according to the current waste emplacement plan, we think that the experimental data from anaerobic incubation without bentonite present are most relevant to expected WIPP conditions. Considering that the current experimental data are mostly for denitrification (Reaction 1), but not sulfate reduction (Reaction 2) and methanogenesis (Reaction 3) (Francis & Gillow, 1994; Francis et al., 1995), we assume that the ranges of the rates of cellulosics biodegradation via sulfate reduction and methanogenesis are equal to those observed for denitrification.

We use CO_2 production data to estimate the rates of cellulosics biodegradation. There are two advantages of using CO_2 production data: (1) there are experimental data available on the CO_2 dissolution in WIPP brine (Telander & Westerman, 1995) and, therefore, it is easy to correct the CO_2 production data for gas dissolution (Appendix I); (2) since cellulosics biodegradation did not reach the stage of methanogenesis in the experiments, according to

Reactions 1 and 2, the consumption of one mole carbon of cellulosics will produce one mole of CO_2. This 1:1 relationship is independent of oxidation state of carbon in cellulosics. Therefore, it is rather straightforward to determine the amount of cellulosics biodegraded from the amount of CO_2 produced.

Experimental data show a strong dependence of CO_2 generation on the concentrations of nutrients and nitrate (Francis & Gillow, 1994; Francis et al., 1995). The maximum CO_2 generation was observed in nitrate-and-nutrient-amended samples. In those experiments, after a short lag phase, CO_2 first linearly increased with time and then approached some limiting value as its production rate diminished. If we assume that biodegradation is nitrate- or nutrient-limited, the experimental data can be explained by Michaelis-Menton kinetics (Chapelle, 1993). Michaelis-Menton kinetics, which describes the dependence of microbial reaction rate on substrate concentration, can be expressed by:

$$V = \frac{V_{\max} S}{K_s + S} \qquad (5)$$

where V is the microbial reaction rate; $V_{\max}$ is the maximum value of the rate; S is the concentration of the limiting substrate; K_s is a constant. Equation (5) states that the microbial reaction rate becomes independent of the substrate concentration, if the latter is high enough, i.e. $S >> K_s$ and $V = V_{max}$. In this circumstance, the reaction product will accumulate linearly with time before the substrate is sufficiently depleted. In other words, in our cases, the linear part of CO_2 vs. time curve will give the estimate of the maximum rate of cellulosics biodegradation.

From the experimental data of Francis & Gillow (1994) and Francis et al. (1995), we estimate the maximum and minimum rates of cellulosics biodegradation under inundated conditions to be 0.3 and 0.01 mole C/kg/year, respectively (Appendix I). The maximum rate is estimated from the data obtained from both NO_3^-- and nutrients-amended experiments, whereas the minimum rate is derived from the data obtained from the inoculated-only experiments without any nutrient and NO_3^- amendment. Under humid conditions, experimental data show no clear correlation between CO_2 production and nutrient concentration. The best estimate of the maximum rate of cellulosics biodegradation under humid condition is 0.04 mole C/kg/year (Appendix I). The minimum of the humid biodegradation rate is set to 0, corresponding to the cases where microbes become inactive due to nutrient and water stress.

- *Biodegradation of Plastics and Rubbers*

The rates of plastics and rubber biodegradation under expected WIPP conditions were measured by Francis et al.(1995). The experimental data show that plastics and rubbers are much less biodegradable than cellulosics, although the data themselves are not sufficient for us to constrain the long-term biodegradation rate for plastics and rubbers. There are two factor that may potentially increase the biodegradibility of those materials: long time scale and cometabolism. Over a time scale of 10,000 years, plastics and rubbers may change their chemical properties and therefore their biodegradibility. Cometabolism means that microbes degrade an organic compound but do not use it as a source of energy or of their constituent elements, all of which are derived from other substrates (Alexander, 1994). In the WIPP repository, plastics and rubbers, which are resistant to biodegradation, may still be cometabolized with cellulosics and other more biodegradable organic compounds. Because of these uncertainties, we recommend a 50% chance for the biodegradation of plastics and rubbers in the event of significant microbial gas generation. We further suggest lumping plastics and rubbers into cellulosics and applying the ranges of cellulosics biodegradation rate to plastics and rubbers. This treatment is conservative in respect of repository pressurization and actinide solubility. We propose to use the following equation to convert plastics and rubbers to the carbon-equivalent quantity of cellulosics (Appendix I):

$$\text{total cellulosics (kg)} = \text{actual cellulosics (kg)} + 1.7 \text{ plastics (kg)} + \text{rubbers (kg)}. \qquad (6)$$

