APPENDIX 5.3

CH-TRU WASTE SAMPLING PROGRAMS AT DOE SITES

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5.3 CH-TRU Waste Sampling Programs at DOE Sites

5.3.1 Summary

Previous and existing sampling programs at U.S. Department of Energy (DOE) sites provide valuable information about the properties and transport parameters of retrievably stored and newly generated waste. Results from these programs have provided a basis for certifying retrievably stored waste with existing records and process knowledge as the primary source of information, and with real-time radiography (RTR) as a verification technique. Actual sampling of a statistically significant number of waste containers can then be used as secondary verification. Although these sampling programs were primarily aimed at meeting the Waste Isolation Pilot Plant Waste Acceptance Criteria (WIPP WAC), they can be extended to meet transportation requirements as well.

Sampling programs also provide a historical perspective of waste generation processes and operations at the sites. Knowledge of these can be used to address some of the issues that are transportation concerns (i.e. production of HCl from payload containers, presence of volatile organics). This Appendix provides a description of the sampling programs and their relevance to the transportation parameters.

5.3.2 Introduction

The objective of this Appendix is to summarize the past and present sampling programs for contact handled transuranic (CH-TRU) waste at sites and to demonstrate how the information obtained through these programs is applicable for qualifying waste for transport. The available data on sampling of TRU waste originates from three sources:

1) The TRU Waste Sampling Program that consists of extensive random sampling programs conducted between 1983-1985 at the Idaho National Engineering Laboratory (INEL).[1]

2) Stored Waste Examination Pilot Plant (SWEPP) Certified Waste Sampling Program conducted from 1986 to present at INEL.[2,3]

3) A controlled study of INEL retrievably stored waste to estimate gas generation rates from CH-TRU waste containers.[4]

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[1] Clements, T. L., Kudera, D. E., September 1985, "TRU Waste Sampling Program: Volume I -- Waste Characterization," EG&G-WM-6503, EG&G Idaho, Inc., Idaho Falls, Idaho.

[2] Arnold, P. M., October 1986, "EG&G Drum Sampling Program Results FY 1986," RFP 4250, Rocky Flats Plant, Golden, Colorado.

[3] Watson, L. E., December 1987, "EG&G Sampling Program Results," RFP 4251 Rocky Flats Plant, Golden, Colorado.

[4] Clements, T. L. and Kudera, D. E., September 1985, "TRU Waste Sampling Program: Volume II -- Gas Generation Studies," EG&G-WM-6503, EG&G Idaho, Inc., Idaho Falls, Idaho.

A background and summary of each of these programs will be provided with an evaluation of the aspects related to the transportation requirements.

5.3.3 TRU Waste Sampling Program at INEL

The INEL TRU Waste Sampling Program[1] randomly selected and sampled 181 TRU unvented waste (payload) containers from retrievable storage. The waste ranged in age from six months to twelve years. The main objectives of the study were to examine the waste contents both visually and by RTR to determine waste form compliance with the WIPP WAC, and to assess the validity of using RTR as a nondestructive certification technique. The sampling program included:

- Analysis of the waste container's headspace gas for composition
- Determination of the packaging configuration
- Description of the waste form
- Reporting the physical state of the waste for each item description code (IDC)

Each of these parameters was assessed by visual, analytical analysis or RTR examination.

It should be noted that the TRU Waste Sampling Program was initiated before the shipping requirements were conceived. However, most of the proposed controls for shipment of TRU waste were examined during the sampling process. These results assist in generating a database that demonstrates a safe history of handling, shipping and storage for the waste.

5.3.4 The SWEPP Sampling Program

The SWEPP Certified Waste Sampling Program has incorporated the results from the TRU Waste Sampling Program described above, to determine acceptable sample sizes. This program has been in progress since 1986, and the percentage of containers to be sampled is updated yearly to incorporate the total number of nonconformances for the previous year's input. The purpose of the SWEPP Certified Waste Sampling Program is to provide quality control in support of the waste certification process. The program consists of selecting a statistically valid portion of the TRU waste containers that have been WIPP WAC certified, and visually examining the contents for compliance. This program supplements 100% RTR of the waste containers.

The combined data from the TRU Waste Sampling Program and the FY-1986 and FY-1987 SWEPP Certified Waste Sampling Program demonstrated that, when all waste forms are taken into consideration only 3 out of 228 (1.32%) sampled containers showed nonconformances to the WIPP WAC. These were uncemented sludge drums that showed no visible liquid during RTR examination, yet actually contained liquid in excess of 0.7 gallons when examined visually. The failure to detect the liquid was because the surface movement was restricted due to formation of a solid layer. It is important to note that the visual examinations did not reveal any problems with any other WIPP WAC requirements, which include restrictions on the presence of non-radioactive pyrophoric materials, explosives, and compressed gases.

An overall WIPP WAC miscertification of 1.3% is considered acceptable for continuation of the SWEPP certification process without requiring any major changes. INEL has defined[5] the sample size and sampling frequencies for FY-1988 based on these results. Sampling 30 out of the 2,900 drums expected to be SWEPP-certified in FY-1988 is expected to give a 95% confidence level that the estimate is correct. This is based on the assumption that 2% of the SWEPP-certified drums are WIPP WAC miscertified, and the actual range of percent of miscertification is 0-7%.

5.3.5 Gas Generation Studies

The gas generation studies of the TRU Waste Sampling Program[4] were conducted to evaluate the effectiveness of different venting devices in maintaining pressure equilibrium between the payload containers and ambient conditions. In addition, concentrations of hydrogen and other gases were measured in an effort to quantify the gas generation rates in the drums.

A total of sixteen newly generated Pu-239 waste drums from the Rocky Flats Plant and six Pu-238 drums from Los Alamos National Laboratory were evaluated under controlled conditions in this study. The Pu-239 drums were vented for a period of 13 weeks and later sealed to measure gas generation rates and temporal variations in composition. Results from these studies are discussed in Section 5.3.6.4 of this Appendix.

5.3.6 Evaluation of Transportation Parameters From Sampling Programs

The transportation parameters and their methods for determination and control are described in the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC). Sampling programs provide confirmatory data on these parameters and the adequacy of the verification techniques used (records and data base, consistency of waste generation processes, RTR, etc.). The transportation parameters that can be addressed in a sampling program are listed below, and each is discussed with respect to the sampling programs below:

- Physical form
- Chemical properties
- Chemical compatibilities
- Gas distribution and pressure buildup

5.3.6.1 Physical Form

The transportation requirements for physical form are the same as WIPP WAC requirements. The previous results from the sampling programs (see Section 5.3.4) have shown the nonconformance rates for these criteria to be very low.[5]

[5] Kudera, D., 1989, Personal Communication.

5.3.6.2 Chemical Properties and Waste Type

The waste type restrictions on payload materials are described in the CH-TRAMPAC. The restrictions on non-radioactive pyrophorics and explosives are regulated by the WAC and the sampling programs show that these requirements are consistently met at the sites.

Sampling programs have demonstrated no visible deterioration of the plastic confinement layers, even for containers that have been in storage for up to fifteen years. This indicates the absence of reactive materials or corrosives in the wastes. Inspections performed on the drums verified that they had not deteriorated appreciably during storage.

All of the content codes from DOE sites are grouped into waste material types (e.g., solidified aqueous or homogeneous inorganic solids, solid inorganics, solid organics, and solidified organics), based on their gas generation potential, which is quantified by the effective G values (see Appendix 3.2 of the CH-TRU Payload Appendices). In order to conform to these limits, the chemicals/materials within a given waste material type are restricted. The waste material types are further classified into shipping categories depending on the type of the payload container and the bagging configuration. The correlations between content codes and shipping categories are listed in the CH-TRU Waste Content Codes (CH-TRUCON) document. Only compatible waste content codes are included in the CH-TRUCON document and considered for transport. The TRU Waste Sampling Program discovered only one payload container in 181 of the sampled containers to have been assigned an incorrect IDC that would have resulted in a change of shipping categories. These results indicated that procedural controls and process technology information have ensured compliance with the waste type restrictions.

5.3.6.3 Chemical Compatibility

5.3.6.3.1 Chemical Compatibility within Payload Containers

Payload materials must be chemically compatible with each other and with the materials of construction of the packaging ICV. The TRU waste sampling program at INEL included examination of several drums that had been in storage for up to fifteen years. No effects of any adverse chemical reactions were detected in any of these drums. Waste containers generated in 1973 and sampled in 1988 showed little or no chemical deterioration of the inner confinement layers, except for coloring of the plastic bags in some cases.[6] The sampling of WAC certified drums in the SWEPP Sampling Program also showed no evidence of adverse chemical reactions. The results of these sampling programs indicate that the waste materials are chemically compatible with themselves and with the payload containers. The detailed chemical compatibility analysis performed on waste from each DOE site demonstrates that no appreciable chemical reactions will occur in the wastes or between the wastes and the payload containers. Details of this analysis are presented in Appendix 6.1 of the CH-TRU Payload Appendices.

[6] Roggenthen, D. K., McFeeters, T. L., Nieweg, R. G., March 1989 (in Press), "Waste Drum Gas Generation Sampling Program at Rocky Flats During FY 1988," RFP-4311, Rocky Flats Plant, Golden, Colorado.

5.3.6.3.2 Occurrence of Free Chlorides

None of the sampling programs reported the presence of HCl gas in the headspace of the sampled containers or (where applicable) in the inner confinement layers. The production of HCl gas is of concern due to its potential for causing stress corrosion cracking of the package. Actual waste data shows that even though HCl production is possible, it is highly improbable that gaseous HCl would ever be produced and released from the payload containers. An analysis of the source terms and release conditions for HCl in the payload materials is presented in Appendix 6.2 of the CH-TRU Payload Appendices.

5.3.6.3.3 Occurrence of Volatile Organic Compounds

Sampling programs also provide information on the relative amounts of volatile organic compounds (VOCs) in the payload materials. VOCs are a concern due to potential incompatibilities with the butyl rubber O-rings of the packaging and due to the potential for pressure buildup from their vapor pressures. A detailed discussion of the existing information on VOCs in the waste from sampling programs is presented in Appendix 6.4 of the CH-TRU Payload Appendices. Results from the sampling programs listed above are:

- The source term for VOCs in the waste is limited.
- Headspace concentrations of VOCs in the payload containers are below the range for saturation values.
- Even in the case of organic sludges (which contain the VOCs in bound form and belong to the test category) the release of the VOCs from the waste is limited.
- VOC release rates from the payload containers are extremely small and the effects of any interaction between the VOCs and the butyl rubber O-rings would be minimal and not affect the sealing properties.
- Ongoing sampling programs show that compared to retrievably stored waste, newly generated waste has much lower concentrations of the VOCs.

5.3.6.4 Gas Concentrations and Pressure Build-Up

Generation of gases from the payload materials is of concern due to the potential for pressure buildup and the occurrence of potentially flammable mixtures of gases. The controls in place to restrict these parameters are described in the CH-TRAMPAC, and are summarized below:

- Restrictions on materials that can be present within each payload (limits on hydrogen generation potential of waste materials).
- Limits on the number of internal layers of confinement within each payload container.
- Limits on the decay heat within each payload container.

The relevance of the sampling programs to each of these parameters is addressed below.

5.3.6.4.1 Restrictions on Materials

The restriction on the materials that can be present in a payload is addressed in Section 5.3.6.2 of this document. Sampling programs show that for waste that is certified to the WAC, the waste type restrictions are consistently met, and none of the sampling programs showed any effects of chemical activity within the drums.

5.3.6.4.2 Restrictions on Packaging Configuration

The second listed control is a packaging requirement, which restricts the maximum number of plastic bag layers that can be present for a given content code. This number is defined for each content code in the CH-TRUCON document. The TRU Waste Sampling Program[1] conducted at INEL documented packaging configurations for each payload container sampled. This includes information on the number and type of liner bags and bagout bags used for waste packaging. This data has provided a basis for the retrievably stored waste to be qualified for shipment. The packaging requirements listed in the CH-TRUCON document for each content code (and correlating IDCs) are consistent with the reported data from the TRU Waste Sampling Program.

5.3.6.4.3 Restrictions on Decay Heat

This parameter controls gas generation in the payload containers by limiting the decay heat of the radionuclides in each shipping category. These decay heats are determined based on an effective G value for generation of flammable gas for each shipping category. An analysis of effective G values measured for real wastes is provided in Appendix 3.1 of the CH-TRU Payload Appendices. An average G value in any waste type (I, II, III) was consistently less than the effective G values being used to establish possible hydrogen generation rates. Experimental results on estimates for hydrogen release rates are provided in Appendix 6.8 of the CH-TRU Payload Appendices. The radionuclide content of a payload container is restricted such that given the release rates and the effective G values, the hydrogen concentration will not exceed 5% in any of the confinement layers. The concentrations of hydrogen predicted in these calculations are derived using steady-state assumptions, and are much higher than those that could be produced in an average drum in a given shipping category. For example, the wattage limit on a drum of Waste Type III with four layers of plastic is 0.0207 watts, or 6.89 grams of weapons grade plutonium.

Sampling programs mentioned above have shown that containers at steady-state with much higher decay heat loadings had hydrogen concentrations well below 5% for payload containers belonging to an analytical category. Especially for retrievably stored waste that had not been vented, the analytical calculations show hydrogen concentrations much greater than the actual measured concentrations. The observed low concentrations could be due to lower hydrogen production rates, matrix depletion (reduction in the G value with time) and/or the escape of hydrogen from the payload containers. Very few of the sealed drums in the sampling programs were overpressurized, indicating possibly low gas generation rates, simultaneous consumption of oxygen or periodic leakage of gas from the drums due to overpressurization (the drums were not vented).

5.3.7 Complexity of Real Waste Sampling

For visual inspection of the waste contents, necessary precautions must be taken to ensure the safety of personnel performing the task. In the handling of materials contaminated with TRU radionuclides, a barrier is always in place between the individual and the radioactive materials (e.g., glove boxes, gloves, bubblesuits, etc). Whenever a waste container is opened for sampling or inspection, necessary precautions must be taken to prevent contamination from the radioactive material. Sites have, in the past, utilized containment structures under ventilation control with the individuals in supplied-air bubblesuits to open and inspect the waste contents. Although the internal exposures have been low, the sites have changed their waste handling techniques by developing in some cases multi-million dollar remote handling concepts to prevent this potential exposure. Due to the unique difficulties associated with actual sampling of the waste (i.e., additional potential exposure to workers and generation of excessive waste as byproduct of waste sampling), alternate and effective nondestructive techniques are necessary to supply the primary source of information on the waste. Visual inspection on a limited basis can then serve as a supplemental verification system.

5.3.8 Conclusions

The following conclusions can be drawn from the waste characterization data obtained through the various sampling programs:

1) A transportation qualification process using a statistical sampling approach is valid for retrievably stored waste when 100% RTR is supplemented with visual examination sampling programs.

2) The use of an RTR system is an adequate non-destructive certification technique for meeting certain WAC requirements, as described in this appendix.

3) Process knowledge, existing records and database information adequately provide primary sources for characterizing the shipping parameter requirements of stored waste. RTR and sampling programs can serve as secondary verification techniques.

4) Existing data on the sampling of real waste and ongoing sampling programs can be used to assess the potential for gas generation and to quantify effective G values.

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APPENDIX 6.1

CHEMICAL COMPATIBILITY OF WASTE FORMS

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6.1 Chemical Compatibility of Waste Forms

6.1.1 Introduction

This appendix describes the method used for demonstrating chemical compatibility in a given payload container, within a given waste type, and among waste types to simulate mixing of waste during hypothetical accident conditions.

6.1.2 Chemical Compatibility Analyses

The chemical compatibility analysis was performed using the methods described in the U.S. Environmental Protection Agency (EPA) document "A Method for Determining the Compatibility of Hazardous Wastes."[1] Content codes are classified as 'incompatible' if the potential exists for any of the following reactions:

- explosion
- heat generation
- gas generation (flammable gases)
- pressure build up (nonflammable gases)
- toxic by-product generation
- fire
- violent polymerization
- solubilization of toxic substances.

Note: Solubilization of toxic substances and toxic byproduct generation is not directly a concern for transportation of waste in the TRUPACT-II or HalfPACT but has been included for completeness.

Each generator and storage site has produced a comprehensive list of chemicals present in an approved content code. The chemical components found in each waste generation process are determined by examining the process technology, by chemical analysis, or by process flow analysis. Under this system, all chemical inputs into the system are accounted for, even though all of these components may not be a part of the waste. For example, generator sites might include both acids and bases in their lists, even though the two groups have been neutralized prior to placement in a payload container.

The chemical concentration levels are reported as either Trace (T)(<1% by weight), Minor (M)(1-10%), or Dominant (D)(>10%). The list is divided into groups based on chemical properties and structure (e.g., acids, caustics, metals, etc.). Table 6.1-1 lists all the groups and their number designations. As noted in the table, the groups and examples listed are only for illustrative purposes, and do not necessarily represent components of waste materials in a payload. A listing of chemicals allowed in the waste in quantities >1% (weight) by waste

[1] Hatayama, H.K., J.J. Chen, E.R. deVera, R.D. Stephens, and D.L. Storm, 1980, "A Method for Determining the Compatibility of Hazardous Wastes," EPA-600/2-80-076, U.S. Environmental Protection Agency, Cincinnati, Ohio.

material type is provided in Section 4.3 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC). Other chemicals or materials not identified in the lists of allowable materials (Tables 4.3-1 through 4.3-8 in the CH-TRAMPAC) as specified by Section 4.3 of the CH-TRAMPAC are restricted to less than 5 weight percent total.

Table 6.1-1 — EPA List of Chemical Groups and Materials*

Group Number	Group Name	Example
1	Acids, Mineral, Non-Oxidizing	Hydrochloric Acid
2	Acids, Mineral, Oxidizing	Nitric Acid (>1%)
3	Acids, Organic	Acetic Acid
4	Alcohols and Glycols	Methanol
5	Aldehydes	Formaldehyde
6	Amides	Acetamide
7	Amines, Aliphatic and Aromatic	Aniline
8	Azo Compounds, Diazo Compounds and Hydrazines	Hydrazine
9	Carbamates	Carbaryl
10	Caustics	Sodium Hydroxide
11	Cyanides	Potassium Cyanide
12	Dithiocarbamates	Maneb
13	Esters	Vinyl Acetate
14	Ethers	Tetrahydrofuran
15	Fluorides, Inorganic	Potassium Fluoride
16	Hydrocarbons, Aromatic	Toluene
17	Halogenated Organics	Carbon Tetrachloride
18	Isocyanates	Methyl Isocyanate
19	Ketones	Acetone
20	Mercaptans and other Organic Sulfides	Carbon Disulfide
21	Metals, Alkali and Alkaline Earth, Elemental	Metallic Sodium
22	Metals, other Elemental and Alloys in the form of Powders, Vapors or Sponges	Titanium
23	Metals, other Elemental and Alloys as Sheets, Rods, Moldings, Drops, etc.	Aluminum
24	Metals and Metal Compounds, Toxic	Beryllium
25	Nitrides	Sodium Nitride
26	Nitriles	Acetonitrile
27	Nitro Compounds	Dinitrobenzene
28	Hydrocarbons, Aliphatic, Unsaturated	Butadiene
29	Hydrocarbons, Aliphatic, Saturated	Cyclohexane
30	Peroxides and Hydroperoxides Organic	Acetyl Peroxide
31	Phenols, Cresols	Phenol

Table 6.1-1 — EPA List of Chemical Groups and Materials[a] (Continued)

Group Number	Group Name	Example
32	Organophosphates, Phosphothioates, and Phosphodithioates	Malathion
33	Sulfides, Inorganic	Zinc Sulfide
34	Epoxides	Epoxybutane
101	Combustible and Flammable Materials, Miscellaneous	Cellulose
102	Explosives	Ammonium Nitrate
103	Polymerizable Compounds	Acrylonitrile
104	Oxidizing Agents, Strong	Hydrogen Peroxide
105	Reducing Agents, Strong	Metallic Sodium
106	Water and Mixtures Containing Water	Water
107	Water Reactive Substances	Sulfuric Acid (>70%)

a Modified from "A Method for Determining the Compatibility of Hazardous Wastes." [1]

NOTE: The chemical groups and materials listed in this table are a comprehensive listing of chemical compounds that may be incompatible. This is not meant to infer that all the listed chemical compounds and materials are present in TRU waste.

Interactions between compounds present in trace quantities (<1 percent by weight) and compounds present in concentrations ≥1 percent by weight (i.e., D x T, M x T, or T x T) do not pose an incompatibility problem for the following reasons:

- The trace chemicals reported by the sites are in concentrations well below the trace limit of less than 1 weight percent. An example is the volatile organic compounds (VOCs) discussed in detail in Appendix 6.4 of the CH-TRU Payload Appendices. Sampling programs show that the concentration levels of these compounds are significantly lower than the upper limit of 1%.

- The trace chemicals are usually dispersed in the waste, which further dilutes concentrations of these materials.

- Trace chemicals that might be incompatible with materials/chemicals >1 weight percent would have reacted during the waste generating process prior to placement in payload containers.

- Because of restrictions imposed by the EPA on reporting of hazardous wastes, some chemicals are listed in trace quantities even if they have already reacted. Hazardous waste regulations as promulgated by the EPA[2] (known as the mixture rule) require that a mixture of any solid waste and a hazardous waste listed in 40 CFR Part 261, Subpart D

[2] U.S. Environmental Protection Agency, Title 40, Code of Federal Regulations, Part 261, Subpart D, U.S Environmental Protection Agency, Washington, D.C.

be considered a hazardous waste subject to RCRA regulations. However, Subpart D does not list minimum concentrations for these listed wastes, with the result that any such mixtures must be considered hazardous waste even if the Subpart D constituent is at or below detection limits.

- The waste is either solidified and immobilized (solidified materials) or present in bulk form as a solid (solid materials). In almost all cases, any possible reactions take place before the waste is generated in its final form.

As specified in the CH-TRAMPAC, the total quantity of chemicals/materials not listed as allowed materials for a given waste material type in any payload container is restricted to less than 5 weight percent total. Potential incompatibilities between minor and dominant compounds have been analyzed for the payload using the lists of allowable materials for each waste material type in Section 4.3 of the CH-TRAMPAC. The analysis combined the lists of allowable materials for all waste material types (to simulate a bounding case where different waste material types may be shipped together in a package) and assigned EPA chemical reactivity group numbers and names to each allowable constituent. The reactivity group numbers were assigned based on information provided in Hatayama, et al.[1] If the allowable material (or chemical) is a non-reactive inorganic material (not covered under the EPA reactivity group numbers), it was assigned a reactivity group number of "0" to reflect a complete analysis for all allowable materials (materials assigned a reactivity group number of "0" do not present a compatibility concern). The compiled list of allowable materials and assigned reactivity group numbers is provided in Attachment A of this appendix.

The list of allowable materials and assigned reactivity group numbers was sorted by reactivity group number and then condensed to form a list of the represented reactivity groups (Attachment B of this appendix).

Using the list of represented reactivity groups, a hazardous waste compatibility chart was generated. The chart, which is provided in Attachment C, is a reduced version of the hazardous waste compatibility chart presented in Hatayama, et al.[1] The chart summarizes the potential types of reactions possible between each of the reactivity groups represented in the lists of allowable materials for each waste material type. The reaction codes and consequences of the reactions are specified for each combination of two reactivity groups.

Using the hazardous waste compatibility chart, a list of potential chemical incompatibilities in the TRU waste was generated. The list, which is presented in Attachment D, also presents explanations why the reaction associated with each of the potential chemical incompatibilities will not occur.

The results of the analysis demonstrate chemical compatibility across all waste material types (I.1, I.2, I.3, II.1, II.2, II.3, III.1, III.2, III.3, and IV.1). As previously discussed, each content code is required to have an associated chemical list. Chemical incompatibilities do not exist in approved content codes. This has been ensured by a knowledge of the processes generating the wastes and the chemical compatibility analysis described in this appendix. The chemical constituents present in quantities >1% (weight) (documented as minor and dominant quantities)

in the chemical list associated with each content code are evaluated for compliance with the list of allowable materials for the appropriate waste material type specified in Section 4.3 of the CH-TRAMPAC. Only content codes with chemical lists that have been evaluated by this process and determined to be compatible shall be approved for shipment in the package. As described in Section 4.3 of the CH-TRAMPAC, any change to the chemical list of an approved content code, as well as requests for additional waste forms, must be submitted to the Cognizant Engineer for evaluation for compliance with the lists of allowable materials of the CH-TRAMPAC.

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Attachment A
Lists of Allowable Materials and Associated Reactivity Groups

Lists of Allowable Materials and Associated Reactivity Groups

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
I.1	Absorbents/adsorbents (e.g., Celite®, diatomaceous earth, diatomite, Florco®, Oil-Dri®, perlite, vermiculite)	Other solidification materials and absorbents/adsorbents	0
I.1	***Acids, inorganic***	Acids, Mineral, Non-oxidizing	1
I.1	***Acids, inorganic***	Acids, Mineral, Oxidizing	2
I.1	Alumina cement	Water reactive substance	107
I.1	Aquaset® products (for aqueous solutions)	Other solidification materials and absorbents/adsorbents	0
I.1	Aqueous sludges	Other solidification materials and absorbents/adsorbents	0
I.1	Aqueous solutions/water	Water and Mixtures containing water	106
I.1	Asbestos	Other Inorganics (non-reactive)	0
I.1	Ash (e.g., ash bottoms, fly ash, soot)	Other Inorganics (non-reactive)	0
I.1	Batteries, dry (e.g., flashlight)	Metals, alkali and alkaline earth, elemental and alloys	21
I.1	Ceramics (e.g., molds and crucibles)	Other Inorganics (non-reactive)	0
I.1	Clays (e.g., bentonite)	Other Inorganics (non-reactive)	0
I.1	Concrete	Other solidification materials and absorbents/adsorbents	0
I.1	Envirostone® (no organic emulsifiers allowed)	Other solidification materials and absorbents/adsorbents	0
I.1	Fiberglass, inorganic	Other Inorganics (non-reactive)	0
I.1	Filter media, inorganic	Other Inorganics (non-reactive)	0
I.1	Firebrick	Other Inorganics (non-reactive)	0
I.1	Glass (e.g., borosilicate glass, labware, leaded glass, Raschig rings)	Other Inorganics (non-reactive)	0
I.1	Graphite (e.g., molds and crucibles)	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
I.1	Grit	Other Inorganics (non-reactive)	0
I.1	Heel (e.g., ash heel; soot heel; firebrick heel; sand, slag, and crucible heel)	Other Inorganics (non-reactive)	0
I.1	Insulation, inorganic	Other Inorganics (non-reactive)	0
I.1	Magnesia cement (e.g., Ramcote® cement)	Water reactive substance	107
I.1	Metal hydroxides	Other Inorganics (non-reactive)	0
I.1	Metal oxides (e.g., slag)	Other Inorganics (non-reactive)	0
I.1	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
I.1	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental and alloy in the form of powders, vapors, or sponges	22

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
I.1	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals and metal compounds, toxic	24
I.1	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Reducing agents, strong	105
I.1	Nitrates (e.g., ammonium nitrate, sodium nitrate)	Oxidizing Agents, Strong	104
I.1	Petroset® products (for aqueous solutions)	Other solidification materials and absorbents/adsorbents	0
I.1	***Portland cement***	Water reactive substance	107
I.1	***Portland cement***	Caustics	10
I.1	Sand/soil, inorganic	Other Inorganics (non-reactive)	0
I.1	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Other Inorganics (non-reactive)	0
I.1	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Fluorides, inorganic	15
I.1	Other inorganic materials	Other Inorganics (non-reactive)	0
I.2	Absorbents/adsorbents (e.g., Celite®, diatomaceous earth, diatomite, Florco®, Oil-Dri®, perlite, vermiculite)	Other solidification materials and absorbents/adsorbents	0
I.2	Alumina cement	Water reactive substance	107
I.2	Aquaset® products (for aqueous solutions)	Other solidification materials and absorbents/adsorbents	0
I.2	Aqueous sludges	Other solidification materials and absorbents/adsorbents	0
I.2	Aqueous solutions/water	Water and Mixtures containing water	106
I.2	Asbestos	Other Inorganics (non-reactive)	0
I.2	Ash (e.g., ash bottoms, fly ash, soot)	Other Inorganics (non-reactive)	0
I.2	Batteries, dry (e.g., flashlight)	Metals, alkali and alkaline earth, elemental and alloys	21
I.2	Ceramics (e.g., molds and crucibles)	Other Inorganics (non-reactive)	0
I.2	Clays (e.g., bentonite)	Other Inorganics (non-reactive)	0
I.2	Concrete	Other solidification materials and absorbents/adsorbents	0
I.2	Fiberglass, inorganic	Other Inorganics (non-reactive)	0
I.2	Filter media, inorganic	Other Inorganics (non-reactive)	0
I.2	Firebrick	Other Inorganics (non-reactive)	0
I.2	Glass (e.g., borosilicate glass, labware, leaded glass, Raschig rings)	Other Inorganics (non-reactive)	0
I.2	Graphite (e.g., molds and crucibles)	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
I.2	Grit	Other Inorganics (non-reactive)	0
I.2	Heel (e.g., ash heel; soot heel; firebrick heel; sand, slag, and crucible heel)	Other Inorganics (non-reactive)	0
I.2	Insulation, inorganic	Other Inorganics (non-reactive)	0

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
I.2	Magnesia cement (e.g., Ramcote® cement)	Water reactive substance	107
I.2	Metal hydroxides	Other Inorganics (non-reactive)	0
I.2	Metal oxides (e.g., slag)	Other Inorganics (non-reactive)	0
I.2	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
I.2	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental and alloy in the form of powders, vapors, or sponges	22
I.2	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals and metal compounds, toxic	24
I.2	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Reducing agents, strong	105
I.2	Nitrates (e.g., ammonium nitrate, sodium nitrate)	Oxidizing Agents, Strong	104
I.2	Petroset® products (for aqueous solutions)	Other solidification materials and absorbents/adsorbents	0
I.2	***Portland cement***	Water reactive substance	107
I.2	***Portland cement***	Caustics	10
I.2	Sand/soil, inorganic	Other Inorganics (non-reactive)	0
I.2	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Other Inorganics (non-reactive)	0
I.2	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Fluorides, inorganic	15
I.2	Other inorganic materials	Other Inorganics (non-reactive)	0
I.3	Absorbents/adsorbents (e.g., Celite®, diatomaceous earth, diatomite, Florco®, Oil-Dri®, perlite, vermiculite)	Other solidification materials and absorbents/adsorbents	0
I.3	Asbestos	Other Inorganics (non-reactive)	0
I.3	Ash (e.g., ash bottoms, fly ash, soot)	Other Inorganics (non-reactive)	0
I.3	Batteries, dry (e.g., flashlight)	Metals, alkali and alkaline earth, elemental and alloys	21
I.3	Ceramics (e.g., molds and crucibles)	Other Inorganics (non-reactive)	0
I.3	Clays (e.g., bentonite)	Other Inorganics (non-reactive)	0
I.3	Concrete	Other solidification materials and absorbents/adsorbents	0
I.3	Fiberglass, inorganic	Other Inorganics (non-reactive)	0
I.3	Filter media, inorganic	Other Inorganics (non-reactive)	0
I.3	Firebrick	Other Inorganics (non-reactive)	0
I.3	Glass (e.g., borosilicate glass, labware, leaded glass, Raschig rings)	Other Inorganics (non-reactive)	0
I.3	Graphite (e.g., molds and crucibles)	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
I.3	Grit	Other Inorganics (non-reactive)	0

