APPENDIX A

APPENDIX A - 1

Sandia National Laboratories

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

date : November 6, 1995

to : R. L. Bisping, DOE/CAO, WQC 3, MS-560

from : L. C. Sanchez, Org 6342, MS-1328 (505)848-0685

subject : **CH and RH-TRU Waste Parameters Potentially Important in WIPP PA**

A) **Requested PA Data From TWBIR**

Below you will find an updated list of waste material parameters that have been identified as being potentially important to the performance analysis of the WIPP repository. It is requested that these parameters be be supplied in Rev. 2 of the Transuranic Waste Baseline Inventory Report (TWBIR). Itemized below you will find the two categories of requested waste parameter data.

1) **Non-radioactive Materials**
The non-radioactive materials are those which influence gas generation potential and those that are needed for mechanical models which predict waste consolidation and shear strength properties. The list of the non-radioactive materials is shown in Table 1.

2) **Radionuclide**
At this time there are no new requests for additional radionuclide inventory data beyond those previously reported in Rev. 1 of the WTWBIR. If there are significant inventory increases in radionuclides due to special circumstances (such as inclusion of residues to the TRU inventory), sufficient footnote explanations should be supplied.

Table 1. Justification of TWBIR Nonradioactive Waste Parameters.

Waste Parameter	Input Variable in Current PA Models		Input Variable in PA Models Under Development	Input Variable in Possible Future PA Models
	Gas Generation	Mechanical Characteristics		
Iron-Based Metals and Alloys	X	X	X	X
Aluminum-Based Metals and Alloys (a)		X	X	
Other Metals		X		?
Other Inorganics		X		?
Cellulosics	X	X	X	X
Plastics	½ (b)	X	X (d)	X
Rubbers	½ (b)	X	X (e)	X
Solidified Inorganics		X	X	X
Solidified Organics Matrix		X	X	X
Soils (c)		X	?	?

(a) Future model for PA does not include aluminum.
(b) Only one-half of material is assumed to generate gas.
(c) May impact colloids.
(d) As is.
(e) Percentage of material to generate gas is unknown at the present time.

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 2. Justification of Special Request Non-PA Non-Radioactive Waste Materials. (a)

Waste Parameter	Input Variable in Current PA Models		Input Variable in PA Models Under Development	Input Variable in Possible Future PA Models
	Gas Generation	Mechanical Characteristics		
Vitrified (b)		X	?	?
Nitrates (NO_3)	X (c)		X	?
Sulfates (SO_4)	X (c)		X	?
Phosphorus	X (c)		X	?
Cement (d)	X		X	?

(a) Information on these additional waste materials are needed for non-PA scoping calculations for assessment of their importance. These waste characteristics can be reported at the "best estimate" level.

(b) New waste parameter corresponding to treatment, identified by some of the sites, to be anticipated in the future.

(c) Input variable is of concern when predicting the rates of microbial action and is used in currently existing reaction path model, which will not become a baseline PA model.

(d) Any concrete or cement (including dry portland cement) that contains calcium oxide.

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]
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MS-1328, L.C. Sanchez (Dept. 6741)
File - SWCF-A WBS 1.1.6.2; PA; PBWAC - WIPP ACTIVITY

APPENDIX A-2

Sandia National Laboratories

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

date : January 11, 1996

to : S. Chakraborti [Science Applications International Corporation]

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

subject : **Information Needed from TWBIR (Rev. 2/Addendum)**

I have read Paul Drez's memo [Ref. DEA-1] about the Rev. 2 of the TWBIR [Ref. BIR-1]. When updated values are available, please send me a memo with the WIPP-scale values (CH & RH waste material parameters -- Tables 3-2 & 3-3 and CH & RH disposal radionuclide inventory data -- Table 3-4). [Note -- **because the anticipated volume of RH waste is much greater than the WIPP disposal volume, the proper volume that should be used to determine the average waste material parameters should be a "truncated volume", i.e., the truncated volume is equal to the existing stored waste plus only the necessary amount of projected waste necessary to reach the WIPP disposal volume limit.**] When regenerating Table 3-4, please add extra columns which also display the "total curies" (in addition to the data displaying the curie volumetric densities) for both CH & RH radionuclides. The volumes to be used for these conversions are: 1) 6.2E+06 cu.ft. = 175,584. cu.m. for CH-TRU waste and 2) 0.25E+06 cu.ft. = 7,080. cu.m. [the unit conversions for volume were done with the factor 1.0 cu.ft. = 2.832E-02 cu.m. taken from Ref. SNL-1].

5.95E+06 — OS 1-12-96

168,504. — OS 1-12-96

A second request, which should be documented in a separate memo, is that CH & RH activity loading tables be generated on a per-waste stream basis. The format for the data should look as close to that shown in Table 1 below. It is also needed that the information be made into an ASCII file and placed on a 3.5" diskette (IBM formatted). There are three versions of this table that are needed: 1) values corresponding to stored waste only, 2) values corresponding to projected waste only, and 3) values corresponding to WIPP disposal volume [Note -- remember to use the truncated volumes for the RH waste].