Anoxic Steel Corrosion

According to current waste inventory estimates, a large amount of steels will be emplaced in the WIPP repository (DOE/CAO, 1996). Those steels will be capable of reacting with the repository brine to form H_2 gas. Both thermodynamic calculations and experimental observations indicate that the H_2 gas can be generated to pressures exceeding the lithostatic pressure at the WIPP horizon, if enough brine enters the repository (Brush, 1990; Telander & Westerman, 1993, 1995). Since the repository will become anoxic shortly after waste emplacement and sealing, we here focus only on anoxic steel corrosion.

- *Steel Corrosion in the Absence of CO_2 and H_2S*

In this case, steel corrosion will follow the reaction (Telander & Westerman, 1993, 1995):

$$Fe + 2\,H_2O \rightarrow Fe(OH)_2 + H_2. \qquad (7)$$

In the Mg-rich WIPP brines (exemplified by Brine A), a significant fraction of Fe in the corrosion product is substituted by Mg. This substitution can substantially increase the stability of the corrosion product. Experimental observations indicate that steel corrosion can still proceed even at an 127 atm H_2 pressure (Telander & Westerman, 1995). Aside from this thermodynamic stability argument, the experimental observations indicate no essential effect of Mg in the brine on the corrosion rate. As a matter of fact, the corrosion rates measured in Mg-rich Brine A are not significantly different from those measured in Mg-depleted Brine ERDA-6 (Telander & Westerman, 1995).

It was observed in the experiments that the steel corrosion rate decreased with time until some limiting rate was achieved (Telander & Westerman, 1995). Our long-term corrosion rate is estimated from the longest-term data available in a WIPP-relevant Brine A environment. The estimated inundated rate is 0.5 μm/year or 0.07 mole Fe /m^2/year (Appendix II). In addition, the corrosion rate is also found to increase with decreasing brine pH (Telander & Westerman, 1993, 1995). Without addition of CO_2 from microbial reactions, the pH in the repository is unlikely to go below its experimental value, which is about 10 (Telander & Westerman, 1993, 1995). Therefore, we recommend using 0.5 μm/year as the upper limit of inundated corrosion rate for the cases without microbial gas generation. On the other hand, the pH in the repository can be ~2 units higher than its experimental value due to the presence of $Ca(OH)_2$ as a cementious material in the waste, and thus, based on the scaling factor (= 0.01) given by Telander & Westerman (1995), the steel corrosion rate could be as low as 0.005 μm/year. In addition, the experimental work *for Source Term Test Program (STTP) at Los Alamose National Laboratory indicates that* salt crystallization on steel surface may possibly prevent the steel from corrosion. To include this possibility, we set the minimum inundated steel corrosion rate to 0.

The corrosion rate observed on specimens exposed to humid conditions is negligible, based on essentially non-existent presence of corrosion product and lack of apparent H_2 generation (Telander & Westerman, 1995). Therefore, we set the humid steel corrosion rate to 0.