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
I.3	Heel (e.g., ash heel; soot heel; firebrick heel; sand, slag, and crucible heel)	Other Inorganics (non-reactive)	0
I.3	Insulation, inorganic	Other Inorganics (non-reactive)	0
I.3	Metal hydroxides	Other Inorganics (non-reactive)	0
I.3	Metal oxides (e.g., slag)	Other Inorganics (non-reactive)	0
I.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
I.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental and alloy in the form of powders, vapors, or sponges	22
I.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals and metal compounds, toxic	24
I.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Reducing agents, strong	105
I.3	Nitrates (e.g., ammonium nitrate, sodium nitrate)	Oxidizing Agents, Strong	104
I.3	***Portland cement***	Water reactive substance	107
I.3	***Portland cement***	Caustics	10
I.3	Sand/soil, inorganic	Other Inorganics (non-reactive)	0
I.3	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Other Inorganics (non-reactive)	0
I.3	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Fluorides, inorganic	15
I.3	Water (maximum of 30 weight percent unbound water)	Water and Mixtures containing water	106
I.3	Other inorganic materials	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Absorbents/adsorbents (e.g., Celite®, Florco®, Oil-Dri®, diatomite, perlite, vermiculite)	Other solidification materials and absorbents/adsorbents	0
II.1 II.2 II.3	Asbestos	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Ash (e.g., ash bottoms, fly ash, soot)	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Batteries, dry (e.g., flashlight)	Metals, alkali and alkaline earth, elemental and alloys	21
II.1 II.2 II.3	Ceramics (e.g., molds and crucibles)	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Clays (e.g., bentonite)	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Concrete/Portland cement (surface contaminated only)	Other solidification materials and absorbents/adsorbents	0
II.1 II.2 II.3	Fiberglass, inorganic	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Filter media, inorganic	Other Inorganics (non-reactive)	0

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
II.1 II.2 II.3	Firebrick	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Glass (e.g., borosilicate glass, labware, leaded glass, Raschig rings)	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Graphite (e.g., molds and crucibles)	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
II.1 II.2 II.3	Grit	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Heel (e.g., ash heel; soot heel; firebrick heel; sand, slag, and crucible heel)	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Insulation, inorganic	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Magnesium alloy	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
II.1 II.2 II.3	Metal oxides (e.g., slag)	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
II.1 II.2 II.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals, Other elemental and alloy in the form of powders, vapors, or sponges	22
II.1 II.2 II.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Metals and metal compounds, toxic	24
II.1 II.2 II.3	***Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)***	Reducing agents, strong	105
II.1 II.2 II.3	Nitrates (e.g., ammonium nitrate, sodium nitrate)	Oxidizing Agents, Strong	104
II.1 II.2 II.3	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	***Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)***	Fluorides, inorganic	15
II.1 II.2 II.3	Sand/soil, inorganic	Other Inorganics (non-reactive)	0
II.1 II.2 II.3	Other inorganic materials	Other Inorganics (non-reactive)	0
II.3	Aqueous solutions/water	Water and Mixtures containing water	106
III.1	Absorbent polymers, organic	Combustible and flammable materials, miscellaneous	101
III.1	Acids, solid, organic	Acids, organic	3
III.1	Asphalt	Combustible and flammable materials, miscellaneous	101

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
III.1	Bakelite®	Combustible and flammable materials, miscellaneous	101
III.1	Cellulose (e.g., Benelex®, cotton Conwed®, paper, rags, rayon, wood)	Combustible and flammable materials, miscellaneous	101
III.1	Cellulose acetate butyrate	Polymerizable compounds	103
III.1	Cellulose propionate	Polymerizable compounds	103
III.1	Chlorinated polyether	Ethers	14
III.1	***Detergent, solid (e.g., emulsifiers, surfactants)***	Esters	13
III.1	***Detergent, solid (e.g., emulsifiers, surfactants)***	Hydrocarbons, Aromatic	16
III.1	***Detergent, solid (e.g., emulsifiers, surfactants)***	Hydrocarbon, aliphatic, unsaturated	28
III.1	***Detergent, solid (e.g., emulsifiers, surfactants)***	Organophosphates, phosphothioates, and phosphodithioates	32
III.1	Fiberglass, organic	Combustible and flammable materials, miscellaneous	101
III.1	Filter media, organic	Combustible and flammable materials, miscellaneous	101
III.1	Greases, commercial brands	Combustible and flammable materials, miscellaneous	101
III.1	Insulation, organic	Combustible and flammable materials, miscellaneous	101
III.1	***Leaded rubber (e.g., gloves, aprons, sheet material)***	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
III.1	***Leaded rubber (e.g., gloves, aprons, sheet material)***	Metals and metal compounds, toxic	24
III.1	***Leaded rubber (e.g., gloves, aprons, sheet material)***	Combustible and flammable materials, miscellaneous	101
III.1	Leather	Combustible and flammable materials, miscellaneous	101
III.1	Oil (e.g., petroleum, mineral)	Combustible and flammable materials, miscellaneous	101
III.1	Organophosphates (e.g., tributyl phosphate, dibutyl phosphate, monobutyl phosphite)	Organophosphates, phosphothioates, and phosphodithioates	32
III.1	Paint, dry (e.g., floor/wall paint, ALARA)	Combustible and flammable materials, miscellaneous	101
III.1	Plastics [e.g., polycarbonate, polyethylene, polymethyl methacrylate (Plexiglas®, Lucite®), polysulfone, polytetrafluoroethylene (Teflon®), polyvinyl acetate, polyvinyl chloride (PVC), polyvinylidene chloride (saran)]	Combustible and flammable materials, miscellaneous	101
III.1	***Polyamides (nylon)***	Combustible and flammable materials, miscellaneous	101
III.1	***Polyamides (nylon)***	Amides	6

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
III.1	Polychlorotrifluoroethylene (e.g., Kel-F®)	Combustible and flammable materials, miscellaneous	101
III.1	***Polyesters (e.g., Dacron®, Mylar®)***	Combustible and flammable materials, miscellaneous	101
III.1	***Polyesters (e.g., Dacron®, Mylar®)***	Esters	13
III.1	***Polyethylene glycol (e.g., Carbowax®)***	Alcohols and Glycols	4
III.1	***Polyethylene glycol (e.g., Carbowax®)***	Combustible and flammable materials, miscellaneous	101
III.1	Polyimides	Hydrocarbons, aromatic	16
III.1	Polyphenyl methacrylate	Combustible and flammable materials, miscellaneous	101
III.1	Polypropylene (e.g., Ful-Flo® filters)	Combustible and flammable materials, miscellaneous	101
III.1	Polyurethane	Combustible and flammable materials, miscellaneous	101
III.1	Polyvinyl alcohol	Alcohols and Glycols	4
III.1	***Resins (e.g., aniline-formaldehyde, melamine-formaldehyde, organic resins, phenol-formaldehyde, phenolic resins, urea-formaldehyde)***	Aldehydes	5
III.1	***Resins (e.g., aniline-formaldehyde, melamine-formaldehyde, organic resins, phenol-formaldehyde, phenolic resins, urea-formaldehyde)***	Phenols and Creosols	31
III.1	Rubber, natural or synthetic [e.g., chlorosulfonated polyethylene (Hypalon®), ethylene-propylene rubber, EPDM, polybutadiene, polychloroprene (neoprene), polyisobutylene, polyisoprene, polystyrene, rubber hydrochloride (pliofilm®)]	Combustible and flammable materials, miscellaneous	101
III.1	***Sand/Soil***	Other Inorganics (non-reactive)	0
III.1	***Sand/Soil***	Combustible and flammable materials, miscellaneous	101
III.1	Waxes, commercial brands	Combustible and flammable materials, miscellaneous	101
IV.1	Acids, organic	Acids, organic	3
IV.1	Alcohols (e.g., butanol, ethanol, isopropanol, methanol)	Alcohols and Glycols	4
IV.1	Esters (e.g., ethyl acetate, polyethylene glycol ester)	Esters	13
IV.1	Ethers (e.g., ethyl ether)	Ethers	14

Waste Material Type	Allowable Chemical/Material[a]	Reactivity Group[b]	
		Name	Number[c]
IV.1	Halogenated organics (e.g., bromoform; carbon tetrachloride; chlorobenzene; chloroform; 1,1-dichloroethane; 1,2-dichloroethane; 1,1-dichloroethylene; cis-1,2-dichloroethylene; methylene chloride; 1,1,2,2-tetrachloroethane; tetrachloroethylene; 1,1,1-trichloroethane; 1,1,2-trichloroethane; trichloroethylene; 1,1,2-trichloro-1,2,2-trifluoroethane)	Halogenated Organics	17
IV.1	***Hydrocarbons, aliphatic (e.g., cyclohexane, n-paraffin hydrocarbons)***	Hydrocarbon, aliphatic, unsaturated	28
IV.1	***Hydrocarbons, aliphatic (e.g., cyclohexane, n-paraffin hydrocarbons)***	Hydrocarbon, aliphatic, saturated	29
IV.1	Hydrocarbons, aromatic (e.g., benzene; ethyl benzene; toluene; 1,2,4-trimethylbenzene; 1,3,5-trimethylbenzene; xylene)	Hydrocarbons, aromatic	16
IV.1	Ketones (e.g., acetone, methyl ethyl ketone, methyl isobutyl ketone)	Ketones	19
IV.1	Trioctyl phosphine oxide	Organophosphates, phosphothioates, and phosphodithioates	32

[a] Chemicals in ***bold italic*** have been assigned to more than one reactivity group.
[b] Reactivity group from Hatayama, H.K., J. J. Chen, E.R. deVera, R.D. Stephens, and D.L. Storm, 1980, "A Method for Determining the Compatibility of Hazardous Wastes," EPA-600/2-80-076, U.S. Environmental Protection Agency, Cincinnati, Ohio.
[c] Non-reactive inorganic materials or chemicals are assigned a reactivity group number of "0."

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Attachment B
List of Unique Reactivity Group Numbers in Lists of Allowable Materials

List of Unique Reactivity Group Numbers in Lists of Allowable Materials

Allowable Chemical/Material[a]	Reactivity Group[b]	
	Name	Number
Absorbents/adsorbents (e.g., Celite®, diatomaceous earth, diatomite, Florco®, Oil-Dri®, perlite, vermiculite)	Other solidification materials and absorbents/adsorbents	0
Acids, inorganic	Acids, Mineral, Non-oxidizing	1
Acids, inorganic	Acids, Mineral, Oxidizing	2
Acids, solid, organic	Acids, Organic	3
Polyethylene glycol (e.g., Carbowax®)	Alcohols and Glycols	4
Resins (e.g., aniline-formaldehyde, melamine-formaldehyde, organic resins, phenol-formaldehyde, phenolic resins, urea-formaldehyde)	Aldehydes	5
Polyamides (nylon)	Amides	6
Portland cement	Caustics	10
Esters (e.g., ethyl acetate, polyethylene glycol ester)	Esters	13
Ethers (e.g., ethyl ether)	Ethers	14
Salts (e.g., calcium chloride, calcium fluoride, sodium chloride)	Fluorides, inorganic	15
Hydrocarbons, aromatic (e.g., benzene; ethyl benzene; toluene; 1,2,4-trimethylbenzene; 1,3,5-trimethylbenzene; xylene)	Hydrocarbons, aromatic	16
Halogenated organics (e.g., bromoform; carbon tetrachloride; chlorobenzene; chloroform; 1,1-dichloroethane; 1,2-dichloroethane; 1,1-dichloroethylene; cis-1,2-dichloroethylene; methylene chloride; 1,1,2,2-tetrachloroethane; tetrachloroethylene; 1,1,1-trichloroethane; 1,1,2-trichloroethane; trichloroethylene; 1,1,2-trichloro-1,2,2-trifluoroethane)	Halogenated Organics	17
Ketones (e.g., acetone, methyl ethyl ketone, methyl isobutyl ketone)	Ketones	19
Batteries, dry (e.g., flashlight)	Metals, alkali and alkaline earth, elemental and alloys	21
Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)	Metals, Other elemental and alloy in the form of powders, vapors, or sponges	22
Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)	Metals, Other elemental, and alloy, as sheets, rods, moldings, vapors, or sponges	23
Leaded rubber (e.g., gloves, aprons, sheet material)	Metals and metal compounds, toxic	24
Hydrocarbons, aliphatic (e.g., cyclohexane, n-paraffin hydrocarbons)	Hydrocarbon, aliphatic, unsaturated	28
Hydrocarbons, aliphatic (e.g., cyclohexane, n-paraffin hydrocarbons)	Hydrocarbon, aliphatic, saturated	29

Allowable Chemical/Material[a]	Reactivity Group[b]	
	Name	Number
Resins (e.g., aniline-formaldehyde, melamine-formaldehyde, organic resins, phenol-formaldehyde, phenolic resins, urea-formaldehyde)	Phenols and Creosols	31
Organophosphates (e.g., tributyl phosphate, dibutyl phosphate, monobutyl phosphite)	Organophosphates, phosphothioates, and phosphodithioates	32
Asphalt	Combustible and flammable materials, miscellaneous	101
Cellulose acetate butyrate	Polymerizable compounds	103
Nitrates (e.g., ammonium nitrate, sodium nitrate)	Oxidizing Agents, Strong	104
Metals (e.g., aluminum, cadmium, copper, steel, tantalum, tungsten, zinc)	Reducing agents, strong	105
Aqueous solutions/water	Water and Mixtures containing water	106
Portland cement	Water reactive substances	107

[a] Chemicals in ***bold italic*** have been assigned to more than one reactivity group.
[b] Reactivity group from Hatayama, H.K., J.J. Chen, E.R. deVera, R.D. Stephens, and D.L. Storm, 1980, "A Method for Determining the Compatibility of Hazardous Wastes," EPA-600/2-80-076, U.S. Environmental Protection Agency, Cincinnati, Ohio.

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Attachment C
Hazardous Waste Chemical Compatibility Chart

Waste Chemical Compatibility Chart

Group No.	Reactivity Group Name	1	2	3	4	5	6	10	13	14	15	16	17	19	21	22	23	24	28	29	31	32	101	103	104	105	106	107
1	Acids, Mineral, Non-Oxidizing	1																										
2	Acids, Mineral, Oxidizing		2																									
3	Acids, Organic		G, H	3																								
4	Alcohols and Glycols	H	H, F	H, P	4																							
5	Aldehydes	H, P	H, F	H, P		5																						
6	Amides	H	H, GT				6																					
10	Caustics	H	H	H		H		10																				
13	Esters	H	H, F					H	13																			
14	Ethers	H	H, F							14																		
15	Fluorides, Inorganic	GT	GT	GT							15																	
16	Hydrocarbons, Aromatic		H, F									16																
17	Halogenated Organics	H, GT	H, F, GT				H, GT	H					17															
19	Ketones	H	H, F					H						19														
21	Metals, Alkali and Alkaline Earth, Elemental	GF, H, F	GF, H, F	GF, H, F	GF, H, F	GF, H, F	GF, H	GF, H	GF, H				H, E	GF, H	21													
22	Metals, Other Elemental and Alloys as Powders, Vapors, or Sponges	GF, H, F	GF, H, F	GF				GF, H					H, E			22												
23	Metals, Other Elemental and Alloys as Sheets, Rods, Drops, Moldings, etc.	GF, H, F	GF, H, F					GF, H					H, F				23											
24	Metals and Metal Compounds, Toxic	S	S	S			S	S										24										
28	Hydrocarbons, Aliphatic, Unsaturated	H	H, F			H										H, E			28								
29	Hydrocarbons, Aliphatic, Saturated		H, F																	29								
31	Phenols and Creosols	H	H, F												GF, H						31							
32	Organophosphates, Phosphothioates, Phosphodithioates	H, GT	H, GT					H, E							H							32						
101	Combustible and Flammable Materials, Miscellaneous	H, G	H, F, GT												H, G, F								101					
103	Polymerizable Compounds	P, H	P, H	P, H				P, H							P, H	P, H	P, H	P, H			P, H			103				
104	Oxidizing Agents, Strong	H, GT		H, GT	H, F	H, F	H, F, GT		H, F	H, F		H, F	H, GT	H, F	H, F, E	H, F, E	H, F		H, F	H, F	H, F	H, F, GT	H, F, G	H, F, GT	104			
105	Reducing Agents, Strong	H, GF	H, F, GT	H, GF	H, GF, F	H, GF, F	H, GF		H, F				H, E	GF, H							GF, H	GT, GF, H	GF, H	H, P, GF	H, F, E	105			
106	Water and Mixtures Containing Water	H	H												GF, H	GF, H		S									106	
107	Water Reactive Substances	<— Extremely Reactive — Do Not Mix with Any Chemical or Waste Material — Extremely Reactive —>																										107
Reactivity Group Number		**1**	**2**	**3**	**4**	**5**	**6**	**10**	**13**	**14**	**15**	**16**	**17**	**19**	**21**	**22**	**23**	**24**	**28**	**29**	**31**	**32**	**101**	**103**	**104**	**105**	**106**	**107**

E	=	Explosion
F	=	Fire
G	=	Innocuous and Non-Flammable Gas Generation
GF	=	Flammable Gas Generation
GT	=	Toxic Gas Generation
H	=	Heat Generation
P	=	Violent Polymerization
S	=	Solubilization of Toxic Substances

Source: Hatayama, H.K., J.J. Chen, E.R. deVera, R.D. Stephens, and D L. Storm, "A Method for Determining the Compatibility of Hazardous Wastes." EPA-600/2-80-076, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1980.

Attachment D
Potential Chemical Incompatibilities

Potential Chemical Incompatibilities

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
1	4	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	5	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	5	Violent Polymerization	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	6	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	10	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; Bases/caustic materials are neutralized and solidified/immobilized prior to shipping
1	13	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	14	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	15	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	17	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	17	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	19	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	21	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	21	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	21	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	22	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	22	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	22	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	23	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	23	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	23	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	24	Solubilization of	Reaction will not occur – Acids are neutralized and

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
		Toxic Substances	solidified/immobilized prior to shipping Additionally, any solubilization of toxic substances will not affect transportation of wastes.
1	28	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	31	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	32	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	32	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	101	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	101	Innocuous and Non-Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	103	Violent Polymerization	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	103	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
1	104	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
1	104	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
1	105	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
1	105	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
1	106	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
1	107	Highly Reactive	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
2	3	Innocuous and Non-Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	3	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	4	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	4	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	5	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	5	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	6	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	6	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	10	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; Bases/caustic materials are neutralized and solidified/immobilized prior to shipping
2	13	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	13	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	14	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	14	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	15	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	16	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	16	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
2	17	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	17	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	17	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	19	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	19	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	21	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	21	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	21	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	22	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	22	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	22	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	23	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	23	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	23	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	24	Solubilization of Toxic Substances	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping Additionally, any solubilization of toxic substances will not affect transportation of wastes.
2	28	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	28	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	29	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	29	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	31	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	31	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
2	32	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	32	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	101	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	101	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	101	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	103	Violent Polymerization	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	103	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
2	105	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
2	105	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
2	105	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
2	106	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume
2	107	Highly Reactive	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
3	4	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	4	Violent Polymerization	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	5	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	5	Violent Polymerization	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
3	10	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; Bases/caustic materials are neutralized and solidified/immobilized prior to shipping
3	15	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	21	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	21	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	21	Fire	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	22	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	24	Solubilization of Toxic Substances	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping Additionally, any solubilization of toxic substances will not affect transportation of wastes.
3	103	Violent Polymerization	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	103	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping
3	104	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
3	104	Toxic Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
3	105	Heat Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
3	105	Flammable Gas Generation	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
3	107	Highly Reactive	Reaction will not occur – Acids are neutralized and solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
4	21	Flammable Gas Generation	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping
4	21	Heat Generation	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping
4	21	Fire	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping
4	104	Heat Generation	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
4	104	Fire	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
4	105	Heat Generation	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
4	105	Flammable Gas Generation	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
4	105	Fire	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
4	107	Highly Reactive	Reaction will not occur – Alcohols and Glycols are solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
5	10	Heat Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; bases/caustic materials are neutralized and solidified/immobilized prior to shipping
5	21	Flammable Gas Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping
5	21	Heat Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping
5	21	Fire	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
5	28	Heat Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping
5	104	Heat Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
5	104	Fire	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
5	105	Heat Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
5	105	Flammable Gas Generation	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
5	105	Fire	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
5	107	Highly Reactive	Reaction will not occur – Aldehydes are solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
6	17	Heat Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping
6	17	Toxic Gas Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping
6	21	Flammable Gas Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping
6	21	Heat Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping
6	24	Solubilization of Toxic Substances	Reaction will not occur – Amides are solidified/immobilized prior to shipping Additionally, any solubilization of toxic substances will not affect transportation of wastes.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
6	104	Heat Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
6	104	Fire	Reaction will not occur – Amides are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
6	104	Toxic Gas Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
6	105	Heat Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
6	105	Flammable Gas Generation	Reaction will not occur – Amides are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
6	107	Highly Reactive	Reaction will not occur – Amides are solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
10	13	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	17	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	19	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	21	Flammable Gas Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	21	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
10	22	Flammable Gas Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	22	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	23	Flammable Gas Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	23	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	24	Solubilization of Toxic Substances	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping; Additionally, any solubilization of toxic substances will not affect transportation of wastes.
10	32	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	32	Explosion	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	103	Violent Polymerization	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	103	Heat Generation	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping
10	107	Highly Reactive	Reaction will not occur – Caustics/bases are neutralized and solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
13	21	Flammable Gas Generation	Reaction will not occur – Esters are solidified/immobilized prior to shipping
13	21	Heat Generation	Reaction will not occur – Esters are solidified/immobilized prior to shipping
13	104	Heat Generation	Reaction will not occur – Esters are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
13	104	Fire	Reaction will not occur – Esters are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
13	105	Heat Generation	Reaction will not occur – Esters are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
13	105	Fire	Reaction will not occur – Esters are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
13	107	Highly Reactive	Reaction will not occur – Esters are solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
14	104	Heat Generation	Reaction will not occur – Ethers are solidified / immobilized prior to shipping. Oxidizing agents are reacted prior to being placed in the waste/shipped.
14	104	Fire	Reaction will not occur – Ethers are solidified / immobilized prior to shipping. Oxidizing agents are reacted prior to being placed in the waste/shipped.
14	107	Highly Reactive	Reaction will not occur – Ethers are solidified / immobilized prior to shipping. Free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
15	107	Highly Reactive	Reaction will not occur – Salts are reacted during use and processing; Free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
16	104	Heat Generation	Reaction will not occur – Aromatic hydrocarbons are solidified/immobilized prior to shipping. Oxidizing agents are reacted prior to being placed in the waste/shipped.
16	104	Fire	Reaction will not occur – Aromatic hydrocarbons are solidified/immobilized prior to shipping. Oxidizing agents are reacted prior to being placed in the waste/shipped.
16	107	Highly Reactive	Reaction will not occur – Aromatic hydrocarbons are solidified/immobilized prior to shipping. Free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
17	21	Heat Generation	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping
17	21	Explosion	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping
17	22	Heat Generation	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping
17	22	Explosion	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping
17	23	Heat Generation	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping
17	23	Fire	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping
17	104	Heat Generation	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
17	104	Toxic Gas Generation	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
17	105	Heat Generation	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
17	105	Explosion	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
17	107	Highly Reactive	Reaction will not occur – Halogenated organics are solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
19	21	Flammable Gas Generation	Reaction will not occur – Ketones are solidified/immobilized prior to shipping
19	21	Heat Generation	Reaction will not occur – Ketones are solidified/immobilized prior to shipping
19	104	Heat Generation	Reaction will not occur –Ketones are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
19	104	Fire	Reaction will not occur –Ketones are solidified/immobilized prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped.
19	105	Flammable Gas Generation	Reaction will not occur –Ketones are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
19	105	Heat Generation	Reaction will not occur –Ketones are solidified/immobilized prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped.
19	107	Highly Reactive	Reaction will not occur – Ketones are solidified/immobilized prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
21	31	Flammable Gas Generation	Reaction will not occur – Phenols and Creosols are solidified/immobilized prior to shipping; metals are typically in oxide form
21	31	Heat Generation	Reaction will not occur – Phenols and Creosols are solidified/immobilized prior to shipping; metals are typically in oxide form

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
21	32	Heat Generation	Reaction will not occur – Organophosphates are solidified/immobilized prior to shipping; metals are typically in oxide form
21	101	Heat Generation	Reaction will not occur – Combustible materials are dry; free liquid content is limited to less than 1% of waste volume; metals are typically in oxide form
21	101	Innocuous and Non-Flammable Gas Generation	Reaction will not occur – Combustible materials are dry; free liquid content is limited to less than 1% of waste volume; metals are typically in oxide form
21	101	Fire	Reaction will not occur – Combustible materials are dry; free liquid content is limited to less than 1% of waste volume; metals are typically in oxide form
21	103	Violent Polymerization	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; metals are typically in oxide form
21	103	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; metals are typically in oxide form
21	104	Heat Generation	Reaction will not occur –Oxidizing agents are reacted prior to being placed in the waste/shipped; metals are typically in oxide form
21	104	Fire	Reaction will not occur –Oxidizing agents are reacted prior to being placed in the waste/shipped; metals are typically in oxide form
21	104	Explosion	Reaction will not occur –Oxidizing agents are reacted prior to being placed in the waste/shipped; metals are typically in oxide form
21	106	Flammable Gas Generation	Reaction will not occur – Free liquids are limited to less than 1% of waste volume; metals are typically in oxide form.
21	106	Heat Generation	Reaction will not occur – Free liquids are limited to less than 1% of waste volume; metals are typically in oxide form.
21	107	Highly Reactive	Reaction will not occur – Metals are typically in oxide form; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
22	28	Heat Generation	Reaction will not occur – Unsaturated aliphatic hydrocarbons are solidified/immobilized prior to shipping
22	28	Explosion	Reaction will not occur – Unsaturated aliphatic hydrocarbons are solidified/immobilized prior to shipping

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
22	103	Violent Polymerization	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping
22	103	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping
22	104	Heat Generation	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped
22	104	Fire	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped
22	104	Explosion	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped
22	106	Flammable Gas Generation	Reaction will not occur – Free liquids are limited to less than 1% of waste volume; water reactive metals are reacted prior to shipping
22	106	Heat Generation	Reaction will not occur – Free liquids are limited to less than 1% of waste volume; water reactive metals are reacted prior to shipping
22	107	Highly Reactive	Reaction will not occur –Water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
23	103	Violent Polymerization	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping
23	103	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping
23	104	Heat Generation	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped
23	104	Fire	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped
23	107	Highly Reactive	Reaction will not occur –Water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
24	103	Violent Polymerization	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping
24	103	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping
24	106	Solubilization of Toxic Substances	Reaction will not occur – Free liquid content is limited to less than 1% of waste volume; Additionally, any solubilization of toxic substances will not affect transportation of wastes.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
24	107	Highly Reactive	Reaction will not occur – Water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
28	104	Heat Generation	Reaction will not occur – Unsaturated aliphatic hydrocarbons are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
28	104	Fire	Reaction will not occur – Unsaturated aliphatic hydrocarbons are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
28	107	Highly Reactive	Reaction will not occur – Unsaturated aliphatic hydrocarbons are immobilized/solidified prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
29	104	Heat Generation	Reaction will not occur – Saturated aliphatic hydrocarbons are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
29	104	Fire	Reaction will not occur – Saturated aliphatic hydrocarbons are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
29	107	Highly Reactive	Reaction will not occur – Saturated aliphatic hydrocarbons are immobilized/solidified prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
31	103	Violent Polymerization	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; phenols and creosols are immobilized/solidified prior to shipping
31	103	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; phenols and creosols are immobilized/solidified prior to shipping
31	104	Heat Generation	Reaction will not occur – Phenols and creosols are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
31	104	Fire	Reaction will not occur – Phenols and creosols are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
31	105	Flammable Gas Generation	Reaction will not occur – Phenols and creosols are immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
31	105	Heat Generation	Reaction will not occur – Phenols and creosols are immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
31	107	Highly Reactive	Reaction will not occur – Phenols and creosols are immobilized/solidified prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
32	104	Heat Generation	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
32	104	Fire	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
32	104	Toxic Gas Generation	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
32	105	Toxic Gas Generation	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
32	105	Flammable Gas Generation	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
32	105	Heat Generation	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
32	107	Highly Reactive	Reaction will not occur – Organophosphates are immobilized/solidified prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
101	104	Heat Generation	Reaction will not occur – Combustible materials are dry; oxidizing agents are reacted prior to being placed in the waste/shipped
101	104	Fire	Reaction will not occur – Combustible materials are dry; oxidizing agents are reacted prior to being placed in the waste/shipped
101	104	Innocuous and Non-Flammable Gas Generation	Reaction will not occur – Combustible materials are dry; oxidizing agents are reacted prior to being placed in the waste/shipped
101	105	Flammable Gas Generation	Reaction will not occur – Combustible materials are dry; reducing agents are reacted prior to being placed in the waste/shipped
101	105	Heat Generation	Reaction will not occur – Combustible materials are dry; reducing agents are reacted prior to being placed in the waste/shipped
101	107	Highly Reactive	Reaction will not occur – Combustible materials are dry; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
103	104	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
103	104	Fire	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
103	104	Toxic Gas Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; oxidizing agents are reacted prior to being placed in the waste/shipped
103	105	Heat Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
103	105	Violent Polymerization	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
103	105	Flammable Gas Generation	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; reducing agents are reacted prior to being placed in the waste/shipped
103	107	Highly Reactive	Reaction will not occur – Polymerizable compounds are reacted or immobilized/solidified prior to shipping; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
104	105	Heat Generation	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped; reducing agents are reacted prior to being placed in the waste/shipped
104	105	Fire	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped; reducing agents are reacted prior to being placed in the waste/shipped
104	105	Explosion	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped; reducing agents are reacted prior to being placed in the waste/shipped

Combination of Reactivity Groups		Reaction Result (A x B)	Explanation of Potential Incompatibility
Group A	Group B		
104	107	Highly Reactive	Reaction will not occur – Oxidizing agents are reacted prior to being placed in the waste/shipped; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
105	106	Flammable Gas Generation	Reaction will not occur – Reducing agents are reacted prior to being placed in the waste/shipped; free liquid content is limited to less than 1% of waste volume
105	106	Toxic Gas Generation	Reaction will not occur – Reducing agents are reacted prior to being placed in the waste/shipped; free liquid content is limited to less than 1% of waste volume
105	107	Highly Reactive	Reaction will not occur – Reducing agents are reacted prior to being placed in the waste/shipped; free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.
106	107	Highly Reactive	Reaction will not occur – Free liquid content is limited to less than 1% of waste volume; water reactive substances are reacted prior to being placed in the waste/shipped. Lime in Portland cement is most common water reactive substance expected in the waste. Portland cement is used as an absorbent and solidification agent for the wastes.