REFERENCES

[DEA-1]
Memo from: P. Drez (Drez Environmental Associates, DEA) to: L.C. Sanchez (Sandia National Laboratories), subject: "BIR Error", dated: January 7, 1996.

[BIR-1]
DOE (U.S. Department of Energy); Transuranic Waste Baseline Inventory Report; DOE/CAO-95-1121; Revision 2; printed December 1995.

[SNL-1]
Sandia WIPP Project. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992. Volume 3: Model Parameters (SAND92-0700/3)*, section: *Conversion Tables For SI and Common English Units*, Table 5, pg. Conversion Tables - 4. SAND92-0700/3. Albuquerque, NM: Sandia National Laboratories.

Table 1. Radionuclide Activity Loading Table
(to be used for human intrusion calculations)

TRU Type	Site ID	Waste Stream ID	Volume of Waste Stream	Curie Loading $\left[\frac{curies}{vol}\right]$	Curie Loading $[curies]$
CH	*LANL*	*LA-?001*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*LANL*	*LA-?002*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*LANL*	*LA-?003*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*LANL*	*LA-?004*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*LANL*	*LA-?005*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*LANL*	*LA-?006*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*LANL*	↓	↓	↓	↓
CH	*LANL*	--	**$\sum$ XXXXX.X**	--	**$\sum$ X.XXE+KK**
CH	*RFETS*	*RF-?001*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
CH	*RFETS*	↓	↓	↓	↓
CH	*RFETS*	--	**$\sum$ XXXXX.X**	--	**$\sum$ X.XXE+KK**
CH	↓	↓	↓	↓	↓
CH	**Total**	--	**$\sum$ XXXXX.X**	--	**$\sum$ X.XXE+KK**
RH	*LANL*	*LA-?001*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*LANL*	*LA-?002*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*LANL*	*LA-?003*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*LANL*	*LA-?004*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*LANL*	*LA-?005*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*LANL*	*LA-?006*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*LANL*	↓	↓	↓	↓
RH	*LANL*	--	**$\sum$ XXXXX.X**	--	**$\sum$ X.XXE+KK**
RH	*RFETS*	*RF-?001*	*XXXX.X*	*X.XXE-KK*	*X.XXE+KK*
RH	*RFETS*	↓	↓	↓	↓
RH	*RFETS*	--	**$\sum$ XXXXX.X**	--	**$\sum$ X.XXE+KK**
RH	↓	↓	↓	↓	↓
RH	**Total**	--	**$\sum$ XXXXX.X**	--	**$\sum$ X.XXE+KK**

LCS:6741:lcs/(96-2096)

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APPENDIX A-3

Sandia National Laboratories

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

date : January 30, 1996

to : S. Chakraborti [Science Applications International Corporation]

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

subject : **Information Needed from TWBIR (Rev. 2/Addendum)**

With regards to the two requests previously made (Ref. LCS-1), the first is no longer needed and an update is needed for the second.

Since the data in the TWBIR (Ref. BIR-1) for projected waste material parameters and radionuclide inventory is based on data for stored waste (Ref. SC-1), the first request for data values to be volume averaged using truncated volume is not necessary (i.e., it would yield the same values).

For the second request from Ref. LCS-1, it has been identified that not all the radionuclide data in the TWBIR are incorporated in the radionuclide activity loading tables which are used for the human intrusion calculations (Refs. SNL-1 & JG-1). Instead, an abbreviated list of 21 radionuclides is all that should be used to generate the curie loading table (see Table 1 of Ref. LCS-1). The list of the 21 radionuclides (for both CH and RH) are shown in Table 1 below (this list is based on Table I of Appendix of Ref. EPA-1). Also, since the projected waste data is based on stored data, values generated are needed only for WIPP disposal volumes (data separated for stored and projected data would have yielded the same values).

REFERENCES

[BIR-1]
DOE (U.S. Department of Energy); Transuranic Waste Baseline Inventory Report; DOE/CAO-95-1121; Revision 2; printed December 1995.

[EPA-1]
"Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radionactive Waste: Final Rule," 40CFR191, *Federal Register*, **50**, 38066 (1985).

[JG-1]Communications with J. Garner [Piru Assoc., SNL/Dept 6749], date: January 30, 1996.

[LCS-1]
Memo from: L.C. Sanchez (Dept. 6741) to: S. Chakraborti (Science Applications International Corporation), subject: "Information Needed from TWBIR (Rev. 2/Addendum)", dated: January 11, 1996.

[SC-1]Communications with S. Chakraborti [Science Applications International Corporation], date: January 25, 1996.

[SNL-1]
Sandia WIPP Project. 1992. *Preliminary Performance Assessment for the Waste Isolation Pilot Plant, December 1992.* (SAND92-0700),

Table 1. Radionuclides That Should Be Used To Generate Curie Loading

	Radionuclide
1	Am-241
2	Cm-248
3	Cs-137
4	Np-237
5	Pa-231
6	Pb-210
7	Pu-238
8	Pu-239
9	Pu-240
10	Pu-242
11	Pu-244
12	Ra-226
13	Sr-90
14	Th-229
15	Th-230
16	Th-232
17	U-233
18	U-234
19	U-235
20	U-236
21	U-238

LCS:6741:lcs/(96-2098)

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

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