- *Steel Corrosion in the Presence of CO_2 and H_2S*

In the event of significant microbial gas generation, steel corrosion can proceed via the following reactions in addition to Reaction (7) (Telander & Westerman, 1993, 1995):

$$Fe + CO_2 + H_2O \rightarrow FeCO_3 + H_2 \qquad (8)$$
$$Fe + H_2S \rightarrow FeS + H_2. \qquad (9)$$

One possible effect of CO_2 and H_2S on steel corrosion is that they may cause passivation of the steel. Steel passivation was observed in the experiments in which large quantities of CO_2 and H_2S were added to the reaction vessels. It usually took place after tens of days and was caused by the formation of a protective layer of $FeCO_3$ or FeS on steel surfaces (Telander & Westerman, 1995). However, we think that this passivation is unlikely to occur under the repository conditions. This is because the microbial production rate of CO_2 and H_2S is too slow and it will take an exceedingly long time period (relative to the experimental time scale) for these gases in the repository to reach their concentration levels required for passivation under the experimental conditions. The conclusion of no steel passivation under the WIPP repository conditions is consistent with other studies (e.g., Ikeda et al., 1983; Schmitt, 1983). In fact, aside from the previously cited work of Telander & Westerman (1993), total passivation of steel by CO_2 and H_2S in low-temperature solutions has not been reported, though varying degrees of corrosion inhibition have been observed.

In the absence of passivation, the microbial generation of CO_2 and H_2S will increase steel corrosion rates in the repository either by lowering the repository pH or by initiating additional reaction pathways (Reactions 8 and 9) (Telander & Westerman, 1995). We take this effect into account by modifying the sampling range of steel corrosion rate. Obviously, Reactions 8 and 9 will be limited by microbial CO_2 and H_2S production, and therefore the upper limit of the reaction rate can be estimated from the maximum cellulosics biodegradation rate, which is 0.3 mole/kg cellulosics/year, equivalent to 6 μm/year of steel corrosion rate (Appendix II). Thus, in the event of significant microbial gas generation, the upper limit of steel corrosion rate is 6.5 μm/year, the sum of the maximum rates of Reactions 7 through 9. The corresponding lower limit will be kept the same as that estimated for the cases without CO_2 production, i.e. 0.0 μm/year. Under humid conditions, experimental results show a negligible effect of CO_2 and H_2S on steel corrosion (Telander & Westerman, 1995). We thus set the humid corrosion rate to 0.

Stoichiometric Factors in the Average-Stoichiometry Model

In the Average-Stoichiometry Model, which is currently implemented in BRAGFLO, microbial gas generation is represented by the overall reaction:

$$\frac{1}{6}C_6H_{10}O_5 \ + \ unknown \ \rightarrow \ y \ gas \ + \ unknown \qquad (10)$$

and H_2 production due to steel corrosion is described by:

$$\mathrm{Fe} + \frac{4+2x}{3}\,\mathrm{H_2O} \rightarrow \frac{4-x}{3}\,\mathrm{H_2} + x\,\mathrm{Fe(OH)_2} + \frac{1-x}{3}\,\mathrm{Fe_3O_4}. \qquad (11)$$

The stoichiometric factors x and y in Reaction 10 and 11 are estimated as follows.

- *Average-Stoichiometric FactorY in Microbial Reaction*

The stoichiometric factor y depends on the extent of the progress of each individual reaction pathway (Reactions 1 through 3). It can be estimated based on the inventory estimates of the transuranic waste to be emplaced in the Waste Isolation Pilot Plant (DOE/CAO, 1996; Drez, 1996).

First, we estimate the maximum quantities (in moles) of cellulosics and steels that will be potentially consumed in 10,000 years:

$$M_{cel}^{\prime} = \min \left\{ \frac{6000 M_{cel}}{162},\ 10000 R_{C}^{\prime} M_{cel} \right\} \tag{12}$$

$$M_{Fe}^{\prime} = \min \left\{ \frac{1000 M_{Fe}}{56},\ 1410 R_{c,i} A \right\} \tag{13}$$