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APPENDIX 6.2

FREE HALIDES IN THE CH-TRU WASTE PAYLOAD—SOURCE TERM AND RELEASE RATE ESTIMATES

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6.2 Free Halides in the CH-TRU Waste Payload-Source Term and Release Rate Estimates

6.2.1 Summary

An evaluation of source terms for halides has demonstrated that very small amounts of halides are available for chemical reaction to cause stress corrosion cracking (SCC) of the Inner Containment Vessel (ICV) of TRUPACT-II or HalfPACT. This is substantiated with sampling data from actual waste drums and radiolysis experiments conducted on TRU waste materials. Extensive sampling programs of both retrievably stored and newly generated waste did not detect hydrogen chloride (HCl) gas in the headspace of any of the payload containers. Experiments designed to simulate alpha and gamma radiolysis of actual bagging and TRU waste materials from generator sites demonstrated HCl gas generation to be very low.

These observations support the conclusions that alpha radiolysis of actual waste produces little or no HCl gas. Any small quantities of HCl gas produced are likely either to dissolve readily in any absorbed water or moisture present in the waste, or to react with the waste contents or payload containers. This will retard the release of HCl gas from the payload containers, precluding the possibility of stress corrosion cracking of the ICV.

6.2.2 Introduction

The production of free halides from radiolysis of the payload materials can potentially cause SCC of the package. The primary material of construction used for the ICV and the Outer Confinement Vessel (OCV) of the package is Type 304 stainless steel (austenitic). This material may be susceptible in the sensitized condition to SCC in the presence of chloride contamination. However, Tokiwai et al.[1], have shown 304 stainless steel to be resistant to SCC at temperatures below 55°C, even for heavily sensitized material at stresses near yield, for maximum allowable levels of NaCl concentration and relative humidities. Normal operating temperatures of the cavity headspace or ICV walls are not expected to exceed 55°C. The following discussion will provide an analysis of the source terms for the halides and their potential to reach the ICV.

6.2.3 Source Terms for Chlorides and Fluorides in Waste Material

The contaminants of concern are hydrogen chloride (HCl) and hydrogen fluoride (HF), which could originate from the radiolysis of polyvinyl chloride or halogenated organics.

6.2.3.1 Potential for Fluoride Production in Waste

Compounds containing fluorides considered as potential sources for HF gas have not been identified in the CH-TRU materials in significant amounts. Only Teflon, inorganic fluoride salts and a trace amount of Freon-113 occur in the waste, and these do not produce HF from radiolysis (Appendix 3.1 of the CH-TRU Payload Appendices).

[1] Tokiwai, M., H. Kimiura, and H. Kusangi, 1985, Corrosion Science, Vol. 25, No. 89, pp. 837-844.

6.2.3.2 Potential for Chloride Production in Waste

The potential for chloride production in the payload materials comes primarily from radiolysis of the chlorinated compounds. Volatile organic compounds (VOCs) capable of generating HCl are not present in sufficient amounts in the waste to be of concern for SCC. Appendix 6.4 of the CH-TRU Payload Appendices discusses the source terms and release rates of VOCs. The only other compound present in the waste with a potential for HCl production is polyvinyl chloride (PVC).

Experimental evidence has shown average G(HCl) (moles of HCl in the gas or liquid state released per 100 eV of energy absorbed) values for radiolysis of commercial grades of plasticized stabilized PVC to be quite small (see Appendix 3.2 of the CH-TRU Payload Appendices). Table 6.2-1 summarizes the available data on generation of HCl from radiolysis of PVC. Three independent experiments of alpha radiolysis on actual waste and packaging material from three U.S. DOE sites revealed very little or no HCl. Contact handled TRU waste to be shipped in the TRUPACT-II or HalfPACT is contaminated predominantly with alpha-emitting radionuclides. For the two gamma radiolysis experiments cited in Table 6.2-1 that measured G(HCl), the quantitative measurement was made by titration of acidity in samples with a weak base. No direct evidence of HCl gas was reported in these experiments other than a qualitative indication of Cl^-.[2]

In conclusion, radiolytic activity within the drums of CH-TRU waste will not result in the generation of any substantial amounts of HCl gas. The source term for HCl gas itself (without any consideration of transport to the ICV) is expected to be insignificant in payload containers transported in the TRUPACT-II or HalfPACT.

6.2.3.3 Gas Sampling of CH-TRU Waste Drums

Sampling programs at Idaho National Engineering Laboratory (INEL)[3] and Rocky Flats Plant[4] did not detect HF or HCl gas in the head space of any of the 249 drums of retrievably stored and newly generated TRU waste that were sampled. In addition to drum headspace sampling, twenty-two drums of retrievably stored and newly generated waste were sampled for gases within successive layers of confinement up to the innermost layer with the waste. In all cases, HF or HCl were never detected in any layers of confinement.

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[2] Kazanjian, A.R, and A.K. Brown, December 1969, "Radiation Chemistry of Materials Used in Plutonium Processing," The Dow Chemical Company, Rocky Flats Division, RFP-1376.

[3] Clements, T.L., Jr., and D.E. Kudera, September 1985, "TRU Waste Sampling Program: Volume I, Waste Characterization," EGG-WM-6503, EG&G Idaho, Inc., Idaho Falls, Idaho.

[4] Roggenthen, D.K., T.L. McFeeters, and R.A. Nieweg, March 1989, "Waste Drum Gas Generation Sampling Program at Rocky Flats During FY 1988," RFP-4311.

Table 6.2-1 — G(HCl) Values for Plasticized Polyvinyl Chloride Materials in CH-TRU Waste

	Irradiation	G(HCl)
Average G(HCl) for Plasticized PVC	α,γ	0.64[a]
Values for Materials used at U.S. DOE site		
PVC bagout bag (Los Alamos National Laboratory)[b]	α	~0[c]
Nine samples of PVC bag material (Rocky Flats Plant)[d]	γ	0.21[e]
Samples of PVC bagout material (Rocky Flats Plant)[f]	α	0
Samples of PVC gloves (Los Alamos National Laboratory)[g]	γ	0
Samples of PVC bags (Savannah River Plant)[h]	γ	<0.01[i]

a Average of 27 literature values for plasticized PVC (Appendix 3.2 of the CH-TRU Payload Appendices).

b Zerwekh, A., 1979, "Gas Generation from Radiolytic Attack of TRU- Contaminated Hydrogeneous Waste," Los Alamos National Laboratory, LA- 7674-MS, June 1979.

c Mass spectrometric analysis of gases did not detect any Cl^- or HCl. Wet chemistry analysis of material inside glass reaction vessel yielded 0.06% Cl^-.

d Kazanjian, A.R, and A.K. Brown, "Radiation Chemistry of Materials Used in Plutonium Processing," The Dow Chemical Company, Rocky Flats Division, RFP-1376, December 1969.

e Tubes of irradiated PVC were opened under water, shaken, and titrated with NaOH. The presence of chlorides in solution was identified qualitatively. Only acid content (not Cl^-) was measured quantitatively. Acid concentration in water could be due to CO_2 dissolved from atmosphere.

f Kazanjian, A. R, "Radiolytic Gas Generation in Plutonium Contaminated Waste Materials," Rockwell International, Rocky Flats Plant, RFP-2469, October 1976.

g Kosiewicz, S.T., "Gas Generation from Organic Transuranic Wastes. I. Alpha Radiolysis at Atmospheric Pressure," Nuclear Technology 54, pp. 92-99, 1981.

h Hobbs, David, Personal Communication, Savannah River Plant, Feb. 1989.

i Personal communication for ongoing experiments.

6.2.4 Mechanisms for Retardation of Chlorides Inside Payload Containers

Production of chlorides by radiolysis of waste materials in payload containers does not necessarily imply the presence of a gaseous phase. Some of the radiolysis experiments did not observe HCl gas in the void space of the experimental apparatus but did measure chlorides after washing of the interior of the reaction vessel.[5] This suggests the existence of mechanisms that can retard the release of gaseous HCl.

6.2.4.1 Solubility of HCl in Water

The presence of any free HCl that is produced in a payload container will be controlled in the headspace by the high solubility of HCl gas in water. Transfer of HCl gas to the aqueous phase occurs with very little resistance in the liquid phase and with very little back pressure of the gas.[6] For small quantities of HCl gas produced in the payload containers, the moisture content of the waste materials would probably be sufficient to absorb the gas generated.

[5] Zerwekh, A., 1979, "Gas Generation from Radiolytic Attack of TRU- Contaminated Hydrogeneous Waste," Los Alamos National Laboratory, LA- 7674-MS, June 1979.

[6] Treybal, R.E., 1980, Mass Transfer Operations, McGraw-Hill Book Company, New York, New York.

The partial pressures of gaseous HCl over aqueous solutions of HCl are extremely small even at appreciable concentrations of HCl, due to its high solubility.[6] Table 6.2-2 provides the partial pressure of HCl above HCl aqueous solutions over a wide range of temperatures.[7] The partial pressures reported in the normal operating ranges of the TRUPACT-II or HalfPACT (Table 6.2-2) would minimize the possibility of HCl being present as a gaseous phase.

Waste types to be transported in payload containers contain varying amounts of adsorbed/absorbed water as a by-product of processes (without the presence of free liquids) in addition to water vapor from atmospheric humidity inside the layers of confinement. Although water vapor was not quantitatively measured in the headspaces of the drums examined at RFP as part of the TRU waste sampling program,[3] water was noted in all gas samples.[8] Hence it is probable that any HCl produced would dissolve within the drums. It should be noted that anhydrous HCl is noncorrosive to 304 stainless steel.[9] Therefore, sufficient moisture exists in the form of adsorbed/absorbed water in layers of containment in payload containers to depress the vapor pressure of any HCl that may be present.

6.2.4.2 Reactivity of Waste Materials and Internal Surfaces of the Payload Containers

For any small quantities of HCl gas that could be present in the payload containers, it is highly unlikely that any chlorides would reach the ICV. The payload containers in which the waste is packaged are either carbon or galvanized steel. HCl is much more reactive with these materials than the 304 SS. HCl will also have an affinity for some contents of the waste. An example of this is hydrolization of cellulose, which is present in substantial amounts in the waste.[10] The small amounts of HCl produced are expected to be consumed in reactions with these materials and therefore be unavailable for transport into the ICV.

6.2.5 Conclusion

In assessing the potential for stress corrosion cracking, it is apparent that the nature of the waste and the conditions under which the waste will be transported, should preclude the possibility of producing significant quantities of free HCl gas in the payload containers. Alpha radiolysis of PVC does not produce appreciable amounts of HCl gas, and any small quantities of the gas generated are likely to be retained in the payload containers, thereby limiting transport to the ICV cavity.

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[7] Perry, C.H., and D. Green, Eds., 1984, Chemical Engineers Handbook, McGraw-Hill Book Company, New York.

[8] Simmons, Bill, Rocky Flats Plant Personal Communications, 1988.

[9] Kirk, R.E., and D.F. Othmer, Eds., 1966, Encyclopedia of Chemical Technology, Vol. 11, John Wiley and Sons, New York.

[10] Young, R. A., and R. M. Rowell, Eds., 1986, Cellulose: Structure Modification, and Hydrolysis, John Wiley and Sons, New York.

Table 6.2-2 — Partial Pressures of HCl Over Aqueous Solutions of HCl mmHg°C[a,b]

%HCL	A	B	0°	5°	10°	15°	20°	25°	30°	35°	40°	45°	50°	60°	70°	80°
2	11.8037	4736	-----	----	0.0000117	0.000023	0.000044	0.000084	0.000151	0.000275	0.00047	0.00083	0.00140	0.00380	0.0100	0
4	11.6400	4471	0.000018	0.000036	0.000069	0.000131	0.00024	0.00044	0.00077	0.00134	0.0023	0.00385	0.0064	0.0165	0.0405	0
6	11.2144	4202	0.000066	0.000125	0.000234	0.000425	0.00076	0.00131	0.00225	0.0038	0.0062	0.0102	0.163	0.040	0.094	0
8	11.0406	4042	0.000118	0.000323	0.000583	0.00104	0.00178	0.0031	0.00515	0.0085	0.0136	0.022	0.0344	0.081	0.183	0
10	10.9311	3908	0.00042	0.00075	0.00134	0.00232	0.00395	0.0067	0.0111	0.0178	0.0282	0.045	0.069	0.157	0.35	0
12	10.7900	3765	0.00099	0.00175	0.00305	0.0052	0.0088	0.0145	0.0234	0.037	0.058	0.091	0.136	0.305	0.66	1
14	10.6954	3636	0.0024	0.00415	0.0071	0.0118	0.0196	0.0316	0.050	0.078	0.121	0.185	0.275	0.60	1.25	2
16	10.6261	3516	0.0056	0.0095	0.016	0.0265	0.0428	0.0685	0.106	0.163	0.247	0.375	0.55	1.17	2.40	4
18	10.4957	3376	0.0135	0.0225	0.037	0.060	0.095	0.148	0.228	0.345	0.515	0.77	1.11	2.3	4.55	8
20	10.3833	3245	0.0316	0.052	0.084	0.132	0.205	0.32	0.48	0.72	1.06	1.55	2.21	4.4	8.5	15
22	10.3172	3125	0.0734	0.119	0.187	0.294	0.45	0.68	1.02	1.50	2.18	3.14	4.42	8.6	16.3	29
24	10.2185	2995	0.175	0.277	0.43	0.66	1.00	1.49	2.17	3.14	4.5	6.4	8.9	16.9	31.0	54
26	10.1303	2870	0.41	0.64	0.98	1.47	2.17	3.20	4.56	6.50	9.2	12.7	17.5	32.5	58.5	100
28	10.0115	2732	1.0	1.52	2.27	3.36	4.90	7.05	9.90	13.8	19.1	26.4	35.7	64	112	188
30	9.8763	2593	2.4	3.57	5.23	7.60	10.6	15.1	21.0	28.6	39.4	53	71	124	208	340
32	9.7523	2457	5.7	8.3	11.8	16.8	23.5	32.5	44.5	60.0	81	107	141	238	390	623
34	9.6061	2316	13.1	18.8	26.4	36.8	50.5	68.5	92	122	161	211	273	450	720	
36	9.5262	2229	29.0	41.0	56.4	78	105.5	142	188	246	322	416	535	860		
38	9.4670	2094	63.0	87.0	117	158	210	277	360	465	598	758	955			
40	9.2156	1939	130	176	233	307	399	515	627	830						
42	8.9925	1800	253	332	430	560	709	900								
44	8.8621	1681	510	655	840											
46	----	----	940													

[a]Perry, C.H., and D. Green, Eds., 1984 Chemical Engineers Handbook, McGraw Hill Book Company, New York, New York.

[b]$Log_{10}pmm = A - B/T$, which, however, agrees only approximately with the table. The table is more nearly correct.

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APPENDIX 6.3

PAYLOAD COMPATIBILITY WITH BUTYL RUBBER O-RING SEALS

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6.3 Payload Compatibility with Butyl Rubber O-Ring Seals

6.3.1 Summary

Payload materials and chemicals in the TRUPACT-II or HalfPACT do not present an incompatibility concern with respect to the butyl rubber O-rings. Chemicals that are of concern are not present in the waste in any significant amounts. Strong oxidizing acids are neutralized or basified prior to being generated as contact-handled transuranic (CH-TRU) waste. Organic solvents of concern that are present in residual amounts in the payload containers are usually bound with the waste materials.

6.3.2 Introduction

This appendix evaluates the compatibility of the payload materials with the butyl rubber O-rings of the package. Chemicals that are reported as potentially incompatible with the butyl rubber O-rings (for liquid immersion or in saturated vapors) include the following:

- Concentrated oxidizing acids, (e.g., nitric acid)
- Aromatic hydrocarbons, (e.g., xylene and toluene)
- Halogenated organic solvents, (e.g., 1,1,2-trichloro-1,2,2-trifluoroethane [Freon-113], methylene chloride, carbon tetrachloride, and 1,1,1-trichloroethane).

6.3.3 Restrictions on Acids

The payload materials do not contain any free liquid acids, because the waste is in a solid form or is solidified. Acidic components from process operations are neutralized or basified before being generated as CH-TRU waste. All aqueous liquids are neutralized or basified to a pH range of 5.5 to 12 prior to solidification. Strong (concentrated) acids are prohibited through restrictions on corrosives.

6.3.4 Restrictions on Aromatic Hydrocarbons

The aromatic hydrocarbons (e.g., xylene) are also flammable and are generally present in concentrations less than or equal to 500 parts per million (ppm) in the headspace of the payload containers. As an upper limit, they are restricted to the mixture lower explosive limit (MLEL) for the total flammable (gas/VOC) mixture as described in Section 5.2 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC). While this is an upper limit, process operations limit the presence and release of these hydrocarbons:

- Very few waste streams use flammable organic solvents at the sites, limiting the number of content codes that could contain these compounds.

- Permeabilities of the aromatic hydrocarbons through the plastic bags used as confinement layers are extremely high.[1] Residual amounts of these compounds should escape from the bags before the waste is emplaced in the payload containers.

- Analysis of solidified aqueous inorganic materials with ppm levels of aromatic hydrocarbons in the waste (Appendix 6.4 of the CH-TRU Payload Appendices) did not have any detectable levels in the headspace above the waste.

This class of compounds is therefore not an incompatibility concern for the payload materials and the package.

6.3.5 Restrictions on Halogenated Organic Solvents

Some of the organic solvents that are incompatible with butyl rubber are used in operations at the sites. Appendix 6.4 of the CH-TRU Payload Appendices evaluates the sources and release of these from the payload materials. Real waste data shows these solvents to be present in extremely small amounts in the waste (Waste Types I, II and III). Any residual amounts of these solvents present will diffuse at very slow rates through the filters in the payload containers. As discussed in Appendix 6.4 of the CH-TRU Payload Appendices, Waste Type IV, which may contain higher levels of VOCs, can be shipped only under the test category.

The total accumulation of organic solvents in the package cavity during transportation is expected to be low (Appendix 6.4 of the CH-TRU Payload Appendices). At these low concentrations, even if the solvents interact with the butyl rubber O-rings, the only possible effect on the O-rings would be a negligible amount of swelling. This should not effect their sealing properties.

6.3.6 Conclusions

In summary, the payload materials in the TRUPACT-II or HalfPACT do not present an incompatibility concern with respect to the butyl rubber O-rings. Chemicals that are of concern are not present in the waste in any significant amounts. Residual amounts of any solvents present are not expected to accumulate above low ppm amounts in the package cavity. These low concentrations are not sufficient to degrade the material properties of the butyl rubber O-rings and affect the sealing properties.

[1] Brandrup, J., and Immergut, E. H., eds., "Permeability Coefficients and Transmission Rates," Polymer Handbook, (Interscience Publishers, New York, 1966).

APPENDIX 6.4

VOLATILE ORGANIC COMPOUNDS (VOC) IN THE CH-TRU PAYLOAD—SOURCE TERM AND RELEASE RATE ESTIMATES

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6.4 Volatile Organic Compounds (VOC) in the CH-TRU Waste Payload—Source Term and Release Rate Estimates

6.4.1 Summary

Volatile organic compounds (VOC) are used by some of the Department of Energy (DOE) sites as part of their process operations. The presence of VOCs in the Transuranic Package Transporter (TRUPACT)-II or HalfPACT payload, and their possible release into the package cavity during transport, are of concern for two reasons: (1) potential damage to the butyl rubber O-ring seals due to interaction with the VOC vapors that could diffuse from the payload containers, and (2) contribution to the overall pressure in the inner containment vessel (ICV) cavity by the vapor pressure that might be exerted by these chemicals. This appendix evaluates these concerns by an analysis of waste generation processes at the sites, current and past sampling programs, and the payload configuration.

Waste types that are known to contain VOCs in appreciable amounts (solidified organics) are restricted from being a part of the payload, unless it can be shown by actual testing that these content codes are safe for transport. The VOCs can be present in the other waste types only in trace amounts of less than one percent by weight. Solidified aqueous or homogeneous inorganic solids (Waste Type I) are processed through a vacuum filtration technique prior to solidification in a payload container. The vacuum filtration process greatly reduces the amount of trace VOCs in the waste. A similar reduction in VOCs also occurs for many inorganic and organic solid wastes (Waste Types II and III) generated in processes that are operated under slightly negative pressures. Examples are wastes generated from glovebox lines. Results from sampling programs support these conclusions.

Any residual amounts of VOCs within the waste in a payload container are impeded from being released during transport because of additional chemical and physical barriers. For waste types with bound water (i.e., solidified aqueous or homogeneous inorganic solids), the vapor pressure of the organics is reduced appreciably. Quantitative analysis, along with data from sampling programs, is presented in following sections.

Due to the multiple processes mentioned above, the source term for the VOCs is limited. VOCs present in residual amounts in the waste are not expected to diffuse from the headspace of the payload containers into the ICV in any significant quantities. Therefore, for the waste types expected to be transported in the TRUPACT-II and HalfPACT, the presence of VOCs in the package cavity should not be an issue of concern.

6.4.2 Introduction

VOCs include those organic compounds that exert appreciable vapor pressures at normal temperatures. Examples are halogenated compounds like Freon-113 and methylene chloride, and lower molecular weight alcohols (e.g., methanol). Some of these compounds are used at the DOE sites as industrial solvents and in decontamination operations. The potential of these volatiles being present in the payload is of concern for the following reasons:

- The vapor pressure exerted by the volatiles may contribute to the total pressure in the package cavity.

- Some of the organic solvents could potentially cause damage to the butyl rubber O-rings in the package during transport.

Hence, evaluation of the VOCs with respect to the payload and the package is necessary in order to ensure safe transport. The following sections discuss the source term of the VOCs in the payload and estimates of the release of these VOCs into the package cavity. Data from past and ongoing sampling programs at the DOE sites and laboratory experiments are analyzed to draw conclusions about these parameters. Wherever relevant, the different waste types expected to be part of the payload are discussed separately. (For a description of the classification of waste materials into waste types, see Appendix 2.1 of the CH-TRU Payload Appendices.

6.4.3 Source Term of VOCS in Different Waste Types

Solidified organics (Waste Type IV) are the only waste type with organic solvents as the main constituents of the waste. At the present time, payload containers belonging to this waste type cannot qualify for shipment unless it can be demonstrated by testing each payload container that it is safe for transport purposes. The test procedure to be followed is detailed in Section 5.2.5 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC). For example, a container in this class would have to be tested under normal transport conditions to demonstrate that the maximum pressure limits imposed on the package are not exceeded. The same is true for the other transport parameters. Testing of a population of payload containers from a content code belonging to Waste Type IV could qualify the content code for shipment.

The remainder of the waste types have VOCs only in trace amounts of less than 1 percent by weight. While this is an upper bound on the amount of VOCs, waste generation procedures limit the VOC concentrations in these waste streams to much lower concentrations:

- Generation of solidified aqueous or homogeneous inorganic solids (Waste Type I) usually involves a vacuum filtration step (to dewater the waste stream), which reduces the amount of trace VOCs in the waste.

- Solid inorganic and organic wastes (Waste Types II and III) are generated from gloveboxes that are operated under negative pressures which acts to reduce the amounts of residual VOCs in the waste.

- Generator and storage sites will cite reportable quantities of some VOCs even if the material is suspected of being present in negligible quantities. This reporting is necessary to comply with Resource Conservation and Recovery Act (RCRA) regulations that a listed material is in a waste until proven to be absent (below testability limit).

6.4.4 Occurrence of VOCs in CH-TRU Waste from Sampling Programs

6.4.4.1 Evidence from Sampling Program at Rocky Flats Plant (RFP)

As part of a recent sampling program at Rocky Flats Plant (RFP),[1] 22 drums were sampled for headspace-gas composition and for organic compounds in the inner confinement layers, and where possible, in the innermost layer of confinement with the waste. Table 6.4-1 lists the results of this sampling along with relevant information on the individual drums. The results of this sampling program are discussed by waste type below.

6.4.4.1.1 Analyses of Solidified Aqueous Inorganic Solids - Waste Type I

Ten drums in this category were tested as part of the sampling program. The drums were analyzed for thirty-six (36) compounds that are listed in Table 6.4-2. The ten waste drums represent a cross section of drums generated at the Rocky Flats Plant and retrievably stored at INEL. Five of the ten drums were filled between 1983 and 1984, two were filled in 1973, and three were newly generated in 1988. Only two of the ten drums had carbon composite filter vents in the drum lids prior to opening. For five of the ten drums, the sludge also was analyzed for volatile organic compounds.

Table 6.4-1 — Summary of Rocky Flats Plant Sampling Program

Drum Number	Waste Type	Date Drum Filled	Gas Sample Analysis[a,b] (Headspace) (Vol %)			
			CCl_4	TRIC	FREON	CH_2Cl_2
62542	I	6-21-88				
59728	I	6-20-88				
62815	I	7-10-88				
7411-2808	I	4-9-73				
7411-2578	I	2-9-73				
7412-03850	I	8-2-84				
7412-02917	I	9-7-83				
7412-03492	I	3-9-84				
41450	III	6-7-88				
58642	III	6-7-88				
74402387	III	1-22-73				
240658	II	6-22-83				
74316881	IV	4-3-84	3.9		0.3	
74317069	IV	12-5-84	1.5		0.8	
741204577	I	3-26-85				

[1] Roggenthen, D.K., T.C. McFeeters, and R.G. Nieweg, "Waste Drum Gas Generation Sampling Program at Rocky Flats During FY 1988," RFP 4311, March 1989.

Table 6.4-1 — Summary of Rocky Flats Plant Sampling Program (Concluded)

Drum Number	Waste Type	Date Drum Filled	Gas Sample Analysis[a,b] (Headspace) (Vol %)			
			CCl_4	TRIC	FREON	CH_2Cl_2
74703446	I	1-7-85				
74316930	IV	5-25-84				
2500484	IV	4-17-85	3.5	0.8		0.8
002800658	II	9-28-82		0.4		
242533	II	2-21-84		0.1		
234906	II	2-21-84				
3201073	II	12-5-83				

[a] $CC1_4$ = Carbon tetrachloride
TRIC = 1,1,1-Trichloroethane
FREON = 1,1,2-Trichloro-1,2,2-trifluoroethane
CH_2C1_2 = Methylene chloride (dichlormethane)

[b] Detection limit: 500 ppm for all gases.

Table 6.4-2 — Organic Compounds Sampled for in Rocky Flats Plant Program

Chloromethane
Bromomethane
Vinyl chloride
Chloroethane
Methylene chloride
Acetone
Carbon disulfide
1,1-Dichloroethene
1,1-Dichloroethane
1,2-Dichloroethene (total)
Chloroform
1,2-Dichloroethane
2-Butanone
1,1,1-Trichloroethane
Carbon tetrachloride
FREON TF
Bromodichloromethane
1,2-Dichloropropane
cis-1,3-Dichloropropene
Trichloroethene
Dibromochloromethane
1,1,2-Trichloroethane
Benzene
trans-1,3-Dichloropropene
Bromoform
4-Methyl-2-pentanone
2-Hexanone
Tetrachloroethene
1,1,2,2-Tetrachloroethane
Toluene
Chlorobenzene
Ethylbenzene
Styrene
Xylenes (total)
Isopropanol
Butanol

None of the drums had detectable quantities of VOCs in the headspace (between the liner and the outer bag), the outer and inner bags or inside the inner bag next to the waste. Analysis of solidified inorganic waste from five retrievably stored drums did not detect any traces of VOCs in four out the five drums (Table 6.4-3). The waste from one drum (No. 7411-2808) contained nine of the organics at low ppm levels (0.9 ppm to 19 ppm). These organics did not appear in any of the containment layers or in the headspace of the drum between the liner and outermost drum liner bag.

Table 6.4-3 — Volatile Organic Analysis of Sludge Samples

Volatile Compounds	Amount (PPM) by Drum Number					
	7411–2808	7412–02917	7412–03492	7412–03850	7411–2578	BLD[b]
1,2-Dichloroethene (Total)	7.8	U[a]	U	U	U	0.1 PPM
Chloroform	1.8	U	U	U	U	0.1
1,1,1-Trichloroethane	8.8	U	U	U	U	0.1
Tetrachloroethene	1.7	U	U	U	U	0.1
1,1,2,2-Tetrachloroethane	4.7	U	U	U	U	0.1
Toluene	0.9	U	U	U	U	0.1
Ethylbenzene	5.3	U	U	U	U	0.1
Styrene	9.6	U	U	U	U	0.1
Total Xylenes	19.0	U	U	U	U	0.1

[a] U = undetected.

[b] BLD = Beyond lower detection limit.

None of the newly generated waste drums showed any traces of the organics in the headspace or layers of confinement. The drum with the ppm levels of some of the organics was the one filled in 1973 and vented at the INEL facility. This means that the drum had been vented for at least a period of eight weeks prior to being part of the sampling program. The absence of detectable quantities of VOCs in nine of ten solidified inorganic solids demonstrates that the vacuum filtration technique for these sludges is effective in lowering the concentration of VOCs in the waste. The presence of ppm amounts of the VOCs in the one sludge and the absence of the VOCs from the headspace (in spite of the vented drum) are evidence to the fact that any residual VOCs tend to stay with the waste. These data support the conclusion that the VOCs present in the waste are in low ppm or less amounts, with the source term itself being very limited.

6.4.4.1.2 Analysis of Solid Inorganics - Waste Type II

Five drums of Waste Type II were analyzed for gaseous components in the different confinement layers and the headspace of the drums. Three of the five drums did not show any of the organics, one (No. 242553) had up to 0.1 volume percent of 1,1,1-trichlorethane, while the fifth drum (No. 002800658) had up to a maximum of 0.4 volume percent of 1,1,1-trichloroethane in some of the individual packages. These drums were made up of mostly glassware, some of which contained residual amounts of the 1,1,1-trichloroethane. The concentrations measured in these drums are well below the saturation concentration of the organic liquid (13% from vapor pressure considerations), indicating that the organic liquid is present in only very small amounts.

6.4.4.1.3 Analysis of Solid Organics - Waste Type III

Three drums belonging to this waste type were analyzed in the sampling program, and none of them had any detectable amounts of the halogenated organics. Low concentrations (0.08 volume %) of hydrocarbons were present in one of the three drums.

