APPENDIX B

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to : R. L. Bisping, DOE/CAO, WQIC 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.

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