with

$$R_{c}^{\prime} = \max \left\{ R_{m,i},\ R_{m,h} \right\} \tag{14}$$

where M_{cel} and M_{Fe} are the quantities (in kg) of cellulosics and steels initially present in the repository; $R_{c,i}$ is the inundated steel-corrosion rate (µm/year); $R_{m,i}$ and $R_{m,h}$ are the sampled rates of cellulosics biodegradation under inundated and humid conditions respectively (mole/kg/year). In Equation (13), we use the factor of 0.141 mole/µm/m^2 to convert steel-corrosion-rate unit from µm/year to mole/m^2/year (Telander and Westerman, 1995). Here, we assume that cellulosics biodegradation and steel corrosion both follow zero order reaction kinetics. Next, we calculate the average stoichiometric factor y by distributing $M_{cel}^{\prime}$ into individual biodegradation pathways. Consider two extreme cases, corresponding to the maximum and minimum values of y: (1) no reaction of microbially produced CO_2 and H_2S with steel and steel-corrosion products; (2) complete reaction of microbially produced CO_2 and H_2S with steel and steel-corrosion products.

If no CO_2 or H_2S is consumed by reactions with steel and steel-corrosion products, we would expect the maximum quantity of microbial gas production in the repository and therefore the maximum value for y. We assume that Reactions 1 to 3 will proceed sequentially. The maximum value of y can be estimated by averaging the gas-yields for all reaction pathways:

$$y_{\max} = \frac{\dfrac{8.4 M_{NO3}}{4.8} + \dfrac{9 M_{SO4}}{3} + \left(M_{cel}^{\prime} - \dfrac{6 M_{NO3}}{4.8} - \dfrac{6 M_{SO4}}{3} \right)}{M_{cel}^{\prime}} \tag{15}$$

where M_{NO3} and M_{SO4} are the quantities of NO_3^- and SO_4^{2-} (in moles) initially present in the repository.

If CO_2 or H_2S reacts with steel and steel-corrosion products, we expect that a significant quantity or, perhaps, all of these microbially produced gases would be consumed, thus forming $FeCO_3$ and FeS. This would result in the minimum value of y. The total gas consumed by those reactions (G) is:

$$G = \min\left\{\frac{6M_{NO3}}{4.8} + \frac{9M_{SO4}}{3} + \frac{3}{6}\left(M'_{cel} - \frac{6M_{NO3}}{4.8} - \frac{6M_{SO4}}{3}\right),\ M'_{Fe}\right\} \tag{16}$$

The minimum value of y can then be estimated by:

$$y_{\min} = \frac{\frac{8.4M_{NO3}}{4.8} + \frac{9M_{SO4}}{3} + \left(M'_{cel} - \frac{6M_{NO3}}{4.8} - \frac{6M_{SO4}}{3}\right) - G}{M'_{cel}} = y_{\max} - \frac{G}{M'_{cel}} \tag{17}$$

For each BRAGFLO simulation, y will be uniformly sampled over $[y_{\min}, y_{\max}]$:

$$y = y_{\min} + \beta(y_{\max} - y_{\min}) \tag{18}$$

with $0 \le \beta \le 1.0$. The calculational scheme proposed here automatically correlates y with waste inventory estimates as well as with reaction rates.

The above calculational scheme does not take into account the SO_4^{2-} that will be brought into repository by brine inflow. Based the previous BRAGFLO simulations for undisturbed cases, the total volume of the brine entering the repository in 10000 years is unlikely to be larger than $2.2\text{x}10^7$ liters, the value corresponding to the case with unrealistically low gas generation and therefore the worst repository flooding. With a typical SO_4^{2-} concentration of 200 mM in WIPP brines (Brush, 1990), we estimate that the amount of SO_4^{2-} brought into the repository by brine inflow would be less than $0.4\text{x}10^7$ moles. This amount of SO_4^{2-} will increase the fraction of sulfate reduction pathway in total cellulosics biodegradation only by less than 1%. Therefore, neglecting the sulfate brought by brine inflow would introduce an error of no more than a few percents in y values.

• *Average-Stoichiometric FactorX in Steel Corrosion Reaction*

While magnetite (Fe_3O_4) has been observed to form on steel as a corrosion product in low-Mg anoxic brines at elevated temperatures (Telander & Westerman, 1995) and in oxic brine (Haberman & Frydrych, 1988), there is no evidence that it will form at WIPP repository temperatures. If Fe_3O_4 were to form, it would be expected that H_2 would be produced (on a molar basis) in excess of Fe consumed. But, the anoxic corrosion experiments did not show the production of H_2 in excess of Fe reacted. Therefore, we set the stoichiometric factor x to 1.0 in Reaction 11.