6.4.4.1.4 Analysis of Solidified Organics - Waste Type IV

As mentioned earlier in this appendix, Waste Type IV belongs in the test category due to the possible presence of appreciable amounts of VOCs in the headspace of the payload containers. Results from the sampling of four of the drums in this waste type are presented here as supporting evidence that the VOCs are generally present in a non-volatile form in the waste. While VOCs could have been present at near-saturation levels in these drums (solidified organics waste type and the drum not vented), the results show that the VOCs are present in fairly low concentrations. One of the four drums (No. 74316930) did not have any detectable quantities of VOCs in any of the confinement layers. No analyses of the organic sludge samples are available. The maximum concentration of any VOC found in the three other drums was 3.9 volume percent for carbon tetrachloride.

These results seem to indicate that even if a finite supply of the organics was available, the nature of the waste limits release of the vapors into the headspace. Until quantified information can be obtained, this waste type is assigned to the test category.

Carbon tetrachloride has the lowest saturated vapor pressure (Table 6.4-4) of the four common solvents found in defense waste (i.e., carbon tetrachloride, Freon-113, methylene chloride and 1,1,1-trichloroethane). The fact that only carbon tetrachloride was detected in the headspace of the solidified organic drums provides evidence that the other organic solvents commonly associated with this waste form have volatilized prior to drum closure.

6.4.4.2 TRU Waste Sampling Program at INEL

The TRU Waste Sampling Program was conducted between 1983-1985 at INEL[2] in an effort to characterize the retrievably stored waste at INEL. In this program, 210 drums were sampled and analyzed for headspace gas composition. Table 6.4-5 summarizes the results on the VOC analyses by waste type and provides maximum, minimum and average concentrations along with the sample size.

Among the thirty-two drums sampled in Waste Type I, four of the VOCs were not present in any of the drums, and average concentrations of the other four ranged between 0.0025 and 0.198 volume percent. This sampling program was conducted even before transport requirements for the package were formulated. The results of the program indicate that by process history, the source term of the VOCs is limited. Similar results can be seen for Waste Types II and III where the average VOC concentrations were orders of magnitude below their saturation levels. Even among the twenty-three drums of Waste Type IV that were sampled, three of the VOCs were not present in the head space at all, and average concentrations of those present were below 1.4 volume percent. These results once again illustrate that the VOCs are in the waste in limited quantities and/or the bound nature of the VOCs even in the case of the organic sludges.

[2] Clements, T.L., and D.E. Kudera, "TRU Waste Sampling Program: Volume I--Waste Characterization," EG&G Idaho, Inc., Idaho Falls, Idaho, EGG-WM-6503, September 1985.

Table 6.4-4 — Vapor Pressures of Organic Solvents Above a Pure Liquid Phase[a]

Compound	Vapor Pressure	Temperature	Vapor Pressure	Temperature
Xylene	20 mm Hg	104°F	60 mm Hg	146°F
1,1,1-Trichloroethane	400 mm Hg	130°F	760 mm Hg	165°F
1,1,2-Trichloro-1,2,2-trifluoroethane (Freon-113)	760 mm Hg	118°F	1520 mm Hg	158°F
Carbon tetrachloride	200 mm Hg	100°F	760 mm Hg	170°F
Methlyene chloride (Dichloromethane)	760 mm Hg	105°F	---	---

[a]Green, D.W., 1984, Perry's Chemical Engineers' Handbook, 6th edition, McGraw-Hill Book Company, New York, New York.

Table 6.4-5 — Summary VOC Analysis in TRU Waste Sampling Program

Waste Type	TRICH[a]	IPROP[b]	TRCETHY[c]	CCl_4[d]	DCM[e]	1,2-DCETHA[f]	FREON[g]	CYCHEX[h]	DCETHY[i]	TOTAL VOC[n]
I[j] MAX	0.94	0	0.04	0.04	0.22	0	0	0	0	1.17
I MIN	0	0	0	0	0	0	0	0	0	--
I AVG	0.1978	0	0.005	0.0025	0.0203	0	0	0	0	--
II[k] MAX	2.84	0	0.17	0.09	0.42	0.4	0.81	0.17	0.03	2.84
II MIN	0	0	0	0	0	0	0	0	0	--
II AVG	0.2669	0	0.0043	0.0029	0.0230	0.0106	0.0103	0.0021	0.0003	--
III[l] MAX	1.06	0.62	0.14	0.29	0.25	0	2.87	0	0	3.37
III MIN	0	0	0	0	0	0	0	0	0	--
III AVG	0.1238	0.0201	0.0087	0.0068	0.0089	0	0.0389	0	0	--
IV[m] MAX	7.48	0	0.14	4.09	0.71	0	10.4	0	0	17.88
IV MIN	0	0	0	0	0	0	0	0	0	--
IV AVG	1.3582	0	0.0213	0.6734	0.0726	0	1.0717	0	0	--

[a]TRICH = Trichloroethane

[b]IPROP = Isopropyl alcohol

[c]TRCETHY = Trichlorethylene

[d]CCl_4 = Carbon tetrachloride

[e]DCM = Dichloromethane

[f]1,2-DCETHA = 1,2-Dichloroethane

[g]FREON = FREON-113 (1,1,2-Trichloro-1,2,2-trifluoroethane)

[h]CYCHEX = Cyclohexane

[i]DCETHY = Dichloroethylene

[j]32 drums Waste Type I were sampled

[k]78 drums Waste Type II were sampled

[l]77 drums Waste Type III were sampled

[m]23 drums Waste Type IV were sampled

[n]Maximum total volatile organic compounds in any drum

6.4.5 Release of VOCs from the Waste into the Payload Container

The vapor pressure of a pure compound is generally not completely exerted when the compound is in a combined form with other substances. Any residual VOCs present in the waste will therefore exert only a portion of their vapor pressures and tend to stay in a bound form. An

example is presented below for the case of methyl alcohol, which is the most volatile alcohol documented in the waste from an analysis of process technology.

The maximum amount of methyl alcohol expected in any of the waste forms based on process technology is 250 ppm. If a waste form contains bound water, the volatility of the alcohol will be reduced. A waste type containing 50% bound water (typical for Waste Type I) and 250 ppm of methyl alcohol would have the alcohol exerting a vapor pressure of only 0.12 mm Hg over the aqueous mixture at 40°C.[3] The vapor pressure at 60°C would be 0.26 mm Hg. The data presented in the previous section for halogenated organic compounds displayed evidence of reduced volatilities in actual waste materials.

6.4.6 Release of VOCs from Payload Containers

All payload containers in the payload are vented as specified in Section 2.5 of the CH-TRAMPAC. Release of the VOCs from the payload containers is seen from the experimental studies conducted at the INEL facility.[4] The concentrations of trichloroethane and methylene chloride in the headspace of a drum of combustible waste (which was vented with a carbon composite filter) remained constant at 6 and 1.5% respectively during thirteen weeks of venting (see Figure A-8d of Clements and Kudera[4]). These concentrations were lower than the saturated concentrations of 13% for trichloroethane and 33% for methylene chloride, which indicates that the source of the VOCs in the waste is limiting. It is also possible that the vapor presence of the organics are depressed by the presence of other compounds. After purging and sealing the drum, the concentration of each VOC remained below 3%, once again indicating that the source term of the VOCs was limited.

6.4.7 Conclusions

The following conclusions can be drawn from an evaluation of existing information on VOCs in CH-TRU waste:

1. For materials expected to be shipped in the TRUPACT-II or HalfPACT, the source term of the VOCs is very small by the very nature of waste generation processes. Waste types known to contain appreciable amounts of VOCs are not allowed to be a part of the payload unless each container is tested under shipping conditions and shown to be safe for transport until sufficient data have been collected to allow a content code to be certified for shipment.

2. Experimental studies show that VOCs present in the waste are well below saturation levels and in ppm levels in most cases.

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[3] Perry, R.H., 1984, Perry's Chemical Engineers' Handbook, 6th edition, McGraw-Hill, Inc., New York, New York, Table 3-8, p. 3-61.

[4] Clements, T.L., and D.E. Kudera, "TRU Waste Sampling Program: Volume II--Gas Generation Studies," EG&G Idaho, Inc., Idaho Falls, Idaho, EGG-WM-6503, September 1985.

3. The residual VOCs in the waste tend to be bound in the waste and do not migrate out of the payload containers. Thus, the residual VOCs do not pose a problem with respect to incompatibilities with the package.

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APPENDIX 6.5

BIOLOGICAL ACTIVITY ASSESSMENT

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6.5 Biological Activity Assessment

6.5.1 Summary

This appendix addresses the impact of biological activity within the waste on TRUPACT-II and HalfPACT shipments. The primary concerns in this regard are the possible generation of gases by biotic processes that might contribute to the build up of pressure in the cavity, or produce potentially flammable gases. An analysis of the waste forms and their environment shows that biological activity will be minimal and will have little impact on the package during a potential shipping period of up to 60-days. Gas production by microbial processes is not a concern for transport of contact-handled transuranic (CH-TRU) waste.

6.5.2 Introduction

Some of the CH-TRU waste forms and most of the packaging inside the payload containers (polyethylene [PE] and polyvinyl chloride [PVC] bags in drums or standard waste boxes) are organic in nature. The potential for microbial activity would exist if a suitable environment exists for the degradation of these organics. As will be shown in the following sections, the waste environment during transport is not conducive for microbial proliferation. Wherever a distinction between retrievably stored and newly generated waste is necessary, it will be made.

6.5.3 Types of Biological Activity

There are different types of microorganisms to be considered in the degradation of CH-TRU waste. Aerobic microorganisms, which produce carbon dioxide (CO_2) and water (H_2O), require oxygen for growth.[1] Anaerobic microorganisms, which can produce CO_2 and hydrogen (H_2, predominantly as an intermediate) or methane (CH_4), as well as other products, degrade materials in anoxic (oxygen-free) environments.[1] Facultative anaerobes can live with or without oxygen. Obligate anaerobes, on the other hand, cannot tolerate any oxygen and will only grow in strict anoxic environments. Microorganisms most likely to be found in waste products include bacteria and fungi. Bacteria utilize only the surface of a material and can be either aerobic or anaerobic. Fungi can access the matrix of the material but are generally only found in aerobic environments. Microorganisms can also be classified based on the optimum temperature they require for growth. Mesophiles have an optimum temperature for growth between 20 and 55°C, while thermophiles grow best at temperatures above 50°C.

[1] Atlas, R. M., 1984, "Microbiology: Fundamentals and Applications," Macmillan Publishing Company, New York , New York.

6.5.4 Waste Forms--Implications of Substrate and Nutrient Availability

Various waste forms will be transported in the package, but, in terms of the potential for gas generation, only one form is important; namely, cellulosic materials (solid organics). Materials made of rubber and plastic are more resistant to microbial actions. The contribution of these compounds to the total gas generated will be negligible, (especially over the shipping period of 60 days) primarily because of their inert nature. Evidence from stored drums (in retrievable storage for periods up to 15 years) that were opened up as part of a sampling program shows little or no degradation of the packaging materials (see Appendix 5.3 of the CH-TRU Payload Appendices). Even under conditions designed to promote microbial proliferation, these compounds degrade very slowly, if at all. Similarly, the solidified inorganic sludges should not exhibit any significant microbial gas generation due to their relatively high alkalinity (pH = 10-12), which would be hostile for most common microorganisms. This aspect is discussed further in the next section on environmental factors affecting microbial growth.

Examples of cellulosic materials that could be present in the payload are cotton, Kimwipes, and paper. Cellulose is a polymer composed of chains of glucose monomers. Biodegradation of cellulose requires the hydrolysis of the polymer into the monomer units. Biological depolymerization is a slow process that can significantly inhibit fermentation rates. Even though there are organisms that can degrade cellulose under different conditions, it is a complex process requiring very specific enzymes. Wood will also be present in TRU waste but is degraded at a much slower rate than cellulose in the form of cotton. Wood contains lignin which is much more resistant to microbial attack than cellulose. In addition, bacterial action is a strong function of surface area and substrate availability. The bulk form and segregated nature of the TRU waste creates conditions that are not very conducive to high microbial metabolic activities, especially during a limited period of sixty days. As shown in subsequent sections, the waste environment is such that, even for stored waste, the relatively long time period in itself is not sufficient to promote active microbial growth.

The availability of the nutrients, nitrogen and phosphorus, is another factor that can severely limit the extent of microbial activity in the package. The dry weight of a bacterial cell typically contains 14% nitrogen and 3% phosphorus.[2] While some of the waste forms do contain sources of nitrogen, phosphorus is limiting in most cases. Even where sources of nitrogen are present, the waste form environments are far from optimum for bacterial growth. An example is inorganic sludges which contain nitrates but are lacking in carbon substrates, and which are basified to a pH of 10-12. In other words, even without any consideration of the non-ideal environmental conditions of the payload, substrate and nutrient limitations by themselves will maintain microbial activity at minimal levels in the cavity.

[2]Bailey, J. E., and D.F. Ollis, 1977, "Biochemical Engineering Fundamentals," McGraw Hill Book Company, New York , New York.

6.5.5 Environmental Factors Affecting Microbial Activity in the Payload

Environmental factors such as temperature, pH, Eh, oxygen, moisture content, and water availability are very important in determining the rates (kinetics) and feasibility (thermodynamic aspects) of microbial activity. For the payload, almost all of these environmental variables are either sub-optimal or hostile. Each of these is considered in detail below.

6.5.5.1 pH and Temperature

The pH is an important factor to consider in the microbial degradation of CH-TRU waste. Usually, most bacteria will be most active at neutral pHs. The sludges to be transported in the package are fairly basic (pH of 10-12), which will inhibit the activity of most bacteria and fungi. Specific organism groups like the methanogens (methane producers) also have sensitive pH ranges for growth.[2] Even under carefully controlled laboratory conditions, methanogenesis has a very long start-up phase and a fairly unstable operating phase. Establishment of an active population of methanogens is therefore unlikely during the shipping period.

As mentioned in Section 6.5.3, microorganisms can be classified based on the optimum temperature they require for growth. Methanogens, for example, have an optimum temperature range between 90 to 100°F. Anaerobic digestion units (aimed at digesting sewage sludge and the production of methane) are usually provided with external heat exchangers to maintain optimum temperatures for methanogenesis.[2] These constant and optimal conditions are not likely to exist even for waste that has been stored for long periods of time. Fluctuations in the temperature also prevent the establishment of a stable microbial population in the waste containers.

6.5.5.2 Eh and Oxygen Availability

Eh (the redox potential) is an indication of whether an environment is oxidizing or reducing. Many microorganisms have strict Eh requirements for growth. Methanogens, for example, require a very reducing environment in which the Eh must be less than -200 mV.[3] They are obligate anaerobes and cannot tolerate even small amounts of oxygen. It is very unlikely that any significant quantities of methane will be produced during transport of CH-TRU waste. Methanogenesis from cellulose requires a complex set of organisms and conditions to be successful and is easily upset if favorable conditions are not maintained. The production of methane requires not only the depletion of oxygen but also the reduction of nitrates and sulfates.[3] Even in a process plant under optimum conditions, it is difficult to produce methane from cellulose. Even experiments done under controlled laboratory conditions showed no methane generation with CO_2 being the major gaseous product.[4] (These experiments are not applicable to

[3]Weiss, A. J., R. L. Tate III, and P. Colombo, 1982, "Assessment of Microbial Processes on Gas Production at Radioactive Low-Level Waste Disposal Sites," BNL-51557, Brookhaven National Laboratories, Brookhaven, New York.

[4]Molecke, M. A., 1979, "Gas Generation from Transuranic Waste Degradation: Data Summary and Interpretation," SAND79-1245, Sandia National Laboratories, Albuquerque, New Mexico.

the transport conditions - a bacterial inoculum was added to synthetic waste along with required nutrients in these experiments.) Radiolytic production of oxygen even in trace quantities would act as an inhibitor of anaerobic activity. In addition, the requirement of having a filter vent on all the waste containers before transport provides a means of communication with the environment, further destabilizing a constant environment even for the stored waste.

6.5.5.3 Moisture Content and Water Availability

One of the prime requirements for microbial proliferation is the availability of sufficient amounts of water. Approximately 80% of a bacterial cell mass is water. Microbial activity can be sustained even at relative humidities below the saturation value, but metabolic activities under these conditions will be very slow. Hence, microbial gas generation rates in short time periods (like the sixty-day shipping period) will be insignificant. As pointed out earlier, even if some of the content codes have pockets of damp waste, other requirements for biological activity (substrate, nutrients, suitable pH and Eh conditions) will not necessarily be present in these areas.

6.5.5.4 Radiation Effects on the Microorganisms

An additional factor that contributes to making the microbial environment non-ideal in the package is the radiation from the payload, which can result in the death of a portion of the microbial population. Radiation effects can potentially compound the existing hostile environment of the microorganisms in the payload.

6.5.6 Source Term of the Microorganisms

The waste packaging configuration in the payload containers restricts the source term for the microorganisms. While an initial microbial inoculum may be present in the waste, the plastic bagging acts as a barrier for the availability of the waste substrates to the microorganisms. In addition, the filter vents on the waste containers have a filtering efficiency of $\geq$99.9%, with 0.3 to 0.5 micron particles, DOP (dioctyl phthalate) smoke (Section 2.5 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control [CH-TRAMPAC]). Typical dimensions of bacteria are between 0.5 to 3 microns.[2] This means that the filter vents would act as effective bacterial filters (though not 100%) to prevent continuous contamination of the waste with microorganisms.

6.5.7 Conclusions

The nature and configuration of the payload for the TRUPACT-II and HalfPACT are such that biological activity will be minimal and of very little concern during the 60-day shipping period. The environment in the cavity will be suboptimal or hostile for the growth of most microorganisms due to the segregation of the waste and essential nutrients and the limitations of usable substrate, nitrogen and phosphorus sources. The following factors support this statement:

1. Cellulose, which is the most likely waste product to be degraded by bacteria, is degraded by a complex process that requires a specific set of organisms. Some of these organisms may be present in the waste but may not be in a sufficient quantity to contribute to the overall gas generation.

2. The proper nutrients (primarily nitrogen and phosphorus) must be present in order for the microorganisms to degrade any material. Nitrogen from the air cannot be efficiently utilized by microorganisms; it must come from a source such as nitrate. Sufficient phosphorus, however, is very likely to be missing or limiting in many drums.

3. It is very unlikely that methane would be produced during transportation of the waste for several reasons:

   - The environment for methanogenesis must be very reducing (no oxygen)
   - Very specific microorganisms are required, which exist in narrow ranges of suitable environments, and
   - The process can be self-poisoning if intermediates produced are not controlled or neutralized.

4. Although hydrogen may be produced during intermediate steps in anaerobic processes, it is very unlikely that it will be present as a final product. It is used as a reducing agent almost as quickly as it is produced.

5. Another factor limiting bacterial degradation is substrate surface area. The cellulosic materials that are put into bags are in a very bulky form that is not easily accessible to surface-decomposing bacteria.

6. Any aerobic decomposition will result in insignificant pressure changes due to the simultaneous consumption of oxygen with the production of carbon dioxide.

7. Even retrievably stored waste does not provide the necessary conditions for continuous and prolonged microbial activity. Fluctuations in environmental variables like the temperature and oxygen availability (due to the filter vent) act to prevent anaerobic biological activity at any significant level. Evidence from sampling programs shows very little deterioration of the packaging materials even after years of storage. In addition, limitations in substrate and nutrient availability and segregation of these nutrients apply to retrievably stored waste as well.

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APPENDIX 6.6

THERMAL STABILITY OF PAYLOAD MATERIALS AT TRANSPORT TEMPERATURES

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6.6 Thermal Stability of Payload Materials at Transport Temperatures

6.6.1 Summary

This appendix describes the thermal stability of payload materials, demonstrating that thermal degradation will be minimal for payload materials during transport in the TRUPACT-II or HalfPACT.

6.6.2 Introduction

The thermal stability of the payload materials is addressed for the wastes inside payload containers, including any dunnage and inserts used, and payload materials outside the payload containers, including the drum binding material (stretch wrap), plastic reinforcement plates, and slip sheets.

Inorganic payload materials will be thermally inert, with the possible exception of small amounts of gases adsorbed on the surfaces, most of which will be water vapor. The pressure calculations performed in the TRUPACT-II and HalfPACT Safety Analysis Reports (SARs) assume saturated water vapor is present in all cases.

Organic materials are placed into shipping categories that are shown to meet transport requirements by analysis or into shipping categories which are shown to meet transport requirements by test, depending on the chemical makeup and decay heat of the wastes. Thermal stability of payload materials is addressed in terms of the threshold decomposition temperatures. The effect of irradiation on the materials at the lowest threshold decomposition temperature is shown to be negligible. For the test shipping categories of Waste Type IV, any gases produced thermally are included in the measurement of total gas generation.

Plasticizers added to polymers to increase flexibility are typically less thermally or chemically stable than the polymers.[1] However, the vapor pressures of most common plasticizers (e.g., phthalates, sebacates, and other esters) are only 1 millimeter of mercury at 160°F (71°C) or above[2] and can be ignored in pressure calculations.

Oxidation is the major degradation process for polymers heated in the presence of oxygen. In a sealed system, oxygen typically is depleted at a rate faster than the rate of formation of oxygen-containing gases such as carbon dioxide or carbon monoxide, leading to a net pressure decrease.

[1] Deanin, R. D., Polymer Structure, Properties and Applications, Chaners Books, Boston, 1972.

[2] AIP Handbook, American Institute of Physics Handbook, Second Edition, McGraw-Hill Book Company, New York, 1963.

6.6.3 Threshold Decomposition Temperatures for Plastics and Other Polymers

Waste material and packaging components may be a combination of cellulosics, plastics, and rubber. Representative materials from each of these categories were studied to determine threshold decomposition temperatures.[3] The temperature at which a material loses weight, not including drying, is the threshold decomposition temperature. Gas generation from thermal decomposition was measured by pressure increases in sealed containers over long periods of time. Experiments were performed in aerobic and anaerobic atmospheres.

The threshold decomposition temperature for materials in air is shown in Table 6.6-1. Pylox gloves (polyvinyl chloride) have the lowest threshold decomposition temperature of 302°F (150°C). Results of anaerobic experiments and experiments with potential catalysts that may be present in the waste yielded no significant lowering of the threshold decomposition temperatures.

The generation of gas through thermal decomposition of the waste materials did not occur at temperatures lower than 302°F (150°C).

In the case of polymeric materials, the large molecules must be broken down into smaller molecules that can vaporize. In most cases, a solid polymer breaks down into a variety of smaller molecular fragments comprised of a number of different chemical species. Heavier molecules may remain in the condensed phase (either solid or liquid) for some time. As decomposition proceeds, solid residues are left behind. These residues can be carbonaceous (char), inorganic, or a combination of both. Volatiles that are produced must pass through the residues to reach the surface. Thus, the carbonaceous chars can considerably slow down further thermal decomposition. Inorganic residues, on the other hand, can form glassy layers that may then become impenetrable to volatiles and protect the underlying layers from any further thermal breakdown. Because of these effects, gas generation due to thermal degradation of waste materials is negligible even at much higher temperatures (up to 100°F) above the threshold decomposition temperature.[4]

6.6.4 Effect of Radiation on Thermal Properties of Materials

Radiation chemically changes materials and can affect their thermal properties. For example, for an absorbed dose of 500 millirad in vacuum, the melting point of polyethylene was decreased about 9°F (5°C).[5]

Polyethylene film irradiated in vacuum or under a nitrogen atmosphere was subsequently heated in the presence of oxygen at 230°F (110°C). The weight change between unirradiated and

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[3] Kosiewicz, S. "Cellulose Thermally Decomposes at 70°C," Thermochimica Acta, Vol. 40, pp 319-326, 1980.

[4] DiNenno (ed), Philip J. SFPE Handbook of Fire Protection Engineering, Third Edition, Section 1, Chapter 7, "Thermal Degradation of Polymers," Society of Fire Protection Engineers, National Fire Protection Association, Quincy, Massachusetts, 2002.

[5] Black, R. M., and A. Charlesby, "The Oxidation of Irradiated Polyethylene-II Thermal Oxidation," Inter. J. Appl. Radiat. Isotopes 7, PP. 134-140, 1959.

irradiated polyethylene films (exposure times up to 1150 hours [hr]) was compared.[6] The major difference between irradiated and unirradiated materials was that the irradiated materials began to absorb oxygen and increase in weight after 50 hr without antioxidant, or after 500 hr with antioxidant.

The rate of weight loss versus temperature of polyethylene was measured for samples irradiated in air and then heated in air.[7] Thermal degradation was detectable above about 302°F (150°C), with only minor differences found between irradiated and unirradiated materials.

The conclusions reached are that while there are measurable differences in the thermal properties of polymers when they are irradiated, the effects are relatively small even near 392°F (200°C), and can be neglected for temperatures less than or equal to 302°F (150°C).

Table 6.6-1 — Threshold Decomposition Temperatures in Air[3]

Material	Temperature (°C)
Cellulosics[a]	
Scott utility wipes	185
Kleenex tissues	185
Diaper paper (PE-backed)	190-185
Cloth (cotton twill)	185
T-shirt (cotton)	185-190
Cheesecloth	205
Wood	175
Fiberboard	185-190
Plastics	
Pylox gloves (PVC)	150
Tygon tubing (PVC)	175
Polyethylene	210
Polypropylene	195-200
Lucite [poly(methyl methacrylate)]	170-175
Teflon [poly(fluoroethylene)]	430-435
Rubbers	
Hypalon	165
Neoprene	175-180
Durasol/neosol	180
Latex	195
Bitumen[b]	275

[a] Water loss observed at 40-110°C.
[b] Not a rubber material.

[6] Kato, K., et al., "Structural Changes and Melting Behavior of Gamma-Irradiated Polyethylene," Jap. J. Appl. Phys. 20, pp. 691-697, 1981.

[7] Igarashi, S., "Thermogravimetric Analysis of the Effect of Ionizing Radiation on Thermal Stability of Polyethylene," J. Appl. Polym. Sci., Vol. 8, pp 1455 - 1464, 1964.

6.6.5 Conclusions

The conclusions reached are that generation of gases through thermal degradation of the waste materials up to 302°F (150°C) will be negligible. While the threshold decomposition temperature in air of 302°F (150°C) is the temperature at which decomposition starts, the contribution to gas generation due to thermal degradation is negligible even at much higher temperatures (up to 100°F above the thermal decomposition temperature).[4]

APPENDIX 6.7

GAS RELEASE ASSESSMENT

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6.7 Gas Release Assessment

6.7.1 Summary

The hydrogen concentration will be maintained below 5% in all void volumes within the payload and packaging inner containment vessel (ICV) during transport of contact-handled transuranic (CH-TRU) materials. This document describes the logic and methodology used in evaluating payload characteristics that meet this requirement. Appendix 6.8 of the CH-TRU Payload Appendices describes the experiments relating to the quantification of hydrogen release rates from the payload containers.

Parameters that govern the maximum decay heat limits per shipping category are listed below:

- Waste configuration (i.e., the number and type of confinement layers).
- Release rates of hydrogen from each of these confinement layers.
- Hydrogen generation rates quantified by the effective G value of a waste material (the number of molecules of hydrogen produced per 100 eV of energy absorbed).
- Operating temperature for the payload in the ICV during a 60-day shipping period.
- Void volume in the ICV outside the payload containers available for gas accumulation.
- Duration of the shipping period.

A computational spreadsheet was used to perform the calculations required to determine the maximum decay heat values based on a pseudo steady-state model of gas release. The computed maximum decay heats are based on an approach that will ensure that hydrogen concentrations are safely maintained below the 5% limit during normal and accident conditions of transport. Among the factors that include a margin of safety to ensure an acceptably low hydrogen concentration are:

- Effective G values used in analytical calculations are higher than values reported for actual waste containers as part of sampling programs (see Appendix 5.3 of the CH-TRU Payload Appendices).
- Minimum measured hydrogen diffusion coefficients through the drum and standard waste box (SWB) filters rather than the average values.
- Minimum drum liner release rate.
- Only the leakage rate from the small bag closure used as the release rate from small bags (i.e., no credit taken for permeation through the plastic bag material).
- Lowest measured total release rate for a large bag was used.

- Void volumes inside each inner confinement layer and in the payload containers assumed to be zero.

- A 60-day shipping period compared to typical shipping periods of 5 days or less.

6.7.2 Introduction

In order to ensure safe transport of the payload in a package, the concentration of hydrogen within any void volume in a layer of confinement of the payload or in the ICV shall be less than or equal to 5% during an assumed 60-day shipping period.[1] The predominant mechanism by which hydrogen is generated within the payload is by radiolysis of the hydrogen-containing waste materials and plastic bags or sheets present in the payload (see Section 5.2 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control [CH-TRAMPAC]). This document describes the logic and methodology used to quantify the maximum decay heats, which will ensure acceptably low hydrogen concentrations.

A description of the payload configuration in the package comprises the next section. The factors affecting and controlling the maximum permissible release rate of hydrogen are discussed in Section 6.7.4. The margins of safety for the parameters that are used to quantify the decay heat limits are discussed in Section 6.7.5. The computational method that was developed to perform the mathematical analysis is described in Appendix 2.3 of the CH-TRU Payload Appendices.

6.7.3 The Payload and the Package

The term "payload" refers to the waste contents that will be transported in the package as defined by the CH-TRAMPAC. The classification of shipping categories is described in Appendix 2.1 of the CH-TRU Payload Appendices. The content codes in the different shipping categories are described in the CH-TRU Waste Content Codes (CH-TRUCON) document.[2] Payloads will be assembled in accordance with the CH-TRAMPAC.

6.7.3.1 Payload Configuration

Typically, for purposes of radiological safety, the CH-TRU waste is packaged in one or more layers of confinement (plastic bags). Bags are closed according to the specifications of Appendix 3.8 of the CH-TRU Payload Appendices. When a drum is the payload container, a punctured or filtered rigid drum liner may separate the waste bags and the steel drum shell (Section 2.9 of the CH-TRAMPAC). Each container is vented in accordance with Section 2.5 of the CH-TRAMPAC. The filter releases generated gases, while acting as a barrier for particulates. Authorized payload containers and payload configurations are specified in Section 2.1 of the CH-TRAMPAC.

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[1] U.S. Nuclear Regulatory Commission, SSINS No. 6835, IE Information Notice No. 84-72: "Clarification of Conditions for Waste Shipments Subject to Hydrogen Generation," September, 1984.

[2] U.S. Department of Energy (DOE), "CH-TRU Waste Content Codes (CH-TRUCON)," DOE/WIPP 01-3194, current revision, U.S. Department of Energy, Carlsbad Field Office, Carlsbad, New Mexico.

6.7.4 Parameters Affecting Release Rates and Decay Heat Limits

Specific parameters that affect these release rates are described below.

6.7.4.1 Permeability of Bags

The permeability coefficient or simply the permeability is a measure of the rate at which a gas passes through a material. Permeability may be defined as the number of moles of gas passing per unit time through a material of unit area that is of unit thickness under a unit partial pressure gradient at a specified temperature. Typical units for permeability are: (mole*cm)/(sec*sq. cm*mmHg). Therefore, the mass flow rate of a gas (e.g., hydrogen) through a material will increase with an increase in the available surface area, an increase in the partial pressure gradient of the gas across the membrane and with a decrease in the thickness of the material, and an increase in temperature.

6.7.4.2 Leakage Through Bag Closures

In addition to permeation through the plastic bags, hydrogen is also released through the closure at the end of the bags (Appendix 3.8 of the CH-TRU Payload Appendices). For bags closed by the twist and tape method, the twisted portion of the bag that is taped generally has a length of six inches. Hydrogen is then released by diffusion through the twisted closure. Bags that are folded and taped would be expected to offer very little resistance to the passage of hydrogen. Vented bags that are heat-sealed are installed with a minimum of one filter vent, with gas release occurring through the filter vent in addition to permeation (Section 2.5 of the CH-TRAMPAC). Bags that are closed with a twist and tape or fold and tape closure may be installed with a filter vent as a measure of safety. The closure methods described in Appendix 3.8 of the CH-TRU Payload Appendices are mandatory for all payload containers to be transported, as specified by Section 5.1 of the CH-TRAMPAC, and hence these release mechanisms for hydrogen will be in operation.

6.7.4.3 Bag Materials

Two kinds of bag materials are typically used by the waste generator sites, polyvinyl chloride (PVC) and polyethylene (PE). The permeability depends on the type of material, and any additives that are added to the polymer during manufacturing. For example, the permeability of a PVC bag generally increases with the amount of plasticizer used in making the film.[3]

6.7.4.4 Radiation Effects on Bags

The radiation from the decay of radionuclides within a bag may affect the properties of the bag including the permeability to hydrogen and other gases. Gamma radiation doses up to 800 Krad seem to have no significant effect on the permeability of PE or PVC to nitrogen, oxygen, carbon dioxide and water vapor.[4] The permeability of these materials to hydrogen can also be expected to yield similar results. Polymers like PE and PVC preferentially crosslink as a result of radiolysis, yet data from Deanin (1972)[3] seem to indicate that significant permeability changes

[3]Deanin R. D., 1972, "Polymer Structure, Properties, and Applications," Chaners Books; Boston, Massachusetts.

[4]Varsanyi, 1975, "Investigations into the Permeability of Polymer Membranes of Food Packaging Quality to Gases and Water Vapour after Radiation Treatment with Radurizing Doses," Acta Alimentaria 4, pp. 169-251.

do not result from this effect. Preliminary permeability data from an actual waste drum, that has been stored for a period of 15 years, indicate that the hydrogen permeability rates through both PE and PVC are higher when compared with new plastic samples.[5]

6.7.4.5 Temperature

Permeabilities are highly dependent on temperature. For this reason, values of permeability are and should be quoted at a specific temperature. The temperature dependence of the permeability may be represented by an Arrhenius type equation:[6]

P "is proportional to the" exp(-E/RT) (Equation 1)

where,

P = permeability
E = activation energy for permeation
R = gas constant
T = absolute temperature.

Typically, for polymeric membranes the activation energies for hydrogen per-meation are between 1 and 10 Kcal/gmole. The estimated activation energies for hydrogen permeating through PE and PVC membranes are 8.2 Kcal/gmole and 1.9 Kcal/gmole respectively.[6] Therefore, the permeability of hydrogen through PE is much more sensitive to changes in temperature than through PVC.

6.7.4.6 Diffusion Coefficients Through Filters

Each container must be vented in accordance with Section 2.5 of the CH-TRAMPAC. These filter vents prevent a potential pressure buildup due to generation of gases by allowing the venting of gaseous products while retaining particulates. Hydrogen molecules diffuse through a filter at a rate that follows Fick's first law of diffusion, which states that the diffusion rate is equal to the product of:

- Effective diffusion coefficient
- Cross-sectional area of the filter, and
- Concentration gradient across the filter.

The temperature dependence of hydrogen release through bag closures is a function of the diffusion process, as well as the closure configuration. While pure diffusion shows a slight decrease with decreasing temperature, actual tests (described in Appendix 6.8 of the CH-TRU Payload Appendices) show that the total release of hydrogen from bags can increase with

[5]Roggenthen, D. K., McFeeters, T. L., Nieweg, R. G., March 1989, "Waste Drum Gas Generation Sampling Program at Rocky Flats During FY 1988," RFP-4311.

[6]Perry, R. H., 1984, "Perry's Chemical Engineers' Handbook," 6th Edition, McGraw Hill Book Company, New York.

decreasing temperature. This aspect is discussed further in Appendix 6.9 of the CH-TRU Payload Appendices.

The effective diffusion coefficient of hydrogen through the filter is a fraction of that in air due to the presence of the solid filter medium.

6.7.4.7 Diffusion Through Drum Liner

If a rigid plastic drum liner is placed inside a drum to be transported, the liner must be punctured with a hole that has a minimum diameter of 0.3 inches, or a filter with hydrogen release rates equivalent to or greater than a 0.3-inch minimum diameter hole. Otherwise, the liner must be treated as any other confinement layer with the associated resistance calculated in accordance with Appendix 2.2 of the CH-TRU Payload Appendices. The release of hydrogen from this liner will therefore be comprised of two components: permeation of the gas through the material and diffusion of hydrogen through the punctured hole. The diffusion rate through the hole will be equal to the product of:

- Cross-sectional area of the hole
- Diffusion coefficient of hydrogen in air
- Concentration gradient of hydrogen.

6.7.5 Quantification of Decay Heat Parameters

6.7.5.1 Margins of Safety in Calculations

The purpose of this section is to identify the margins of safety associated with the parameters that determine the maximum permissible decay heat for each payload shipping category. The watts of decay heat have been derived incorporating several margins of safety as explained in the following sub-sections. The maximum decay heat values will ensure that the concentrations of hydrogen will be below the 5% limit during normal and accident conditions of transport.

6.7.5.2 Temperature and Pressure

The temperature dependence of hydrogen release rates is discussed in Appendix 6.9 of the CH-TRU Payload Appendices.

The pressure being used in the hydrogen release calculations is assumed to be constant at 1 atm. Since production of any gases would tend to increase the pressure (and reduce mole fractions of hydrogen), neglecting gas generation and any decrease in ambient pressure should not alter the margins of safety being used in the release calculations. Any increase in pressure in the inner confinement layers due to gas production would result in flow of the gases and higher release rates.

6.7.5.3 High G Values

The effective G values provided in Appendix 3.2 of the CH-TRU Payload Appendices bound the worst-case hydrogen producing material while allowing credit for weight percent water in the waste and self-absorption of alpha decay energy by radioactive particulates. For Waste Types II

and III, the assumption is made that all of the decay heat is absorbed by the material with the highest G value for hydrogen.

6.7.5.4 Minimum Hydrogen Diffusion Coefficients

Each payload container to be shipped will be vented as specified in Section 2.5 of the CH-TRAMPAC. The filters provide for venting of gaseous products while retaining particulates. A total of 18 filters of the carbon composite filter design (12 drum and 6 SWB) have been tested for hydrogen diffusivity[7] to calculate the hydrogen diffusion coefficient for each. Four of the Kevlar filters to be used in the bins have also been tested for their hydrogen diffusivity characteristics. As a margin of safety, the hydrogen diffusion coefficient assumed for the drum filter vent decay heat limit calculations is the lowest diffusion coefficient which has been measured. The value of this parameter is 1.90E-6 mole/sec/mole fraction[7] as opposed to the average value of 3.10E-6 mole/sec/mole fraction (Table 6.7-1). The value of the lowest measured diffusion coefficient for the SWB filter vent is 3.70E-6 mole/sec/mole fraction whereas the average was 4.87E-6 mole/sec/mole fraction (Table 6.7-2). This minimum hydrogen diffusivity value for the SWB filter vent is also used for

the bin filter vents, even though the hydrogen diffusivities of these filter vents are about four times higher than this value (Table 6.7-3). Testing and hydrogen diffusivity values for filter vents used in bags are discussed in Appendix 3.11 of the CH-TRU Payload Appendices.

6.7.5.5 Minimum Drum Liner Release Rate

If a rigid plastic liner is used in a drum, the liner must have a hole with a minimum diameter of 0.3 inches or a filter with hydrogen release rates equivalent to or greater than a 0.3-inch minimum diameter hole. Otherwise, the liner must be treated as any other confinement layer with the associated resistance calculated in accordance with Appendix 2.2 of the CH-TRU Payload Appendices before the drum can be transported. Release of hydrogen through the liner will occur by two mechanisms:

- Diffusion through the punctured hole or filter vent and
- Permeation through the material.

As a margin of safety, no credit will be taken for the release of hydrogen by permeation through the liner material. The release rate through the punctured hole is equal to the product of:

[7]Peterson S. H., July 1988, "Determination of Hydrogen Flow and Diffusion Properties of Selected Graphite Filters," Westinghouse Research and Development Center, Chemical and Process Development Department, Pittsburgh, Pennsylvania.

Table 6.7-1 — Hydrogen Diffusion Coefficients Through Drum Filters

Filter ID #	Diffusion Coefficient (mole/sec/mole fraction)
NFT-D1	3.60E-6
NFT-D2	3.30E-6
NFT-D3	5.70E-6
NFT-D4	4.23E-6
NFT-D5	3.22E-6
NFT-E5	3.38E-6
NFT-16	2.46E-6
NFT-17	2.43E-6
NFT-18	1.90E-6
NFT-21	2.10E-6
NFT-22	2.37E-6
NFT-23	2.50E-6

Source: Peterson S. H., July 1988, "Determination of Hydrogen Flow and Diffusion Properties of Selected Graphite Filters," Westinghouse Research and Development Center, Chemical and Process Development Department, Pittsburgh, Pennsylvania.

Table 6.7-2 — Hydrogen Diffusion Coefficients Through SWB Filters

Filter ID #	Diffusion Coefficient (mole/sec/mole fraction)
NFT-9026	5.43E-6
NFT-9027	3.70E-6
NFT-9032	5.19E-6
NFT-9033	4.80E-6
NFT-9034	5.19E-6
NFT-9035	4.90E-6

Source: Peterson S. H., July 1988, "Determination of Hydrogen Flow and Diffusion Properties of Selected Graphite Filters," Westinghouse Research and Development Center, Chemical and Process Development Department, Pittsburgh, Pennsylvania.

Table 6.7-3 — Hydrogen Diffusion Coefficients Through Kevlar Bin Filters

Filter ID #	Diffusion Coefficient (mole/sec/mole fraction)
K-23	7.7E-6
K-25	7.2E-6
K-27	7.4E-6
K-28	7.3E-6
K-25 (repeat)	7.7E-6

Source: Peterson S. H., and E. E. Smeltzer, August 1990, "Determination of Flow and Hydrogen Diffusion Characteristics of Kevlar Filters for WIPP," Westinghouse Science and Technology Center, Pittsburgh, Pennsylvania.

- Minimum cross sectional area of the hole (0.456 sq. cm)
- Diffusion coefficient of hydrogen in air, and
- Concentration gradient of hydrogen across the hole.

Another margin of safety that has been incorporated is that the diffusion coefficient of hydrogen in air at -29°C will be used in calculations of decay heat limits. With this value of the diffusion coefficient (0.511 sq. cm/sec) the release rate through the drum liner has been computed as 5.09E-5 mole/sec/mole fraction. Since the diffusion coefficient varies with temperature to the 1.75 power[6] the release rate would be higher by a factor of 1.42 at 25 °C but is not considered in the calculations for the decay heat limits. The sites that use a carbon composite filter to vent the liner will ensure that the release rate is equal to or higher than this value.

6.7.5.6 Release Rates From Bags

Several margins of safety have been incorporated in deriving the release rates from bags. These may be summarized as follows:

- For small bags (not large drum liner bags), such as those used to bag-out solid inorganics and organics, only the leakage through the worst-case bag material closure has been used as the release rate. All decay heat is assumed to be in the innermost layer of confinement. These bags do have a finite surface area which is typically around 0.6 sq. meters which would correspond to an additional release rate of around 2E-7 mole/sec/mole fraction at 25°C.

- Credit has been taken for only one closure, although the majority of the small bags have two closures. The release rate by this mechanism has been quantified as 5.58E-7 mole/sec/mole fraction based on experimental measurements (Appendix 6.8 of the CH-TRU Payload Appendices).

- For large bags the total release (closure leakage and bag permeation) as measured at three different temperatures (Appendix 6.8 of the CH-TRU Payload Appendices). For purposes of calculating the decay heat limits, the lowest measured total release rate of 4.67E-6 mole/sec/mole fraction was used.

- For the SWB and ten-drum overpack (TDOP) liners the total release rate is the sum of the release rates by permeation through the liner and the release rate through the small bag closure. The actual release rates through the SWB and TDOP liners are expected to be much higher due to the fold and tape closures that offer minimal resistance.

- For filtered small bags, only the diffusion through the filter vent has been used as the release rate. The lowest measured value for the hydrogen diffusivity was used in calculating decay heats.

- For filtered large bags, the total release consists of permeation through the bag and diffusion through the filter vent. The lowest measured values for the hydrogen diffusivity and permeation from the liner bags are used in calculating decay heats.

6.7.5.7 Void Volumes

A pseudo-steady-state analysis was used to compute the decay heat limit for each shipping category and will be described in detail in the following section. For the purpose of these calculations, an assumption of zero void volume inside each of the layers of confinement in a payload container has been made. This results in higher calculated concentrations of hydrogen in the different confinement layers and the ICV cavity. (The smaller the available volume for a given amount of hydrogen, the higher its concentration.) For fixed release rates of hydrogen through the various layers of confinement, this approach gives the lowest decay heat limits.

6.7.6 Decay Heat Limits for Shipping Categories

The method of arriving at a decay heat limit for the different shipping categories is presented in Appendix 2.3 of the CH-TRU Payload Appendices. The decay heat limit in watts per generator for each payload shipping category is presented in the CH-TRAMPAC.

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APPENDIX 6.8

GAS RELEASE TESTING

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6.8 Gas Release Testing

6.8.1 Summary

This document provides a summary of a testing program designed to obtain data on hydrogen release rates from confinement layer configurations that mimic real waste drums of contact-handled transuranic (CH-TRU) waste. Several different confinement layer configurations have been tested.

A test consists of simulating hydrogen gas generation in the innermost bag by a controlled release of hydrogen and monitoring the resulting hydrogen concentration within each of the void volumes between layers of confinement. All layers of confinement are initially purged with nitrogen. The tests are terminated when steady state conditions are achieved, (i.e., when the hydrogen volume percentage remains constant in all void volumes for twelve consecutive hours with a concentration of around 4.0 percent in the inner bag.) A mass balance for hydrogen at steady state permits the computation of effective release rates from each of the confinement layers since the flowrates across each layer are equal to each other and to the hydrogen gas injection rate.

The release of hydrogen from a waste confinement layer consists of two components:

- Permeation through the bag material
- Release through the bag closure ("twist and tape" or "fold and tape"), or through the filter vents in heat-sealed bags.

Only the release rate through the bag closure (5.6E-7 mole/sec/mole fraction) was used as the total release rate from small inner bags (Appendix 6.7 of the CH-TRU Payload Appendices). This value was computed as the difference in values obtained from Tests 9A and 9C. The contribution of bag permeation was not considered in the calculations in order to provide a margin of safety. Results of test 9B demonstrate that the bag permeability for small bags is nearly 80% of the value being used for the bag closure of the small bag.

The lowest measured total release rate (4.67E-6 mole/sec/mole fraction), based on Test 10C, was used as the total release rate from large drum liner bags in the computations of decay heat limits. These release rates serve as inputs to the hydrogen release estimates described in Appendix 6.7 of the CH-TRU Payload Appendices.

6.8.2 Introduction

The purpose of this document is to provide a summary of whole-bag hydrogen release tests that were conducted at Pacific Nuclear Systems, Inc., Richland, Washington. The objective of this test program was to obtain data on the release rates of hydrogen from each of several layers of confinement in drums that simulate the typical packaging configuration of CH-TRU waste.

The scope of the testing program is presented in the next section (6.8.3). A description of the experimental equipment can be found in Section 6.8.4. The details of the experimental procedure that was used are contained within Section 6.8.5. The quality assurance and quality control measures pertinent to the testing program are discussed in Section 6.8.6. The final section contains an analysis and summary of the experimental results.

6.8.3 Test Program

6.8.3.1 Task

The scope of the testing program is to obtain hydrogen release rate data for different configurations that mimic typically packaged CH-TRU waste drums (payload container). For purposes of radiological safety, the CH-TRU waste is packaged in multiple layers of plastic bags that are closed by one of the allowable methods specified in Appendix 3.8 of the CH-TRU Payload Appendices and subsequently placed in a payload container. The payload containers are vented as specified in Section 2.5 of the CH-TRAMPAC.

6.8.3.2 Configuration of Test Drums

The drums used to measure hydrogen release rates were generally configured as follows (from the drum to the innermost layer of confinement):

- 55-gallon drum (with gasket) and with a carbon composite filter installed in drum lid.
- 90-mil rigid high density polyethylene (HDPE) liner, punctured with 0.75"-diameter hole (bung removed).
- One or more layers of plastic bagging.

A detailed description of the test apparatus is presented in the following section.

6.8.4 Equipment Description

The purpose of this section is to describe the equipment that was used in conducting the hydrogen release tests. A schematic diagram of the external test equipment assembly is presented in Figure 6.8-1.

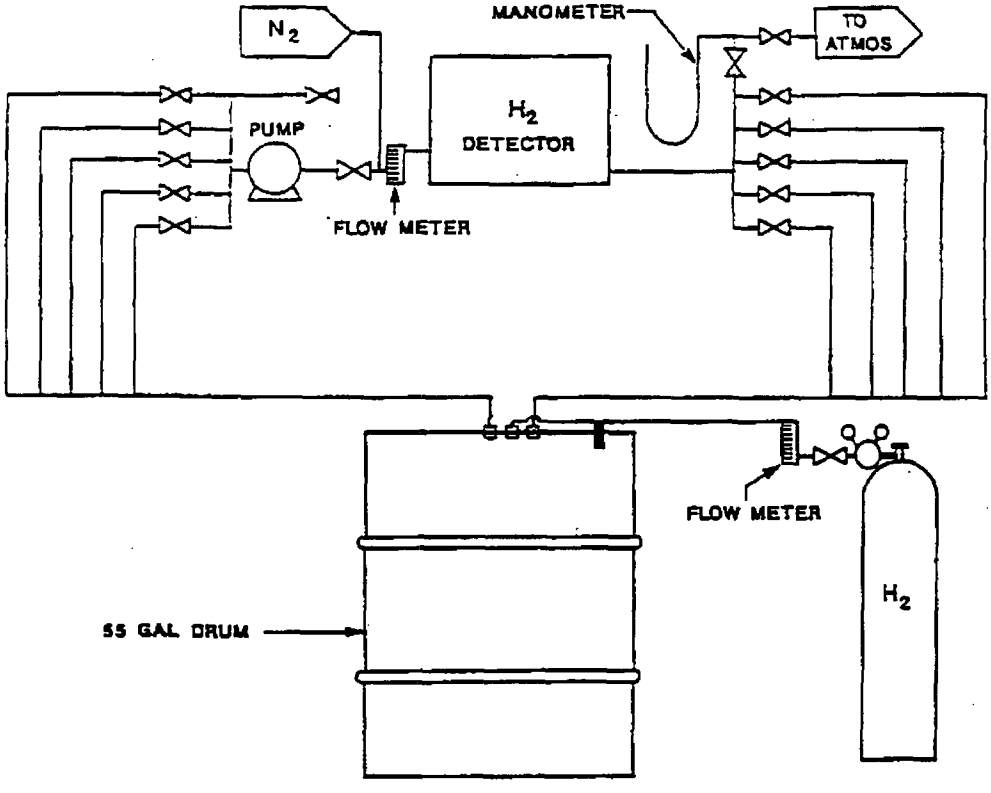

Figure 6.8-1—External Test Equipment Assembly

6.8.4.1 Plastic Bags

The four different types of bags used in the experiments were:

- 9 - 14 mil, 55-gallon PVC O-ring drum liner bag manufactured by Vinyl Tech Inc, used by Rocky Flats Environmental Technology Site (RFETS) and typical of bags used at all sites.
- 10 - 12 mil, 55-gallon PE round-bottom drum liner bag manufactured by the Hedwin Corp, used by RFETS and typical of large drum liner bags used at all sites.
- 9 - 14 mil, PVC bag-out (small inner bag) manufactured by Vinyl Tech Inc., used by RFETS and typical of bags used at all sites to bag-out waste from gloveboxes.
- 5-mil PE (small inner bag) manufactured by Parade Packaging Materials, used at RFETS and typical of bags used at all sites.

6.8.4.2 Drum Liner

This is a rigid, 90-mil, high density polyethylene (HDPE) liner for a 55-gallon drum, which is black opaque with a removable lid and seal. The lid has a 0.75-inch diameter hole near the center of the lid (after removal of the bung).

6.8.4.3 55-Gallon Drum

A drum made of carbon steel and painted white. The drum has a white neoprene rubber gasket between the body and lid. A filter vent is installed in the drum lid.

6.8.4.4 Filter Vents

The specifications for the filter vents are provided in Section 2.5 of the CH-TRAMPAC. The filters are installed in the lids of a drum. The filters release any gases that might be generated in the payload containers, while acting as a barrier for particulates (efficiency in excess of 99.9%). Model numbers and characteristics of the filters used in the hydrogen release tests are:

- Model 012, which is in service at RFETS. Two filters of this model, lot numbers NFT-17 and NFT-21, were used in the tests. The 3/4-inch threaded bung plug is made of mild steel.
- Model 013, which is in service at Savannah River Site (drums) will be used in SWBs. Two filters of this model, lot numbers NFT-9034 and NFT-9035, were used in the tests. The lid to this filter is distinct in that it is suspended 1/16-inch in the air by dimples stamped onto the lid. The 3/4-inch threaded bung plug is made of 304 stainless steel.

- Model 020, Lot number NFT-E filter, is used at the Idaho National Engineering and Environmental Laboratory and the Nevada Test Site. The 7/16-inch self-tapping threaded plug is made of 303 stainless steel.

6.8.4.5 Whole Drum Configuration

The experiments were set up with one, two, three, or four bags. Examples of the test configurations are shown in Figures 6.8-2 to 6.8-5 for Tests 4 to 7. The shaded areas in the figures represent a three-dimensional cage that was used inside the test apparatus to prevent the bags from collapsing and to sustain their shape. The experimental procedures for the tests are summarized in Table 6.8-1. Table 6.8-1 lists the exact configuration of each test set-up. The parameters that are listed in the table are defined below, in the order in which they appear.

PARAMETER	DEFINITION
Test Number	Uniquely identifies each test. For Tests 4 - 7, the B test was a repeat of the A test.
Temperature At Steady State (°F)	The temperature of the room measured at steady state.
Dimensions (in)	The dimensions of the bag as specified by the manufacturer.
Total Surface Area (sq. ft.)	Effective surface area of bag in test. (Does not include the closure area).
Confinement Layers	The confinement layer configuration for each test. (See next section for a complete description of each layer.)
Filter Type and Number	The filter (identified by model lot and serial numbers) that is installed in the lid of the drum.
Bulkhead -Duct Seal Used/Unused	A yes or no denotes whether duct seal was used to seal the bulkhead connections.
Type of Bag Seal	Denotes whether the method of sealing the bag was twist and tape or heat-sealing (for experimental purposes only).
Notes	Refers to the figure number in this appendix that depicts the confinement layer configuration.

Most of the experiments were set up to simulate typical waste configurations at the sites, except for Tests 9B and 9C that were specifically designed to measure individual components of the release rates (i.e., bag plus bulkhead plus closure, bag plus closure and bag only). The bag used in these tests was heat sealed for the purpose of the experiments. The following descriptions of the components of the test assembly refer to the experimental set up shown in Figure 6.8-1.