Table 1. Gas-Generation Parameters for the Long-Term WIPP Performance Assessment

Parameter	Estimated Value
Probability of occurrence of significant microbial gas generation	50%
Probability of occurrence of plastics and rubber biodegradation in the event of significant gas generation	50%
Rate of inundated cellulosics biodegradation	0.01 - 0.3 mole C/kg/year
Rate of humid cellulosics biodegradation	0.0 - 0.04 mole C/kg/year
Rate of inundated steel corrosion for the cases without microbial gas generation	0.0 - 0.5 μm/year[1]
Rate of humid steel corrosion for the cases without microbial gas generation	0.0 μm/year
Rate of inundated steel corrosion for the cases with microbial gas generation	0.0 - 6.5 μm/year
Rate of humid steel corrosion for the cases with microbial gas generation	0.0 μm/year
Stoichiometric factor x in Reaction 11	1.0
Stoichiometric factor y in Reaction 10	calculated from Eqn. (18)
Factor β in Equation 18	0 - 1.0
NO_3^- initially present in the waste[2]	2.6×10^7 moles
SO_4^{2-} initial present in the waste[2]	6.6×10^6 moles

1. Multiplying 0.141 mole/μm/m^2 will convert the unit of steel corrosion rate from μm/year to mole/m^2/year (Telander & Westerman, 1993). 2. See Appendix I.6.

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Appendix I. Hand Calculations for Estimating Microbial Gas generation Parameters

Name of person performing the calculations: Yifeng Wang, Jan. 26, 1996 Yifg W
Name of person reviewing the calculations: Larry Brush, Jan. 26, 1996 Larry Brush

I.1 Correction for CO_2 Dissolution in the Brine

Data and definition of variables:

TCO_2: Total CO_2 produced in an incubating experiment (moles)
n: Measured CO_2 in headspace (moles)
C_l: Dissolved CO_2 (moles/l)
V_l: Brine volume = 0.104 (l) (Gillow, per. comm.)
V_g: Headspace volume 0.046 (l) (Francis & Gillow, 1994)
P: Partial pressure of CO_2 (atm)
K: Partition coefficient of CO_2 between brine and gas phase = 0.01 (mole/l/atm) (Telander & Westerman, 1995)
R: Gas constant = 0.082 (l•atm/mole/K)
T: Temperature = 303.15 (K)

Assumption: Gaseous CO_2 approximately follows the idea gas law during these experiments.

Calculations:

$$TCO_2 = V_l*C_l + n = K*P*V_l + n = K*V_l*n*R*T/V_g + n = (K*V_l*R*T/V_g + 1)*n = (0.01*0.104*0.082*303.15/0.046 + 1)*n = 1.56*n \text{ (moles)}.$$

I.2 Estimate of the Maximum Inundated Cellulosics Biodegradation Rate

Data:

Source: Francis et al. 1995, p. 41, 148-149.
Experimental conditions: anaerobic inoculated, nutrients and nitrate amended

We only take the linear part of CO_2 vs. time curve:

time	CO_2
69 days	6.1 µmol/g of cel.
411 days	163 µmol/g of cel.

Calculations:

(1) Rate = (163 - 6.1)/(411 - 69) = 0.459 micro-moles/g/day = 0.168 mole/kg/year.
(2) Correcting it for dissolved CO_2 (see I.1), we finally have:
maximum rate = 0.168*1.56 = 0.3 mole/kg/year.

I.3 Estimate of the Minimum Inundated Cellulosics Biodegradation Rate

Data:

Source: Francis et al. 1995, p. 148-149.
Experimental conditions: anaerobic, inoculated only,

time	CO_2
0 days	2.1 µmol/g of cel.
1034 days	14.0 µmol/g of cel.