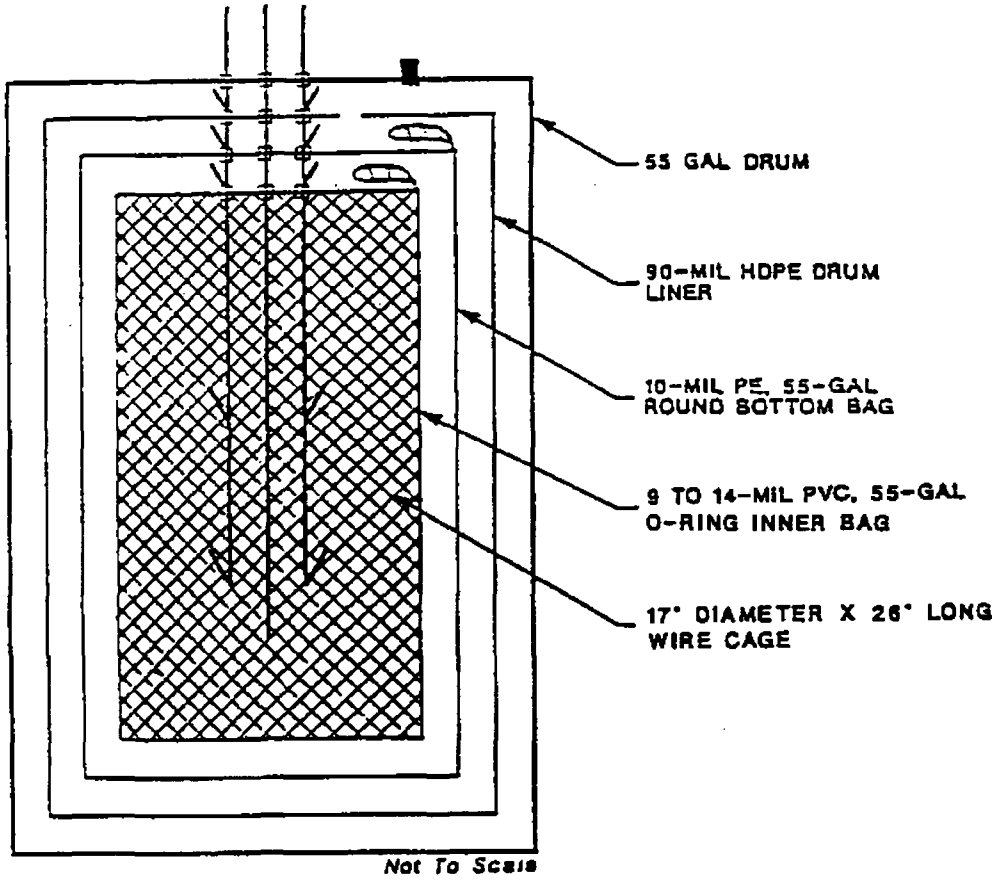

Figure 6.8-2—Test 4. Confinement Layer Configuration

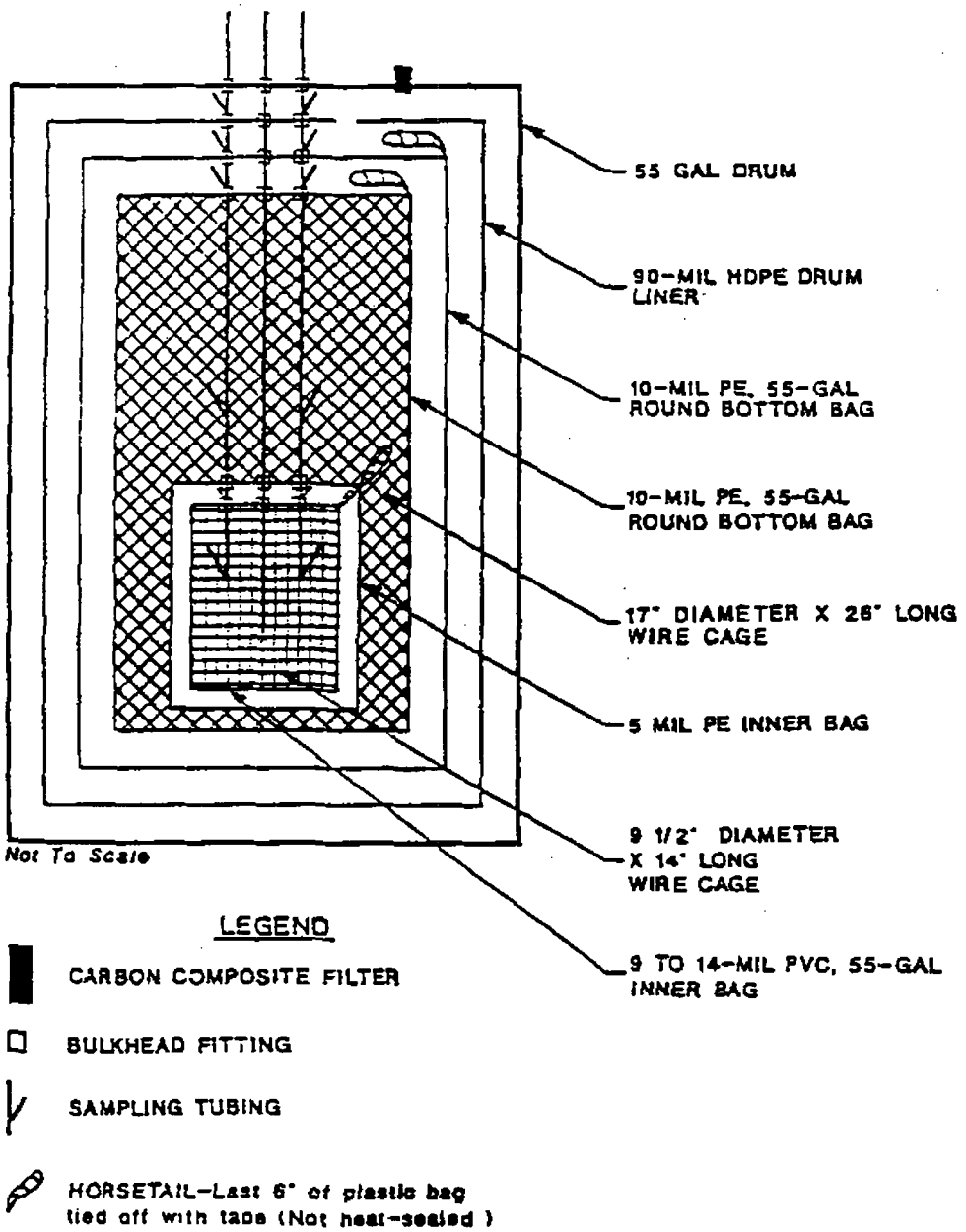

Figure 6.8-3—Test 5. Confinement Layer Configuration

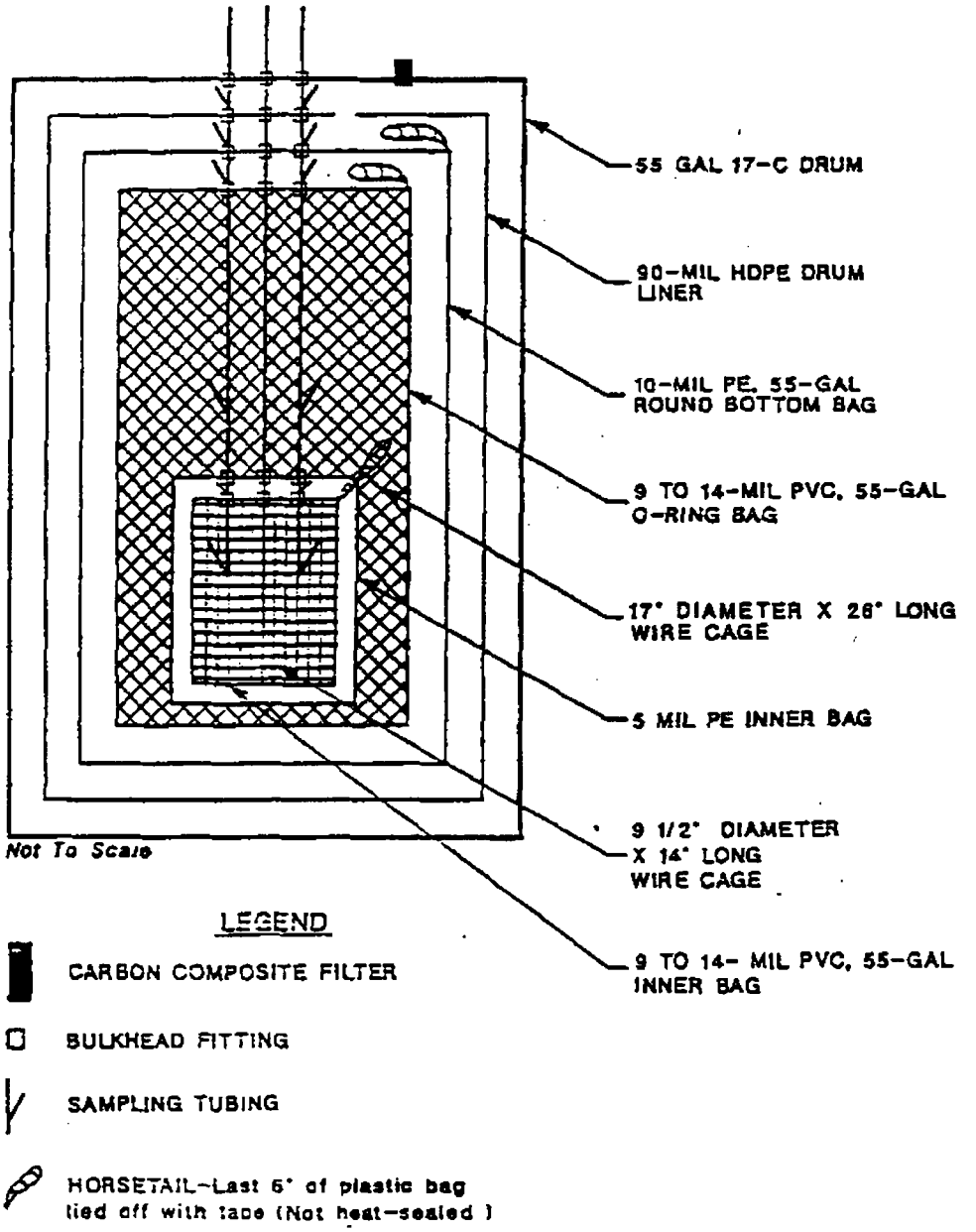

Figure 6.8-4—Test 6. Confinement Layer Configuration

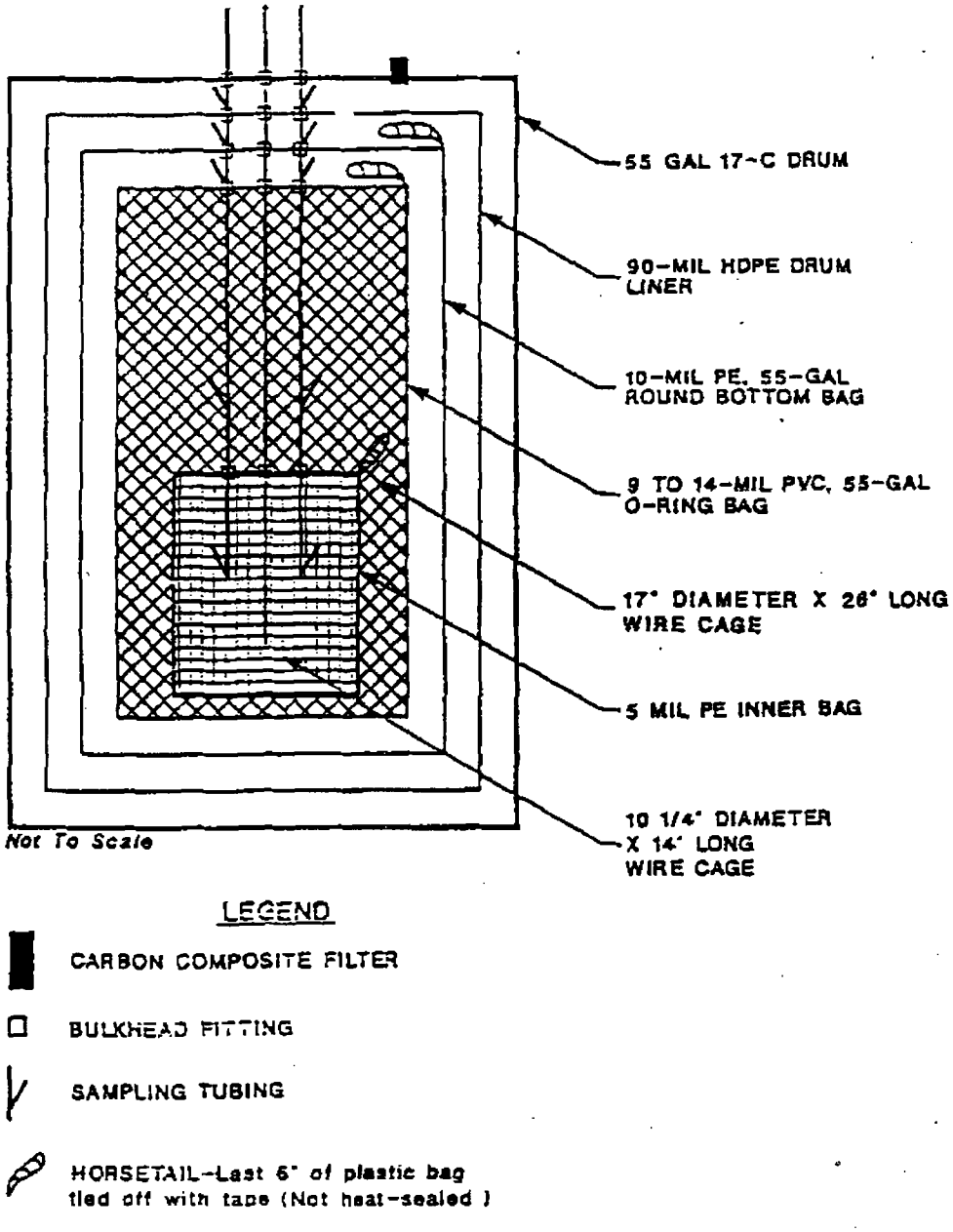

Figure 6.8-5—Test 7. Confinement Layer Configuration

Table 6.8-1 — Test Descriptions

Test Number	Temperature at Steady State (°F)	Dimensions (in.)	Total Surface Area (ft^2)	Confinement Layers	Filter Type and Number	Bulkhead Duct Seal Used	Type of Bag Seal	Notes
4A	74.0	36.875 x 86.5 37.625 x 58	36.6 29.4	14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-E INEL Design	No	Twist and tape closure	Figure 6.8-2
4B	76.0	36.875 x 86.5 37.625 x 58	36.6 29.4	14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-21 RFP Design	No	Twist and tape closure	Figure 6.8-2
5A	78.0	10 x 72 24.625 x 30.5 37.625 x 58 37.625 x 58	6.3 8.4 29.4 29.4	14 mil PVC inner bag-out 5 mil PE inner bag 10 mil PE liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-21 RFP Design	No	Twist and tape closure	Figure 6.8-3
5B	82.0	10 x 72 24.625 x 30.5 37.625 x 58 37.625 x 58	6.3 8.4 29.4 29.4	14 mil PVC inner bag-out 5 mil PE inner bag 10 mil PE liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-21 RFP Design	No	Twist and tape closure	Figure 6.8-3
6A	68.0	10 x 72 24.625 x 30.5 36.875 x 86.5 37.625 x 58	6.3 8.4 36.6 29.4	14 mil PVC inner bag-out 5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-17 RFP Design	No	Twist and tape closure	Figure 6.8-4
6B	66.0	10 x 72 24.625 x 30.5 36.875 x 86.5 37.625 x 58	6.3 8.4 36.6 29.4	14 mil PVC inner bag-out 5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-21 RFP Design	No	Twist and tape closure	Figure 6.8-4
7A	77.0	24.625 x 30.5 36.875 x 86.5 37.625 x 58	8.4 36.6 29.4	5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-17 RFP Design	No	Twist and tape closure	Figure 6.8-5
7B	71.0	24.625 x 30.5 36.875 x 86.5 37.625 x 58	8.4 36.6 29.4	5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	NFT-17 RFP Design	No	Twist and tape closure	Figure 6.8-5
9A	70.0	10 x 72	6.3	14 mil PVC inner bag-out	NFT-17 RFP Design	No	Twist and tape closure	

Table 6.8-1 — Test Descriptions (Concluded)

Test Number	Temperature at Steady State (°F)	Dimensions (In.)	Total Surface Area (ft^2)	Confinement Layers	Filter Type and Number	Bulk Head Duct Seal Used	Type of Bag Seal	Notes
9B	50.0	10 x 72	6.3	14 mil PVC inner bag-out	NFT-9035 SRP Design	Yes	Heat sealed	
9C	59.0	10 x 72	6.3	14 mil PVC inner bag-out	NFT-9035 SRP Design	No	Heat sealed	
10A	10.0	37.625 x 58	29.4	10 mil PE liner bag	NFT-17 RFP Design	Yes	Twist and tape closure	
10B	-18.0	37.625 x 58	29.4	10 mil PE liner bag	NFT-17 RFP Design	Yes	Twist and tape closure	
10C	57.0	37.625 x 58	29.4	10 mil PE liner bag	NFT-9034 SRP Design	Yes	Twist and tape closure	
11A	63.0	36.875 x 86.5	36.6	14 mil PVC liner bag	NFT-21 RFP Design	Yes	Twist and tape closure	

6.8.4.6 Sampling Tubing

Small diameter (0.125-inch O.D., 0.08-inch I.D.) Nylaflow tubing is used to penetrate the confinement layers to allow recycling of gas to measure H_2 concentration in confinement layers and to input H_2 into the innermost confinement layer.

6.8.4.7 Manometer

A water-filled manometer measures the pressure inside each confinement layer or void volume to a sensitivity of 0.1 inch of water. These measurements were discontinued once it was established that there is no pressure differential across any of the layers of confinement.

6.8.4.8 Hydrogen Cylinder and Two-Stage Regulator

A hydrogen cylinder (high purity), fitted with a two-stage regulator model #TSA-15-350, provides a steady flow of H_2 irrespective of changes in pressure inside the cylinder. Both of these items are manufactured by Oxarc Inc., Pasco, Washington.

6.8.4.9 Hydrogen Rotameter Assembly

A precision flowmeter, model FL-310, manufactured by Omega Engineering, Stanford, Connecticut, provides a flow rate of 0.03 to 30 ml/minute of H_2 at ambient temperature and pressure to the innermost bag confinement layer.

6.8.4.10 Bulkhead Fittings

All plastic (Nylaflow) tubing used to sample head spaces in layers of confinement were guided through bulkhead fittings to provide leak-tight seals. A combination of plastic, threaded bulkhead fittings with neoprene seal rings and multi-tube compression fittings (i.e., conax type) are used to prevent leakage of gases between confinement barriers around tubing penetrations. These fittings were supplied by Harrington Plastics, Seattle, Washington.

For the initial tests (Tests 4, 5, 6, and 7), a bubble test was used to detect any leaks that may occur around the bulkhead fittings. For the quantification of minimum release rates, the bubble test proved to be inadequate, and a special duct seal was used around the bulkheads to completely seal all possible areas of gas leakage. An independent study, utilizing Freon gas and commercial leak detection equipment, confirmed that with the duct seal, the system did not have any detectable gas leaks. The details for each individual test are summarized in Section 6.8.7.

6.8.4.11 Hydrogen Analyzer

A Beckman Model No. 6139-1-1-0-0-1-000 thermal conductivity analyzer is used for detecting hydrogen in nitrogen mixtures in the range of 0-5 percent by volume. The sensitivity of these detectors is ±0.05 percent H_2 by volume.

6.8.4.12 Gas Manifolds

Two valve manifolds are used for directing the flow from each of the different sample lines through the hydrogen analyzer (Figure 6.8-1).

6.8.4.13 Pump

A rotary, peristaltic, tygon tubing pump shown in Figure 6.8-1 is used for recirculating the atmosphere of each void volume between confinement layers. After aligning the appropriate inlet and return valves, the pump draws the gas out of a selected void volume and discharges it through the hydrogen analyzer (to measure H_2 concentration). The exhaust from the analyzer is returned (recycled) back to the same void volume through a gas diffuser.

6.8.4.14 Gas Diffuser

A porous plastic gas diffuser is used on each sample return line to reduce the gas velocity at the tubing exit.

6.8.4.15 Nitrogen Supply

Nitrogen gas is used for purging the atmosphere within the test drum and within each bag at the initiation of the experiment.

6.8.4.16 Nitrogen Purged Filter Vent Assembly

The open end of an inverted plastic beaker is sealed to the surface of the drum lid, covering the drum filter vent. A stream of nitrogen gas will continually purge the beaker to prevent the diffusion of air into the drum during testing. A small hole in the closed end of the beaker will allow introduction of a nitrogen purge tube and escape path for nitrogen purge.

6.8.4.17 Timer Solenoid H_2-Flow Control

A programmable timer, electric solenoid, and air-operated bellows valve system automatically control the H_2 flow rate. The timer can be programmed to supply H_2 for a desired amount of time per time period. This allows very low flow rates of H_2 to be supplied to the innermost bag. If the hydrogen flow is below the rotameter range or if the rotameter accuracy/repeatability is in question over a given hydrogen flow range, the hydrogen metering valve and regulator pressure

can be set at a fixed setting and the timer on/off cycle can be varied to provide the desired hydrogen injection rate. These are all manufactured by Seattle Valve and Fitting, Bellevue, Washington.

6.8.5 Experimental Procedure

6.8.5.1 General Requirements

The general requirements for all of the hydrogen release tests can be summarized as follows:

- All fittings for tubing penetrations into confinement layers are ensured to be gas tight in order to prevent leakage of hydrogen. For initial experiments, a soap bubble test was used for all fittings. Additional testing demonstrated that the seal in the bulkheads was not adequate. Starting with Test 9B, duct seal is used in all experiments to prevent any gas leakage around fittings.

- The atmosphere within the test drum and within each void volume is purged and replaced by inert nitrogen prior to the introduction of hydrogen for safety purposes.

- Hydrogen is injected into the inner bag until a concentration of 5 volume percent is attained. The hydrogen supply is turned off and the inner bag void volume is allowed to decay to four percent. The purpose of this is to obtain an approximate estimate of the hydrogen release rate from each layer.

- Hydrogen gas concentration is analyzed at regular time intervals from each void volume and recorded. Utilizing the timer and the hydrogen solenoid valve, the flow rate of hydrogen is adjusted to achieve steady state at 4 percent in the inner bag.

- The test is terminated when steady state is achieved in all void volumes between confinement layers with a concentration of approximately 4 percent in the innermost bag. The test is continued for approximately 12 hours after steady state conditions are achieved.

For each test, the pertinent information is recorded on a "Datasheet." A copy of a sample Datasheet is included as Table 6.8-2. In addition to the parameters listed on the Datasheet, the confinement layer configuration (i.e., type and number of bags), vendor, and sizes are also included to completely define each test.

The following sections describe the detailed experimental procedure that was followed for each test.

Table 6.8-2 — Example Datasheet For Hydrogen Release Experiments

			Pressure			
Time	Sample	H_2 Conc. (% Vol)	Static (in of H_2O)	Baro.	Temp. (F^o)	Observations/Initials
2/1/89						
0000	Drum	1.14			70	
	Inner Bag	3.99				
0800	Drum	1.15			69	
	Inner Bag	3.99				
1000	Drum	1.15			72	
	Inner Bag	3.99				
2330	Drum	1.15			71	
	Inner Bag	3.99				

Date HYDROGEN RELEASE TEST FOR TYPICAL
RFETS CH-TRU DRUM

6.8.5.2 Installation of the Gas Flow Tubing

- Make the penetrations through confinement layers and install the bulkhead fittings and sample tubes through the drum lid, drum liner lid (if used), and each bag.
- Install a gas diffuser on the end of each sample return line in the bags.
- Label the outside ends of the tubing.
- Assemble the appropriate bag configuration system for each test per instructions (list of tests is in Table 6.8-1).
- Place the appropriate bag system adjacent to the drum liner lid and place the drum liner lid adjacent to the 55-gallon drum.
- Adjust the tubing lengths so that they are placed in the desired area of the appropriate bag or container lid. Tighten the compression fitting nut on the tubing seals approximately 1/3 turn from hand tight. Then apply duct seal putty to all bulkhead fittings if applicable to the particular test.
- Verify that the outside end of each tube is attached to the appropriate connection on the gas manifolds. Cycle the gas flow pump to ascertain that unrestricted flow can occur through each tube.

6.8.5.3 Closure of the 55-gallon Drum

- Cut the small 14-mil PVC bag-out bag in concurrence with dimensions of the bag listed in Table 6.8-1 and insert a rigid frame (wire cage) inside the bag to maintain the size of the bag for Tests 5, 6, 9, and 11. For Tests 4 and 7, cut the 14-mil PVC 55 gallon O-ring drum liner bag as identified in Table 6.8-1 and insert rigid frame inside the bag to maintain the size of the bag (Figures 6.8-2 to 6.8-5 show typical configurations of these bags). Utilize maximum size frame in all cases. For Test 7, place maximum size frame inside the 5-mil PE bag. Record dimensions and details of frame construction on Datasheet.
- Place wire frame inside third bag to support bag volume around inner and second bag for Tests 5 and 6. For Test 7, place the second wire frame inside second bag to support bag volume around the inner bag. Record dimensions and details of frame construction on Datasheet.
- Insert nitrogen purge tube into bottom of each bag. Purge for five to ten minutes. Remove purge tube and then, if not a heat-sealed bag (only experiments 9B and 9C), make a twist-and-tape closure as follows:
  - Twist top 6 inches of bag into "horsetail" closure. Twist the 55-gallon PVC O-ring bag and the 55-gallon PE round-bottom bag each four turns at 180 degrees

each. Twist both the small PVC bag-out bag and the small PE bag six turns at 180 degrees each.

— Hold the twisted end, tape around the horsetail, starting at the bag end of the twist and wrapping in upward spirals until the end of the horsetail is reached. Continue wrapping up and down horsetail until three or four layers of tape have been reached.

— Repeat nitrogen purge and seal open end of each bag used as per Table 6.8-1.

- Insert carefully the bags with internal frames inside the 90 mil rigid liner if used (refer to Table 6.8-1). Install the lid of the 90-mil liner on top of the liner and snap it into place. Adjust tubing lengths through bulkhead fittings and tighten the compression fitting nut on the tubing seals approximately 1/3 turn from hand tight. Then apply duct seal to bulkhead fittings as per the individual test procedure.

- Guide all the sampling lines through the holes in the lid for the 55-gallon drum as the lid is placed and secured to the top of the 55-gallon drum. After placement of the 55-gallon drum lid, adjust tubing lengths through the bulkhead fittings and tighten the compression fitting nut on the tubing seals approximately 1/3 turn from hand tight. Do not kink or crimp the nylon tubing.

- Test the manifolds for any leaks.

6.8.5.4 Purging of Drum

- Start nitrogen purge of drum and 90-mil rigid drum liner by removing drum bung and connecting nitrogen supply to drum return tubing and 90-mil drum liner inlet tubing. Establish flow of nitrogen into drum cavity while performing the next step. Adjust the nitrogen flow to produce noticeable flow of nitrogen out of the open bung hole.

- Place inverted plastic beaker on top center of drum lid and seal with RTV or duct seal. Insert N_2 purge tube through small hole in top of beaker.

- Isolate nitrogen purge on drum and 90-mil drum liner and reinstall bung in drum lid.

- Test static pressure inside each bag void volume with water manometer. Record on Datasheet. Open return valves as required to vent all bags to atmosphere until pressure inside each bag is less than 1/8-inch water prior to starting test. Following commencement of test no static pressure readings are required.

6.8.5.5 Testing of Drum

- Record actual flowrate of hydrogen or timer interval on Datasheet. The source of hydrogen for the experiment will be a cylinder with a two-stage regulator that will

provide a large decrease in pressure to the rotameter and help stabilize the flowrate as the pressure in the cylinder decreases with usage. The two-stage regulator will be connected to the hydrogen rotameter.

- Verify zero and span calibration of hydrogen monitor as described in Section 6.8 by connecting calibration gas to the nitrogen inlet of the hydrogen monitor. Record data on Datasheet.

- Sample for gas analysis from each void volume at periodic intervals as follows. Three samples per day at approximately 8-hour intervals until steady state is reached. Record data on Datasheet.

- Turn off or reduce the hydrogen supply after the inner bag attains 4.5 to 5% hydrogen and allow the system to decay to approximately 4%. Initiate hydrogen gas input into the inner bag to sustain a 4% hydrogen level. Utilizing the timer and hydrogen solenoid valve, adjust flowrate to achieve steady state at 4% in inner bag. Terminate test when steady state is achieved in all void volumes with a concentration of around 4% in the innermost bag for 12 consecutive hours.

6.8.5.6 Sampling of Gases

- The sampling procedure is based upon the following operational parameters of the Beckman Thermal Conductivity Analyzer. Important operating parameters are:

  — A sample of nitrogen gas should always be flowing through the hydrogen monitor, except during valve manipulations.

  — A flow of 100 to 200 cc/min of sample gas is required during recirculation of gas within a layer of confinement void volume.

  — If sample gas flow must be interrupted for more than 1 hour, it will be necessary to turn off the hydrogen monitor. Operations should be planned to avoid deenergizing the hydrogen monitor to prevent delays caused by heat up stabilization and recalibration.

  — The sampling order is:
    1. Drum
    2. Drum Liner
    3. Large Bag
    4. Second Large Bag (If used)
    5. Inner Bag
    6. Bag-out Bag

- Sample all void volumes as follows:
  — Verify hydrogen meter reads zero percent. If meter is more than 0.05 percent off zero, recalibrate as described in next section.

- Isolate nitrogen purge gas to monitor by closing upper nitrogen valve and then close gas out valve on return manifold.

- Record temperature at each recording on Datasheet.

- Turn on sample pump to 35% to 45% speed to provide 100 to 200 cc/min sample gas flow through monitor. Open and then close appropriate inlet and return valves for desired void volume to allow sample gas to flow through manifold. Continue sample gas flow for 1 to 5 minutes until hydrogen monitor stabilizes. Record hydrogen concentration on Datasheet.

- After all void volumes are sampled, verify that all sample valves are closed and the pump is on.

- Open gas-out and manometer valves and throttle open lower nitrogen valve to provide nitrogen purge flow (10-50 cc/min) to pump and monitor through the inlet manifold.

- Close lower nitrogen valve (inlet manifold) and then stop sample pump.

- Throttle open upper nitrogen valve to provide a continuous nitrogen purge (10-50 cc/min) to monitor. Verify purge flow is directed to inverted beaker on top of drum.

- Repeat the sampling of gases per schedule.

- Repeat calibration check on hydrogen monitor as described in the next section.

6.8.5.7 Calibration Check

- Check calibration of hydrogen monitor with known calibration gas (5 percent hydrogen by volume in nitrogen) as follows:

  - Verify hydrogen monitor reads zero percent with nitrogen purge gas at 50-200 cc/min to monitor. Rezero by changing zero dial as required.

  - Disconnect nitrogen inlet to monitor and connect calibration gas.

  - Meter in calibration gas carefully and stabilize flow at 50-200 cc/min. Allow monitor to stabilize, one to five minutes. Recalibrate monitor to full scale (5 percent) by changing span dial, as required. Record hydrogen concentration on Datasheet.

  - Isolate calibration gas and disconnect.

— Reinstall nitrogen purge tubing and valve in nitrogen purge flow (10-50 cc/min) to monitor.

6.8.6 Quality Assurance and Quality Control

6.8.6.1 Documentation

The following information is recorded throughout the test program for each test on the Datasheet:

- Chronological log with time at each sampling
- Hydrogen concentrations within each containment layer void volume at each sampling
- Temperature in the testing room at each sampling
- Any visual observations.

6.8.6.2 Verification of Rotameter Calibration

The hydrogen rotameter factory calibration is verified by flowing hydrogen through the rotameter into a water-filled, inverted graduated cylinder provided with a water seal.

6.8.6.3 Verification of Hydrogen Monitor Calibration

The hydrogen monitor (i.e., Beckman thermal conductivity analyzer) calibration should be verified as described in Section 6.8.5.7 at the beginning and end of the test, or more frequently if sufficient drift in the calibration is observed. Record the hydrogen calibration check on the Datasheet.

6.8.7 Analysis of Experimental Data

6.8.7.1 Testing Program Versus Waste Generation Procedures at Sites

The testing program described here has been formulated to obtaining release rates of hydrogen through systems that were representative of real waste, but with a margin of safety. The bag closure methods used in these tests (described in Section 6.8.5.3), for example, are more stringent (tighter wrapping and more layers of plastic tape) than what is usually practiced at the sites. The tie off procedure in the tests is usually carried out by two individuals in order to obtain as tight a closure as possible. Independent (and qualitative) tests were also performed using easily detectable gases (i.e., Freon) to verify that variations in closure methods including double bent tie offs are not less restrictive than the procedure used for closure during the testing. Soap

bubble tests were also performed to determine the relative amount of release through the closure. All of these tests showed that in most cases, the leakage of hydrogen through the closure was the dominant release mechanism. At some of the U.S. Department of Energy sites, two or more of the bags are sometimes tied off in single tieoffs, which should further increase the release of hydrogen (compared to two layers with independent closures). Results from these tests are therefore expected to provide a reasonable margin of safety in estimating release rates of hydrogen.

6.8.7.2 Determination of Release Rates

6.8.7.2.1 Introduction

The tests were terminated when steady state conditions were achieved, i.e., when the hydrogen volume percentages remained constant in all void volumes. Figures 6.8-6 through 6.8-20 are plots of the hydrogen concentration in each of the bag layers in a given test versus time. The test numbers can be correlated with the test configuration through Table 6.8-1. When steady state conditions are achieved, the hydrogen concentrations in the different layers do not change with time. The figures also serve to highlight the relative resistances of the different layers to the release of hydrogen. Higher the gradient of hydrogen across a barrier, higher is its resistance. For example, from Figure 6.8-8, it can be seen that the concentration gradient of hydrogen across the liner is very small. This is because the punctured liner offers very little resistance to the release of hydrogen compared to the other bag layers.

Once steady state is achieved, the molar flowrates of hydrogen across each of the confinement layers are equal to each other and to the hydrogen generation rate (simulated in the tests by injection of a controlled stream of hydrogen). The flowrate across a layer is equal to the product of the hydrogen release rate and the mole fraction difference across a layer of confinement. The gas injection rate was converted from a volumetric flowrate in (ml/hr) to a molar flowrate in (mole/sec) via the ideal gas law equation. The pressure was assumed to be atmospheric (i.e., 1 atm.). The temperature at steady state for each test was used in the ideal gas law equation.

The release rate for a confinement layer was therefore computed using the following relation:

$$R_r = \frac{CG\,x\,P/(RT)\,x\,hr/3600\,\text{sec}}{Delta\,x}$$

where,

R_r	=	Release rate from a confinement layer (mole/sec)
CG	=	Hydrogen gas injection rate (ml/hr)
P	=	Atmospheric pressure (1 atm)
R	=	Gas law constant (82.054 atm*ml/mole*K)
T	=	Absolute temperature at steady state (K)
Delta x	=	Volume (mole) fraction hydrogen gradient across the confinement layer.