Calculations:

(1) Rate = (14.0 - 2.1)/(1034 - 0) = 0.0115 µmol/g/day = 0.004 mole/kg/year.
(2) Correcting it for dissolved CO_2 (Appendix I.1), we finally have:
minimum rate = 0.004*1.56 = 0.01 mole/kg/year.

I.4 Estimate of the Maximum Humid Cellulosics Biodegradation Rate

Data:

Source: Francis et al. 1995, p. 80.
Experimental conditions: anaerobic, inoculated only;
anaerobic, inoculated and amended

time	CO_2
6 days	(7.7 + 13.3)/2 = 10.5 µmol/g of cel.
415 days	(83.1 + 28.8)/2 = 56 µmol/g of cel.

Calculations:

Maximum rate = (56 - 10.5)/(415 - 6) = 0.11µmol/g/day = 0.04 mole/kg/year.

I.5 Convert Plastics and Rubbers to the Equivalent Quantity of Cellulosics

Data:

Source: Molecke (1979)

Celllulosics: $C_6H_{10}O_5$	M. W. = 162 g/mole
Polyethylene: $(-C_2H_4-)n$	M. W. = 28 g/mole
Polyvinychloride: $(-C_2H_3Cl-)n$	M. W. = 62 g/mole
Neoprene: $(-C_4H_5Cl-)n$	M. W. = 88 g/mole
Hypalon: $(-(C_7H_{13}Cl)_{12}-(CHSO_2Cl)_{17}-]n$	M. W. = 3488 g/mole

Assumption:

Plastics: 80% polyethylene, 20% polyvinychloride
Rubbers: 50% neoprene, 50% hypalon
Based on Molecke (1979).

Calculations:

The P kilograms of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:

$$Q = (0.8*2*162/28/6 + 0.2*2*162/62/6)*P + (0.5*4*162/88/6 + 0.5*101*162/3488/6)*R = 1.7\ P + R \text{ (kilograms)}$$

I.6 Moles of NO_3^- and SO_4^{2-} Initially Present in the Waste

NO_3^- : 1.62×10^6 kg (Drez, 1996) = $1000/62*1.62\times10^6 = 2.6\times10^7$ moles
SO_4^{2-} : 6.33×10^5 kg (Drez, 1996) = $1000/96*6.33\times10^5 = 6.6\times10^6$ moles

Appendix II. Hand Calculations for Estimating Steel Corrosion Parameters

Name of person performing the calculations: Yifeng Wang, Jan. 26, 1996
Name of person reviewing the calculations: Larry Brush, Jan. 26, 1996 Larry Brus

II.1 Estimate of the Maximum Inundated Steel Corrosion Rate for the Cases without Microbial Gas Generation

Data:

(1) Anoxic corrosion rate obtained from the 12th to 24th month experimental data = 0.71 μm/year (Telander & Westerman, 1993, p. 6-14).
(2) Scaling factor for the long-term rate = 70% (Telander & Westerman, 1995, p. 6 - 19).

Calculation:

The maximum long-term steel corrosion rate = 0.71*70% = 0.5 μm/year.

II.2 Estimate the Maximum Inundated Steel Corrosion Rate for the Cases with Microbial Gas Generation

Data:

Total transuranic waste volume: $1.5\text{x}10^5$ m^3 (DOE/CAO, 1996)
Drum volume: 0.208 m^3 (DOE/CAO, 1996)
Surface area of steel: 6 m^2/drum (Brush, 1995)
Maximum cellulosics biodegradation rate: 0.3 mole/kg/year (Appendix I.2)
Maximum inundated steel corrosion rate for the cases without microbial gas generation: 0.5 μm/year.
Total cellulosics (including plastics and rubbers): $2.1\text{x}10^7$ kg (DOE/CAO, 1996; Appendix I.5)
NO_3^- initially present in the waste: $2.6\text{x}10^7$ moles (Appendix I.6)
SO_4^{2-} initial present in the waste: $6.6\text{x}10^6$ moles (Appendix I.6)

Assumption:

Reactions 8 and 9 will be limited by microbial CO_2 and H_2S production rate.

Calculations:

(1) Number of drums = $1.5\text{x}10^5/0.208 = 7.2\text{x}10^5$ drums.
(2) Total moles of C in cellulosics = $6*2.1\text{x}10^7*1000/162 = 7.74\text{x}10^8$ moles of C.

Molar fraction of cellulosics biodegraded via denitrification =
$2.6x10^{7}/7.74x10^{8} = 3\%$.
Molar fraction of cellulosics biodegraded via sulfate reduction =
$6.6x10^{6}/7.74x10^{8} = 1\%$.

(3) Maximum CO_2 and H_2S production rate for the whole repository = (0.03 + 1.5*0.01 + 0.5*0.96)*0.3*2.1x10^{7} = 3.3x10^{6} moles CO2/year.

(4) Total steel surface area = 6*7.2x10^{5} = 4.32x10^{6} m^{2}.

(5) The maximum rate of steel corrosion via Reactions 8 and 9 = 3.3x10^{6}/4.32x10^{6} = 0.8 mole Fe/m^{2}/year = 6 µm/year.

(6) The upper limit of inundated steel corrosion rate for the cases with microbial gas generation = 0.5 + 6 = 6.5 µm/year.

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Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

WCA Attachment WCA.8.18

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WPO36044

Sandia National Laboratories

Albuquerque, New Mexico 87185-1341

date: March 13, 1996

to: R. Vann Bynum 6831 MS 1395

from: Kurt Larson 6751 MS 1341

subject: Brine-Waste contact volumes for scoping analysis of organic ligand concentration

You requested information on the volume of brine required in the repository prior to possible release, for the purpose of estimating bounds to the possible concentration of organic ligands.

I have discussed your question with Palmer Vaughn and Peter Swift, and suggest the following.

In general, assume that a 75% brine saturation is required in any unit volume of waste prior to releases being possible up an intrusion borehole. It is considered that this is a lower but still reasonable value, in that such a high gas saturation (25%) would likely segregate brine near the base of any region intersected by a borehole and effectively prevent upward flow. In other words, higher saturations would likely be required to initiate and sustain flow upward through a borehole, but can't be proven at this time given your need for immediate information on this subject.

There are two time scales that you should be aware of with respect to brine contacting waste. In the long-term and for undisturbed conditions, it is reasonable and the project position that no barriers constructed within the repository will be effective in isolating regions from fluid flow.

In the short time frame, perhaps up to two hundred years, panel closures, or closures on other scales such as the room scale (if constructed), will be relatively effective in isolating the intersected, closed off volume from the rest of the repository volume. This is especially true if boreholes are assigned high permeabilities in PA. High permeability boreholes could allow saturation with Castile brine of intruded waste regions because flow into them could occur more rapidly than flow through closures would drain the intruded area. Because a project position on borehole properties has not been established, I cannot speculate further.

In the following table, I present excavation volumes, and consolidated void volumes for several divisions of the repository. These volumes are taken from or calculated based on [1] Sandia WIPP Project, (1992, V. 3, 3-4) and [2] Freeze et al., (1995, 2-7 to 2-8).

Scale	Excavated Volume m^3	Room Equivalents	Consolidated Porosity[1]	Consolidated Void Volume m^3	Brine Volume (saturation) m^3
room	3644. [1]	1	0.22 [2]	343. [2]	257. (75%)
exterior panel	46100. [1]	12.65	0.22 [2]	4339.	3254. (75%)
waste region	420881.[2] [1]	116	0.22 [2]	39788.	29841. (75%)

[1] assumes no gas generation, a bounding case

[2] excluding panel closure volume

References:

Freeze, G.A., Larson, K.W., and Davies, P.B., 1995. A Summary of Methods for Approximating Salt Creep and Disposal Room Closure in Numerical Models of Multiphase Flow. CENT.-0251. Albuquerque, NM: Sandia National Laboratories.

Sandia WIPP Project, 1992. Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. CENT.-0700/3. Albuquerque, NM: Sandia National Laboratories.

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