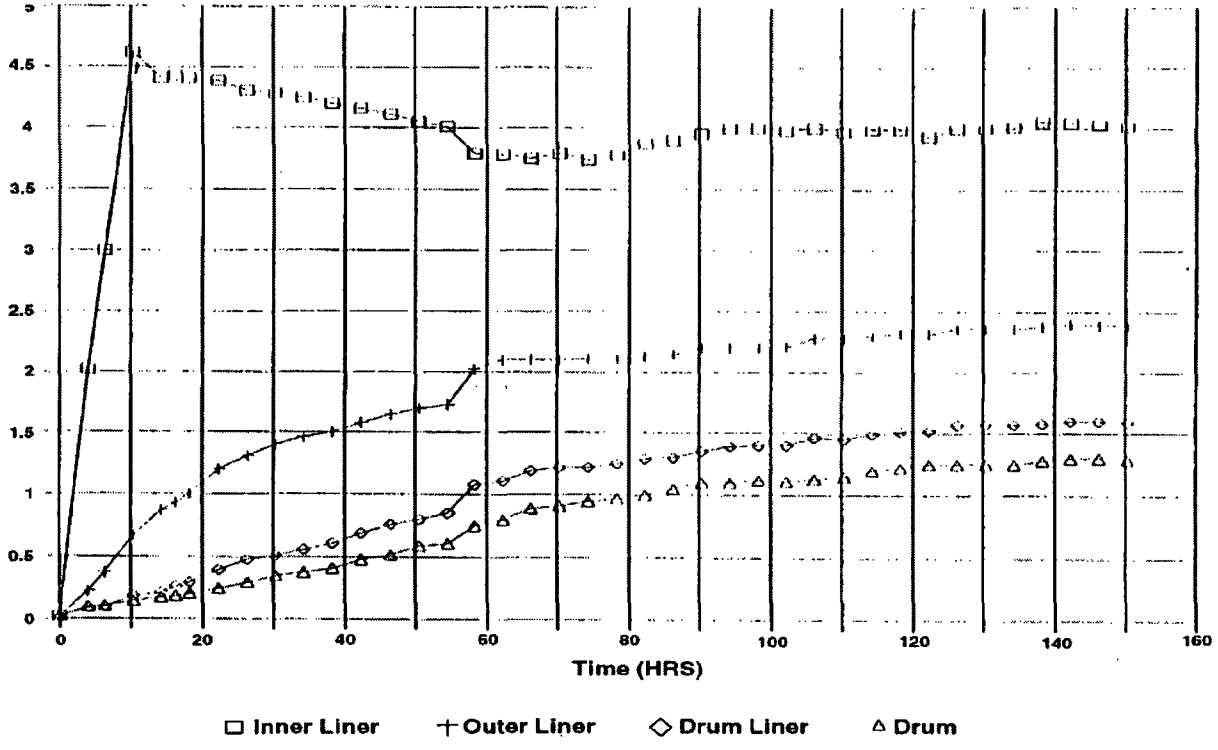

Figure 6.8-6—Hydrogen Concentration Profiles in Confinement Layers, Test Number 4A

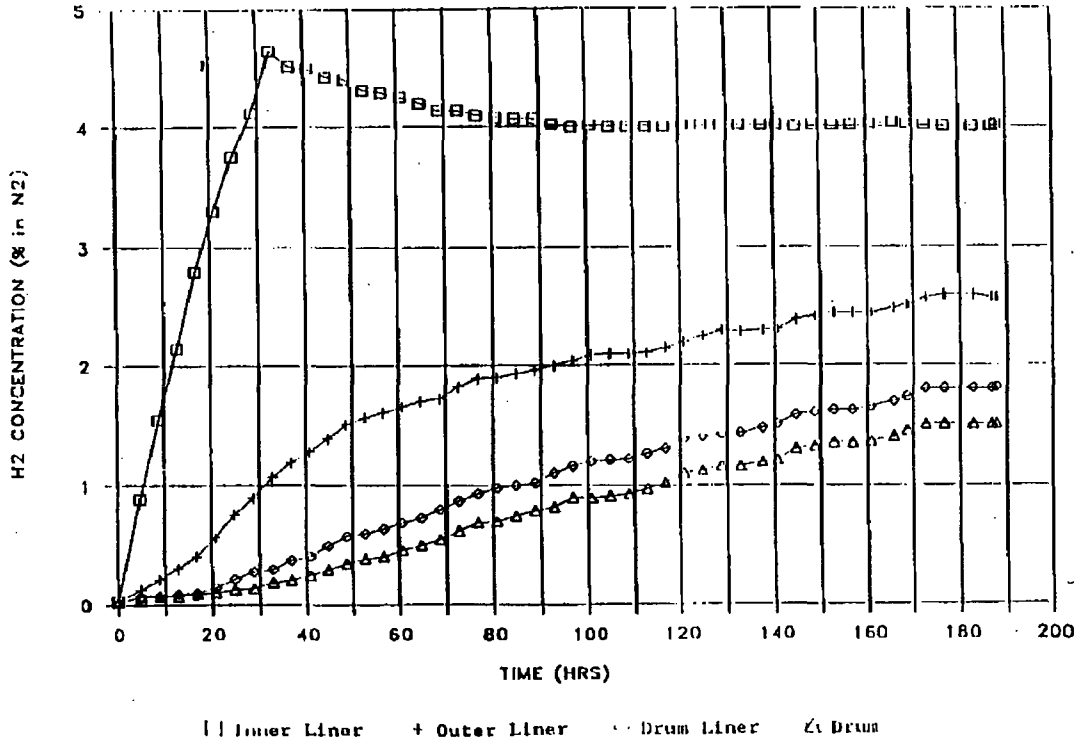

Figure 6.8-7—Hydrogen Concentration Profiles in Confinement Layers, Test Number 4B

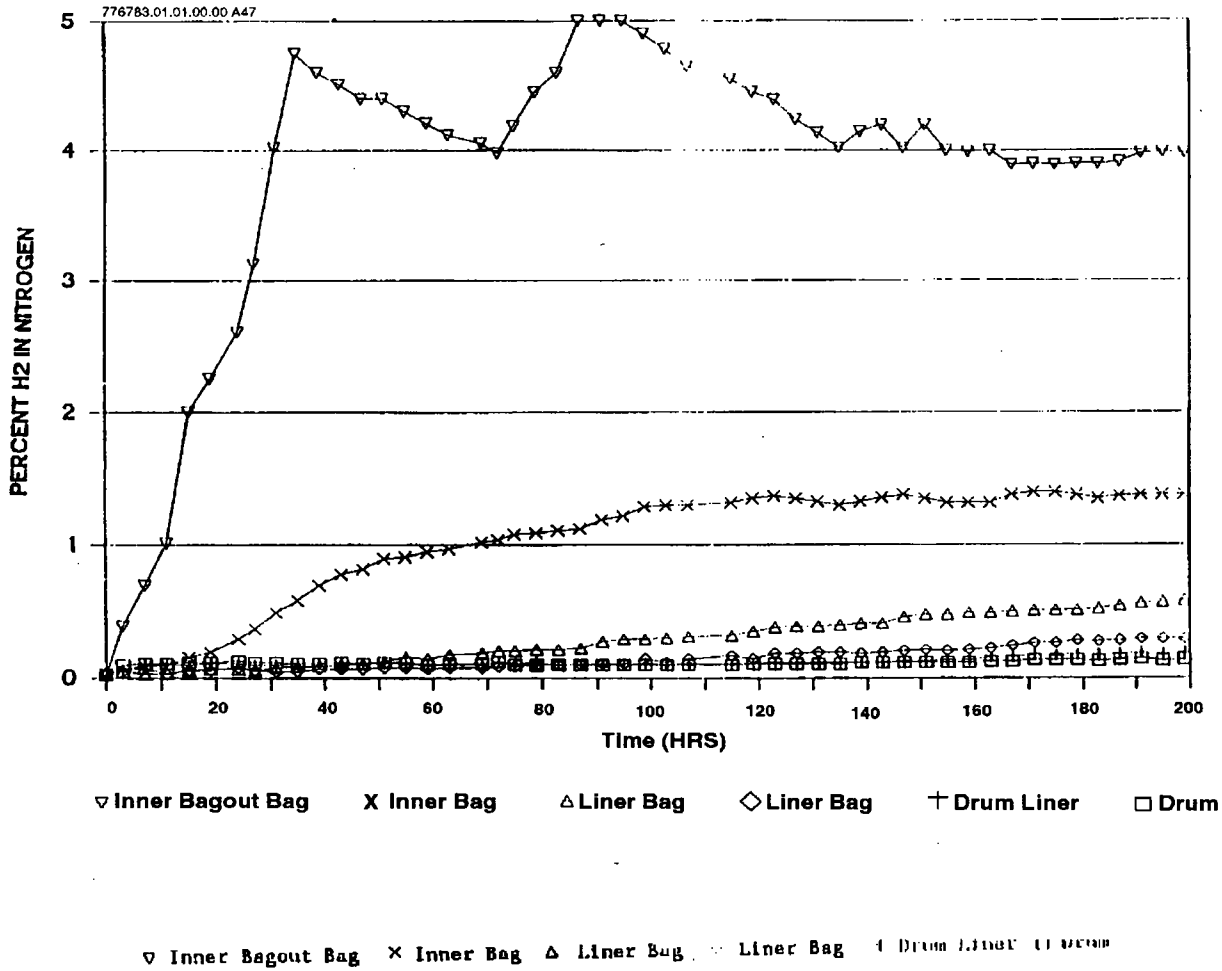

Figure 6.8-8—Hydrogen Concentration Profiles in Confinement Layers, Test Number 5A

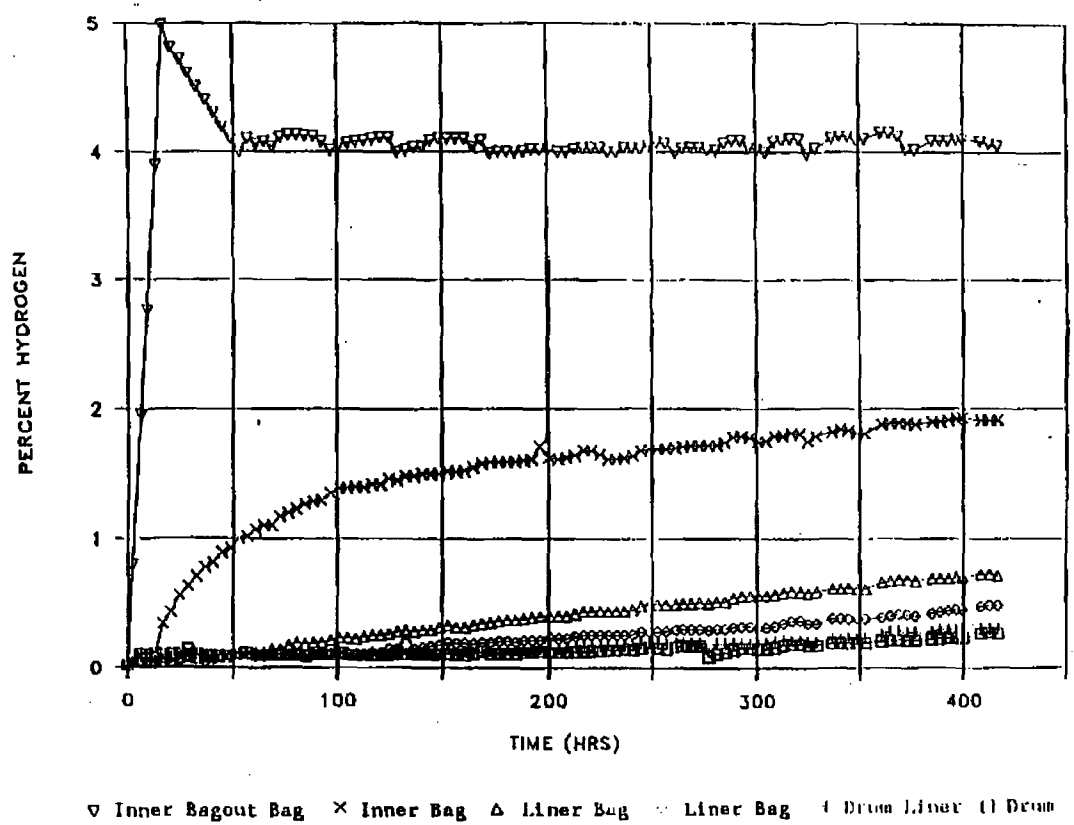

Figure 6.8-9—Hydrogen Concentration Profiles in Confinement Layers, Test Number 5B

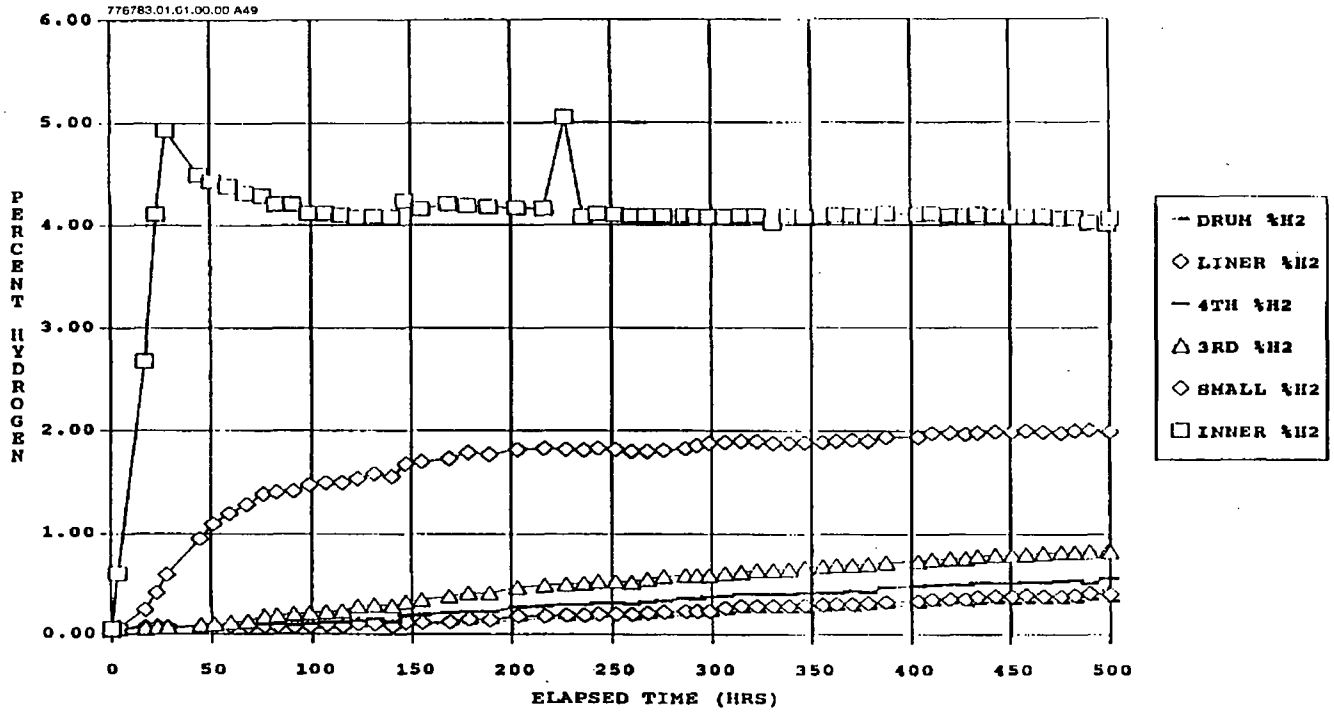

Figure 6.8-10—Hydrogen Concentration Profiles in Confinement Layers, Test Number 6A

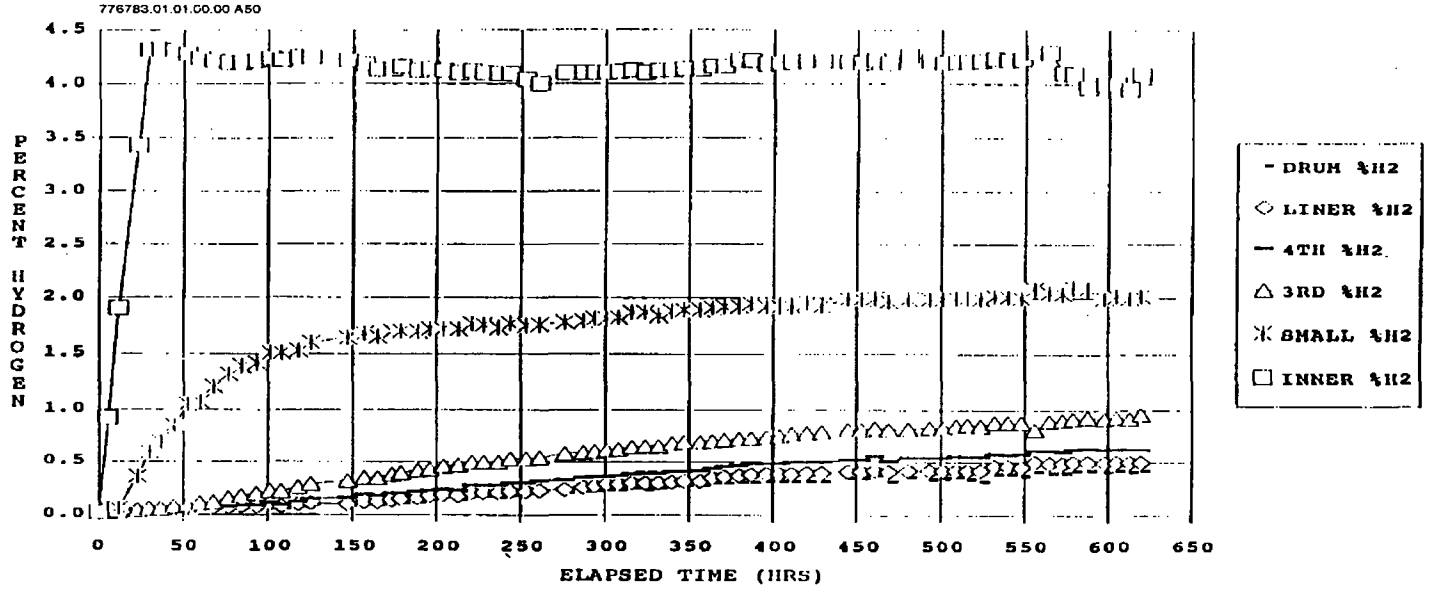

Figure 6.8-11—Hydrogen Concentration Profiles in Confinement Layers, Test Number 6B

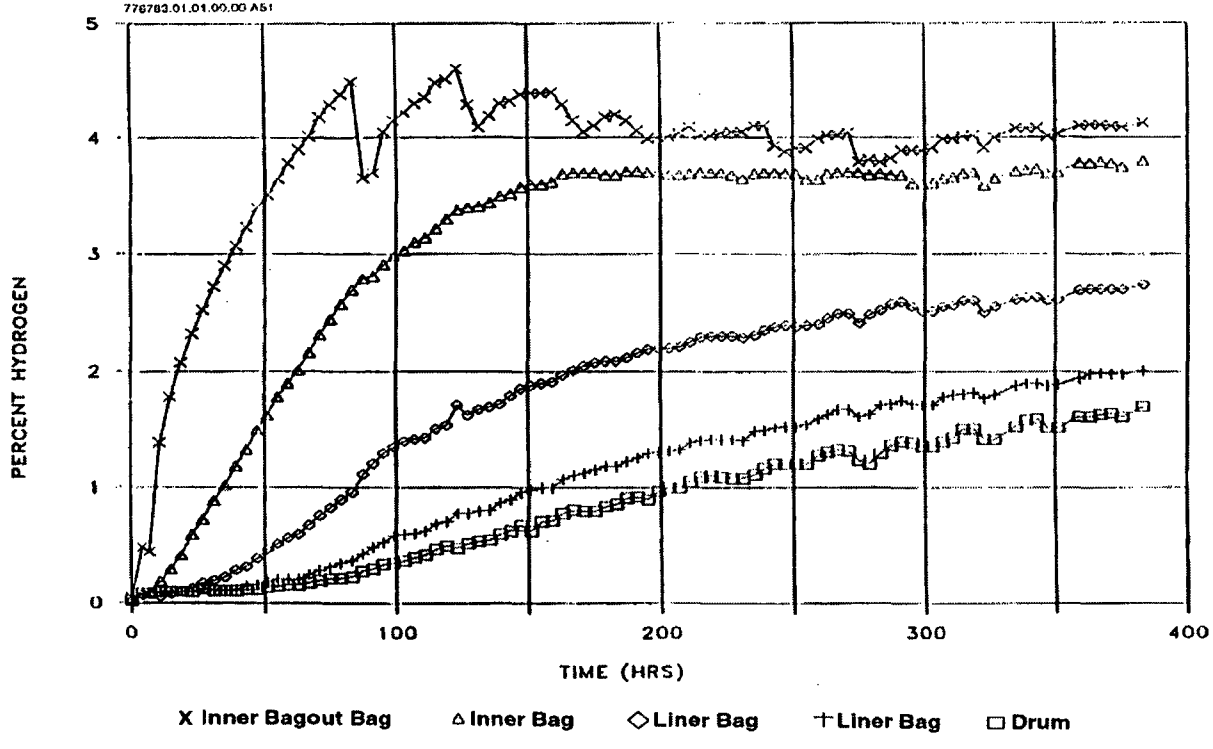

Figure 6.8-12—Hydrogen Concentration Profiles in Confinement Layers, Test Number 7A

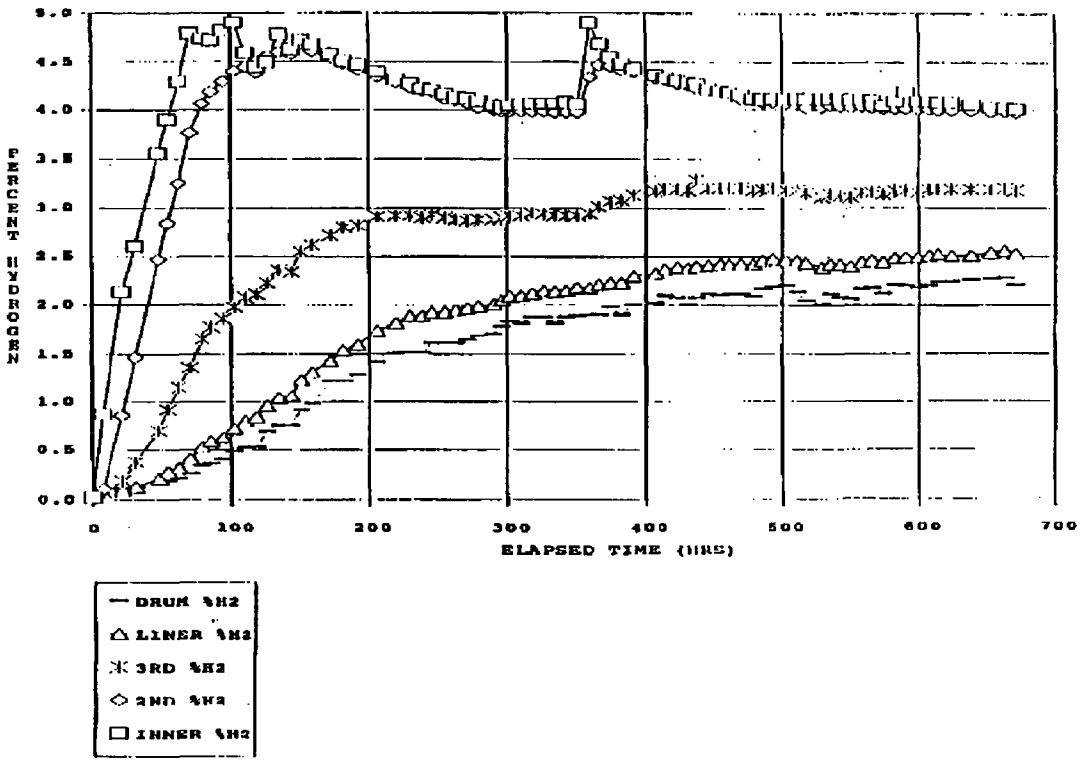

Figure 6.8-13—Hydrogen Concentration Profiles in Confinement Layers, Test Number 7B

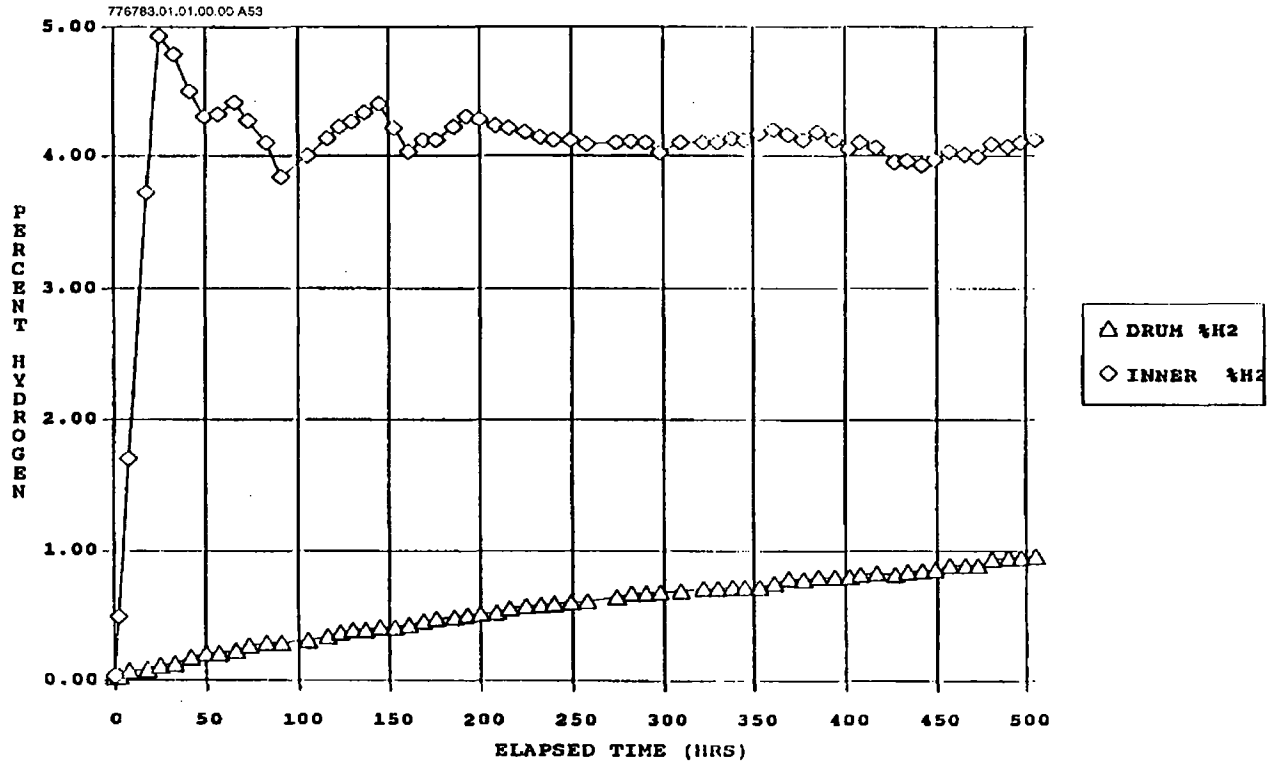

Figure 6.8-14—Hydrogen Concentration Profiles in Confinement Layers, Test Number 9A

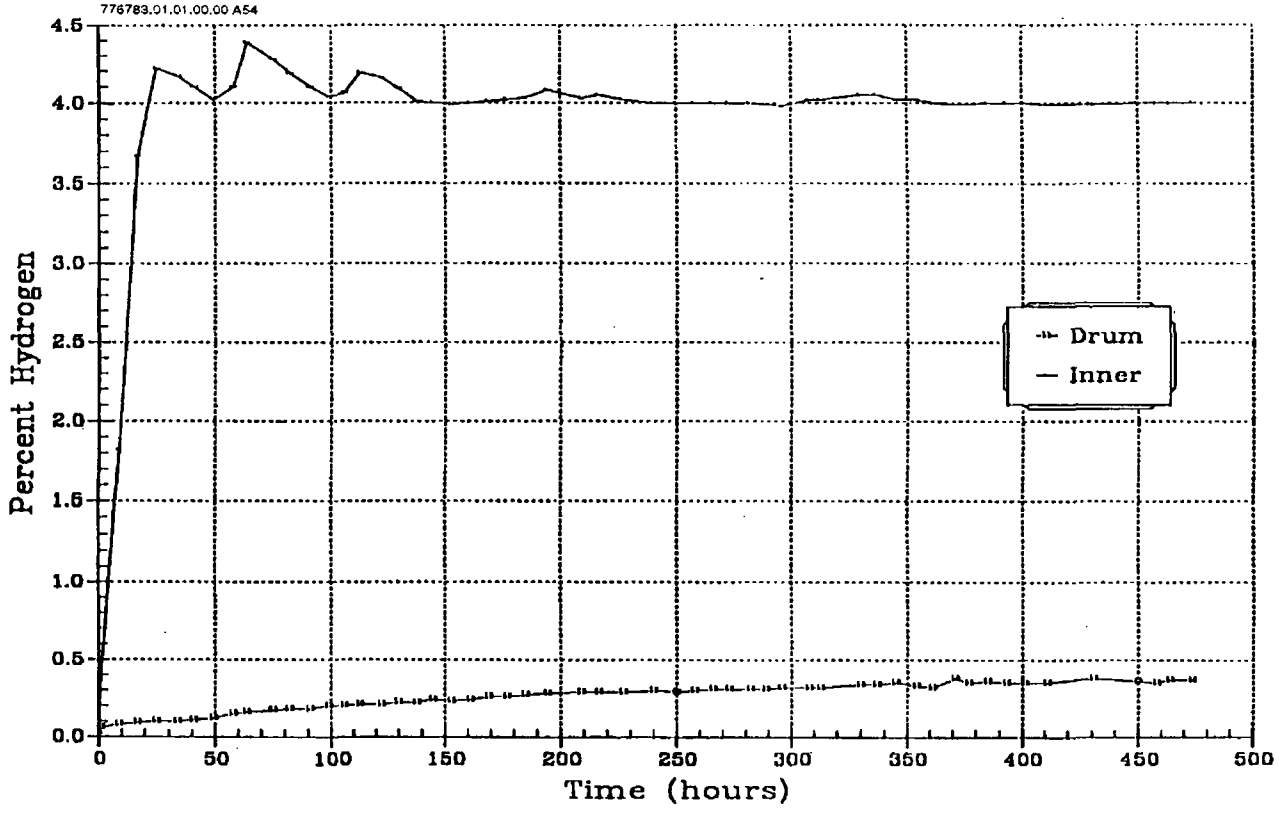

Figure 6.8-15—Hydrogen Concentration Profiles in Confinement Layers, Test Number 9B

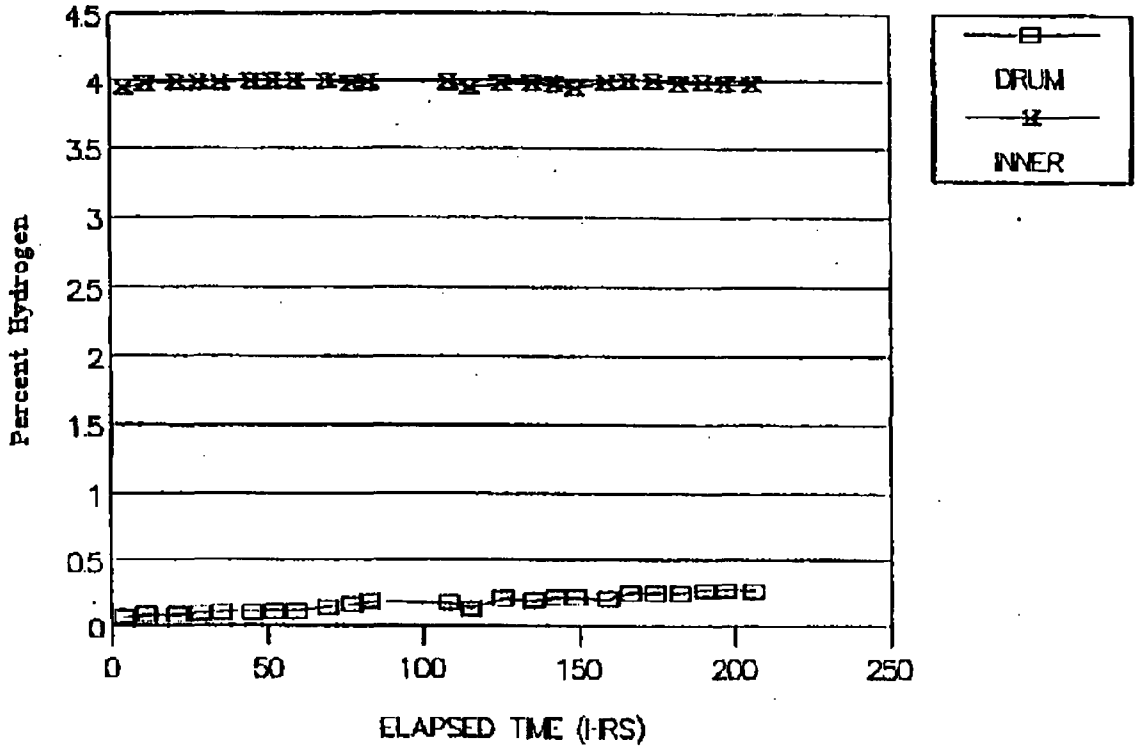

Figure 6.8-16—Hydrogen Concentration Profiles in Confinement Layers, Test Number 9C

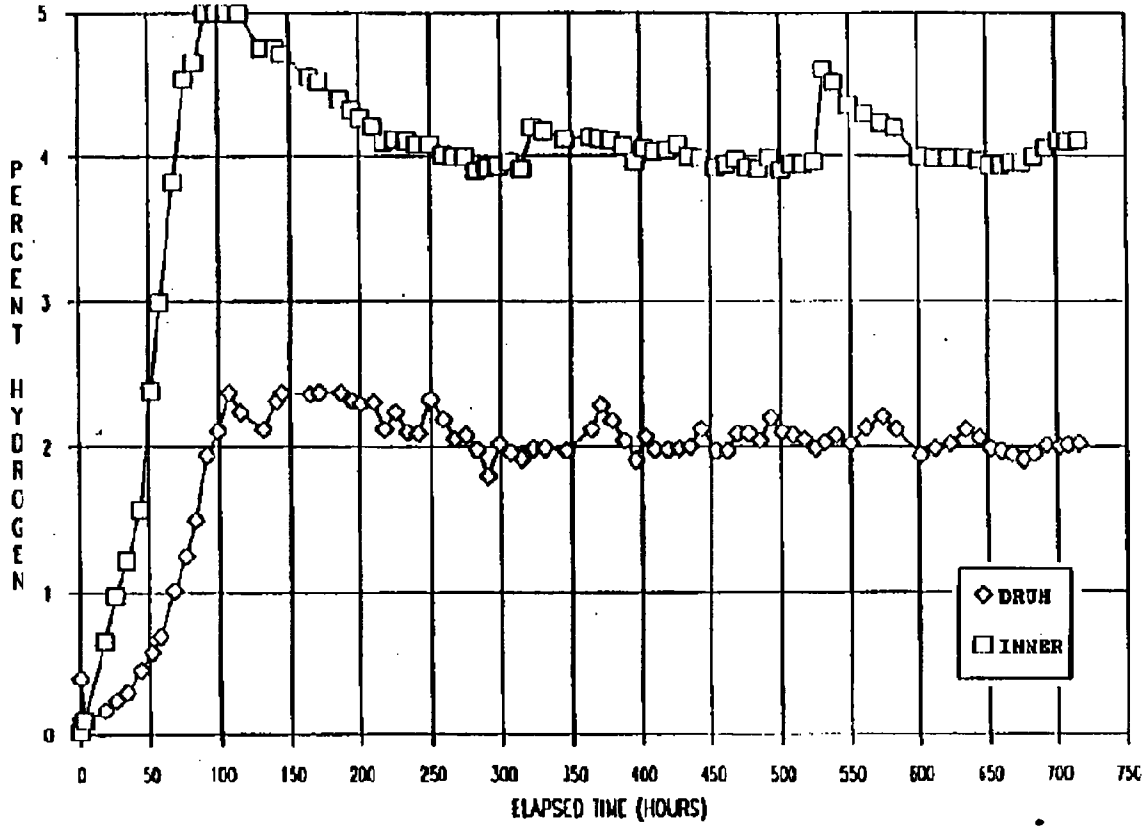

Figure 6.8-17—Hydrogen Concentration Profiles in Confinement Layers, Test Number 10A

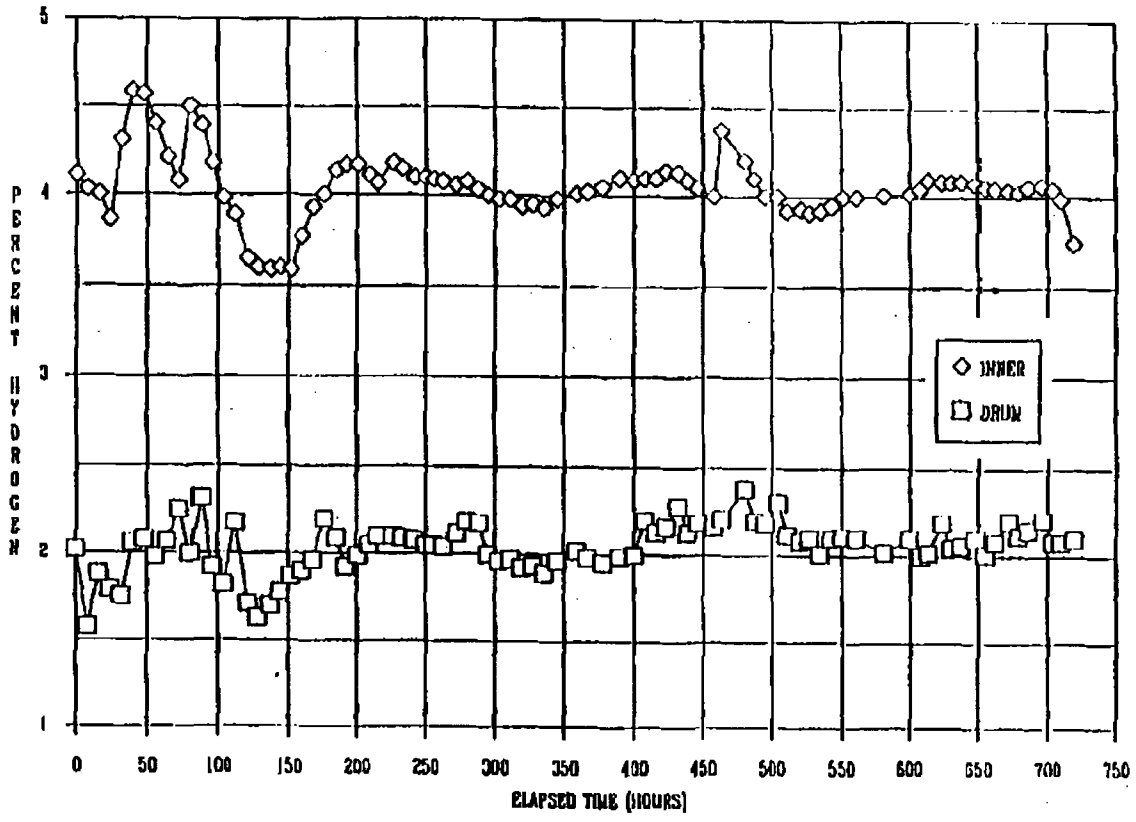

Figure 6.8-18—Hydrogen Concentration Profiles in Confinement Layers, Test Number 10B

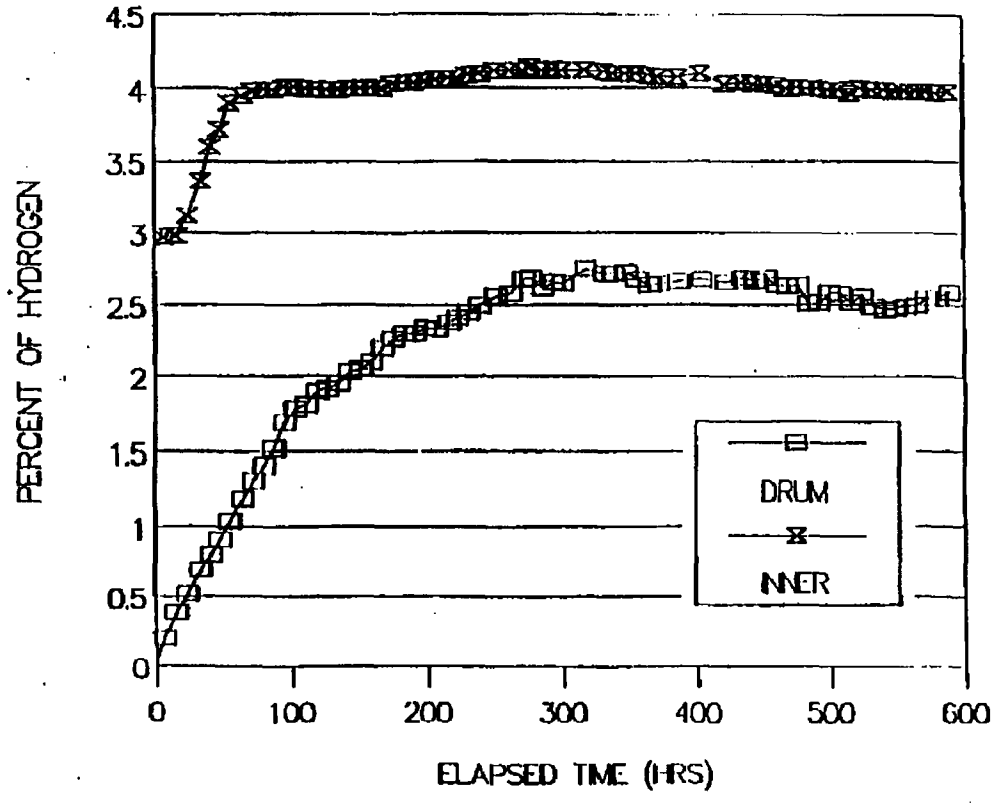

Figure 6.8-19—Hydrogen Concentration Profiles in Confinement Layers, Test Number 10C

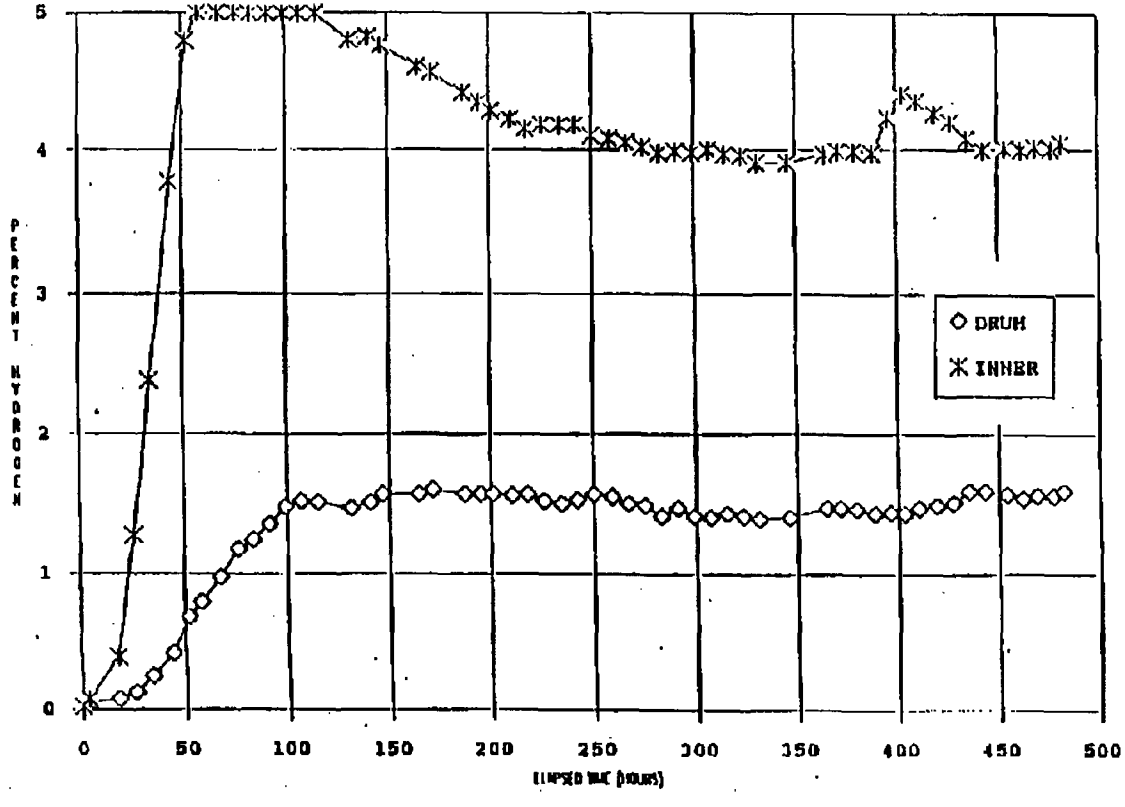

Figure 6.8-20—Hydrogen Concentration Profiles in Confinement Layers, Test Number 11A

For each test, the number of the test, hydrogen injection rate, temperature at steady state, bag type, the mole percent hydrogen in the void volume of each confinement layer at steady state, and the computed release rates for each of the plastic bag confinement layers are summarized in Table 6.8-3. Similar information for the filters is provided in Table 6.8-4.

The contribution to the total release rate by any leakage of hydrogen around the bulkhead fittings was eliminated in experiments 9B, 10A, 10B, 10C, and 11A with the use of the duct seal. The release rate data of Tests 4, 5, 6, and 7 have not been used in quantifying the total release rates from bags since only the lowest measured release rates were being used as inputs into the calculations (Appendix 6.7 of the CH-TRU Payload Appendices).

6.8.7.2.2 Release Rates from Small Inner Bags

Tests 9A through 9C were conducted specifically in order to quantify the various contributions to the total release rate in the case of the small inner bags. The various contributions are summarized in Table 6.8-5.

The release rate by permeation through the small inner bag is equal to the total release rate from Test 9B, since there was no leakage around the bulkhead fitting nor through the twisted closure because this test had the twist-and-tape closure cut off and the end heat-sealed. The leakage through the closure is equal to the difference of the values measured in Test 9A and 9C, that is, 5.6E-7 mole/sec/mole fraction. The leakage rate around the bulkhead fitting is the difference between Tests 9B and 9C or 2.96E-7 mole/sec/mole fraction.

6.8.7.2.3 Temperature Dependence of Gas Release

Tests 10A through 10C were conducted in order to quantify the temperature dependence of the total release rate at the low end of the operating temperatures. The results show that the total release rate at the low temperatures (Tests 10A and 10B at 10°F and -18°F, respectively) do not decrease as would be predicted by considerations of pure permeation and diffusion. The total release rate at 10°F was approximately 70% higher than the release rate at 57°F. The release rates at 10°F and at -18°F appear to be the same. The increased release rates at the low temperatures probably result from a stiffening of the plastic material and changes in the closure configuration. The similar release rates at 10°F and -18°F suggest that the dependence of release rates on these low temperatures is not functional. That is, there would not be a continuous decrease in the release rate with increasing temperatures. At higher than room temperature, the normal dependence of diffusion on temperature (increasing as the 1.75 power of temperature) would be valid.

6.8.7.2.4 Bounding Release Rate for Decay Heat Calculations

The release rate from the small PVC bag closure leakage (5.6E-7 mole/sec/mole fraction) was used as the total release rate from small bags in computations of decay heat limits (Appendix 6.7 of Payload Appendices). As mentioned earlier, the bag permeability was not considered in this case even though its contribution to the release of hydrogen is approximately equal to the closure release rate (Table 6.8-5). This should provide a margin of safety in keeping concentrations of hydrogen at lower concentration than what is predicted by analytical calculations. The lowest

measured total release rate (4.67E-6 mole/sec/mole fraction) based on Test 10C results (Table 6.8-3) was used as the total release rate from large bags (Appendix 6.7 of Payload Appendices).

The filter diffusivities presented in Table 6.8-4 are not actual measurements on the filters but are effective diffusivities in the configuration of the waste. For the purposes of specifying a minimum diffusivity for the filters, actual diffusivity measurements on the filters have been used since these are representative of what would be measured by the manufacturer. In a drum (or SWB) configuration, release of hydrogen can depend on the way the filter is installed, hydrogen leakage through the gasket material and any other available paths for the hydrogen.

In summary, this test program determined the release rates through different bagging configurations that serve as conservative inputs into the decay heat calculations outlined in Appendix 6.7 of the CH-TRU Payload Appendices. Release rates in actual waste drums are expected to be much higher than what is predicted by this experimental data. This, coupled with the lower hydrogen production rates (as opposed to the effective values being used in the calculations), should provide a high margin of safety for safe transport of the CH-TRU waste. Sampling programs at the sites prove this to be true and are discussed in Appendix 5.3 of the CH-TRU Payload Appendices.

Table 6.8-3 — Summary of Total Release Rates from Plastic Confinement Layers

Test Number	H_2 Flow Rate (Ml/hr)	Temperature at Steady State (°F)	Confinement Layer	Steady State Hydrogen mol%	Total Release (mol/sec/mol fraction)
4A	15.6	74.0	14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.02 2.39 1.59	1.09E-05 2.23E-05 5.94E-05
4B	13.6	76.0	14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.01 2.58 1.81	1.08E-05 2.00E-05 4.99E-05
5A	3.1	78.0	14 mil PVC inner bag-out 5 mil PE inner bag 10 mil PE liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.00 1.93 0.90 0.50 0.29	1.35E-06 4.45E-06 1.21E-05 3.19E-05 7.03E-05
5B	3.5	82.0	14 mil PVC inner bag-out 5 mil PE inner bag 10 mil PE liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.05 1.91 0.72 0.49 0.31	1.84E-06 3.31E-06 1.71E-05 2.19E-05 9.84E-05
6A	2.8	68.0	14 mil PVC inner bag-out 5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.06 1.99 0.83 0.56 0.40	1.56E-06 2.79E-06 1.20E-05 2.02E-05 4.62E-05
6B	2.2	66.0	14 mil PVC inner bag-out 5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.09 2.02 0.96 0.62 0.50	1.23E-06 2.40E-06 7.47E-06 2.12E-05 3.18E-05
7A	17	77.0	5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.09 3.75 2.70 1.98	5.68E-05 1.84E-05 2.68E-05 5.22E-05
7B	2.8	71.0	5 mil PE inner bag 14 mil PVC liner bag 10 mil PE liner bag 90 mil HDPE drum liner	4.02 3.98 3.18 2.53	8.07E-05 4.04E-06 4.97E-06 1.01E-05
9A	3.7	70.0	14 mil PVC inner bag-out bulkhead; not sealed	4.12	1.35E-06
9B	1.5	50.0	14 mil PVC inner bag-out less horsetail; bulkhead; end sealed	4.00	4.94E-07
9C	2.5	59.0	14 mil PVC inner bag-out less horsetail; no duct seal used on bulkhead fittings	3.98	7.90E-07
10A	25	10.0	10 mil PE liner bag	4.11	1.55E-05
10B	20.9	-18.0	10 mil PE liner bag	4.02	1.52E-05
10C	5.9	57.0	10 mil PE liner bag	3.98	4.67E-06
11A	12.5	63.0	14 mil PVC liner bag	4.01	5.97E-06

Table 6.8-4 — Summary of Total Release Rates from Filters

Test Number	H_2 Flow Rate (ml/hr)	Temperature at Steady State (°F)	Filter Type and Number	Steady State Hydrogen mol%	Total Release Rate (mol/sec/mol fraction)
4A	15.6	74.0	NFT-E INEL Design	1.29	1.38E-05
4B	13.6	76.0	NFT-21 RFP Design	1.50	1.03E-05
5A	3.1	78.0	NFT-21 RFP Design	0.22	2.51E-05
5B	3.5	82.0	NFT-21 RFP Design	0.27	1.46E-05
6A	2.8	68.0	NFT-17 RFP Design	0.33	9.80E-06
6B	2.2	66.0	NFT-21 RFP Design	0.42	6.05E-06
7A	17	77.0	NFT-17 RFP Design	1.61	1.20E-05
7B	2.8	71.0	NFT-17 RFP Design	2.21	1.46E-06
9A	3.7	70.0	NFT-17 RFP Design	0.96	4.44E-06
9B	1.5	50.0	NFT-9035 SRP SRP Design	0.37	4.85E-06
9C	2.5	59.0	NFT-9035 SRP SRP Design	0.26	1.13E-05
10A	25	10.0	NFT-17 RFP Design	2.02	1.60E-05
10B	20.9	-18.0	NFT-17 RFP Design	2.12	1.36E-05
10C	5.9	57.0	NFT-9034 SRP Design	2.49	2.80E-06
11A	12.5	63.0	NFT-21 RFP Design	1.57	9.28E-06

Table 6.8-5 — Summary of Release Rates for Small Bag Confinement Layers

Contributor to Total Release Rate	Permeation Through Small PVC	Bag Closure Leakage	Bulkhead Fittings Leakage
Relation to Tests	9B	9A-9C	9C-9B
Value*	4.94E-7	5.6E-7	2.96E-7

*Values reported in mole/sec/mole fraction.

APPENDIX 6.9

TEMPERATURE DEPENDENCE OF HYDROGEN GAS GENERATION AND RELEASE RATES

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6.9 Temperature Dependence Of Hydrogen Gas Generation And Release Rates

6.9.1 Summary

The temperature dependence of hydrogen gas generation and release rates is presented in this document. These parameters determine the maximum allowable decay heat limit for each shipping category. The assumptions and equations used in calculating the analytical decay heat limits are presented in this document. The analysis presented here demonstrates that for Waste Types II and III, under worst-case assumptions, the minimum decay heats occur at room temperatures. The minimum decay heat limits for shipping categories in Waste Type I occur at the lowest operating temperature, -20°F (-29°C). As examples of the results from determining the decay heat limits from each shipping category, plots of the decay heat limit as a function of temperature are provided for the shipping categories II.1A4 and I.1A3.

For Waste Types II and III, the total hydrogen release rate (from the different layers of confinement in a payload container) and the hydrogen generation rate (calculated using the temperature corrected effective G value) increase with increasing temperatures. The resultant decay heat limit varies only minimally with temperature [a difference of 2.2% between the extremes of the operating temperature range from -20°F (-29°C) to 154°F (68°C) applicable to analytical category waste], and room temperatures result in the minimum values for the decay heat limits.

For Waste Type I, the effective G value does not change with temperature (see Appendix 3.2 of the CH-TRU Payload Appendices). Using the same set of assumptions for the hydrogen release rate (as for Waste Types II and III), the total hydrogen release rate increases with increasing temperatures and are a minimum at the lowest operating temperature, -20°F (-29°C). Since the effective G value does not decrease with decreasing temperature for Waste Type I (while the equations show a decrease in the hydrogen release rates with decreasing temperatures), the minimum decay heat limit is obtained at the lowest operating temperature in each shipping category.

Experiments conducted at lower than room temperature show the release rates from plastic bags to be much higher than those assumed in these calculations (Appendices 6.7 and 6.8 of the CH-TRU Payload Appendices). No credit is taken for the experimentally measured increased hydrogen release rates through the twist-and-tape closure of the bags at the low temperatures. These assumptions add a margin of safety to the decay heat limit used for each payload shipping category in Waste Type I and Waste Material Type II.3.

An example calculation for obtaining the decay heat limit for the shipping category II.1A4 at the maximum operating temperature is presented in Attachment A. This attachment presents the steps for obtaining the decay heat limit for any shipping category at any temperature. The analysis presented in Attachment A of this appendix shows that porosity effects on the twist-and-tape closure are negligible in calculating the decay heat limits. Any decrease in porosity of the closure at high temperatures is offset by increased diffusion.

Attachment B of this appendix provides example calculations for decay heat limits using less restrictive assumptions (taking credit for increased permeation from the liner bags at higher temperatures, etc.). These values are provided for illustrative purposes only.

6.9.2 Introduction

The release of hydrogen gas from the layers of plastic bags and the payload containers occurs by two mechanisms. The first is release of hydrogen by diffusion through the twist-and-tape closure of the bags, through the drum liner lid hole, and drum filter. The second is permeation of the hydrogen through the bag materials. The temperature dependence of pure diffusion and permeation processes is well characterized. Diffusion is directly proportional to the 1.75 power of the absolute temperature.[1] Permeation through plastics increases exponentially with temperature, with an activation energy characteristic of a given material.[1] In the flammable gas calculations presented in Appendix 2.3 of the CH-TRU Payload Appendices, the release rates used to calculate the decay heat limit for each payload category assume the following (see Appendix 6.7 of the CH-TRU Payload Appendices for details):

- Room temperature conditions are assumed for Waste Material Type II.1 and Waste Type III. Minimum operating temperature conditions [-20°F (-29°C)] are assumed for Waste Type I and Waste Material Type II.3. As shown in this appendix, the most conservative decay heat limits are obtained under these conditions.

- For small inner bags (excluding the drum liner bags), only the diffusion through the twist-and-tape closure is used in determining the total release rate. No credit is taken for permeation through the bag material.

- For the drum liner bags, the sum of diffusion through the bag closure and permeation of the bag material is used in determining the total release rate. The lowest measured total hydrogen release rate at three different test temperatures [-18°F (-28°C), 10°F (-12°C), and 57°F (14°C)] (Appendix 6.8 of the CH-TRU Payload Appendices) is used as the hydrogen release rate.

- For the rigid drum liner, the diffusion through a 0.3" diameter hole at -20°F (-29°C) is used to determine total hydrogen release rate (see Appendix 6.7 of the CH-TRU Payload Appendices). No credit is taken for permeation through the liner material.

- For the filter vents in the payload containers, the lowest measured diffusion coefficient is used to determine the total hydrogen release rate (Appendix 6.7 of the CH-TRU Payload Appendices) and is corrected for temperature as described by equation (2) of Table 6.9-1.

[1] Perry, R.H., "1984, Perry's Chemical Engineers Handbook," 6th Edition , McGraw Hill Book Company, New York, New York.

Table 6.9-1 —Equations Summarizing Temperature Dependence Of Decay Heat Parameters*

1. Effective G Value for Hydrogen

   The effective G value for hydrogen is calculated using an Arrhenius type dependence on temperature (see Appendix 3.2 of the CH-TRU Payload Appendices). The effective G value, $G_{eff(T2)}$, at temperature T_2 is computed as:

   $$G_{eff(T2)} = G_{eff(T1)} \exp[(E_G/R)\{(T_2-T_1)/(T_2 \times T_1)\}] \quad (1)$$

2. Release through Drum Filter

   The mechanism of release through the filter is by diffusion, which varies with temperature raised to the 1.75 power. Using the minimum measured diffusion coefficient of $1.9(10)^{-6}$ mole/sec at 70°F (21°C) (Appendix 6.7 of the CH-TRU Payload Appendices), the total release rate of hydrogen from the filter, RS(drum filter) at temperature, T_2 is:

   $$RS(\text{drum filter},T_2) = 1.9(10)^{-6} \text{ mole/sec } (T_2/T_1)^{1.75} \quad (2)$$

3. Release through Punctured Rigid Drum Liner

   The release rate from the rigid drum liner is the minimum value based on diffusion of hydrogen in air at -20°F (-29°C). The value of this release rate is:

   $$RS(\text{drum liner},T) = 5.09(10)^{-5} \text{ mole/sec} \quad (3)$$

4. Release through Liner Bags

   The lowest measured total release rate is used as the release rate at all temperatures. The value of this release rate is:

   $$RS(\text{liner bag},T) = 4.67(10)^{-6} \text{ mole/sec} \quad (4)$$

5. Release through Inner Bags

   The release rate is corrected for temperature and closure porosity dependence. The dependence of the porosity (ϵ) on temperature is discussed in Attachment A of this appendix. The release rate at temperature, T_2 is:

   $$RS(\text{inner bag},T_2) = 1.58(10)^{-7}(T_2/T_1)^{1.75} \ (\epsilon_2/\epsilon_1)^2 \text{ mole/sec} \quad (5)$$

* All variables are defined in Table 6.9-2.

Table 6.9-2 — Nomenclature List For Variables

E_G	Hydrogen generation activation energy. [0.8 kcal/g-mole] for polyethylene (Waste Material Type II.1 and Waste Type III) [0.0 kcal/g-mole] for water (Waste Type I and Waste Material Type II.3)) (Appendix 3.2 of the CH-TRU Payload Appendices)
E_p	Activation energy for hydrogen permeation through polyethylene. [8.2 kcal/g-mole] (Appendix 6.7 of the CH-TRU Payload Appendices)
R	Gas law constant. $[1.987(10)^{-3}$ kcal/g-mole K]
T_1	Absolute temperature at which the reference value of a decay heat parameter is specified. [294 °K] (70 °F).
T_2	Absolute temperature at which the value of a decay heat parameter is to be evaluated (K).
$G_{eff(T1)}$	Reference effective G value for hydrogen [1.70 molecules/100eV] at 70 °F for Waste Material Type II.1 [1.60 molecules/100eV] at 70 °F for Waste Material Type I.1 (Appendix 3.2 of the CH-TRU Payload Appendices)
$G_{eff(T2)}$	Temperature corrected effective G value for hydrogen at temperature, T_2.
ϵ_1	Porosity of the twist-and-tape closure at temperature, T_1.
ϵ_2	Porosity of the twist-and-tape closure at temperature, T_2.
RS(I)	Total release rate from confinement layer "I" (mole/sec).
r(i)	Resistance of confinement layer "I" to the flow of hydrogen; equal to the reciprocal of the total release rate = 1/RS(I) in (sec/mole).
r_{eff}	Effective resistance of all layers of confinement. $r_{eff} = \Sigma$ r(I) for I = 1 to number of confinement layers (sec/mole).
CG	Allowable hydrogen gas generation rate per innermost confinement layer (mole/sec).

Table 6.9-2 — Nomenclature List For Variables (Concluded)

X_{inner}	Maximum permissible concentration (mole fraction) of hydrogen in innermost confinement layer. [0.05]
t	Shipping period duration. [60 days]
n_{gen}	Number of hydrogen generators per packaging. • 14 for drums • 8 for overpack of drums in an SWB • 2 for SWBs and bins overpacked in SWBs
N_{tg}	Total moles of gas inside the packaging inner containment vessel (ICV) cavity. [101.56 moles for drums and 72.54 moles for SWBs] (Appendix 2.3 of the CH-TRU Payload Appendices)
Q_i	Decay heat per innermost confinement layer (watt).
N_A	Avogadro's number. [$6.023(10)^{23}$ molecules/g-mole].

6.9.3 Temperature Dependence Of Parameters In Decay Heat Calculations

The temperature dependent parameters in the decay heat limit calculations include the effective G value for hydrogen, porosity of the twist-and-tape closure, and the hydrogen release rates through the different layers of confinement. The equations describing these temperature dependencies, and the values for parameters used in these equations, are described in this section. The nomenclature for the variables in the equations is presented in Table 6.9-2. A summary of the variables as a function of temperature is presented in Table 6.9-2, and each is discussed in detail below:

1. G value for Hydrogen: The effective G values for hydrogen generation used for Waste Material Type II.1 and Waste Type III are based on polyethylene (Appendix 3.2 of the CH-TRU Payload Appendices). The effective G values have an Arrhenius type dependence with temperature with an activation energy of 0.8 kcal/g-mole for polyethylene (Appendix 3.2 of the CH-TRU Payload Appendices). For Waste Type I and Waste Material Type II.3, the effective G values for hydrogen are due to water. These effective G values do not vary as a result of temperature changes; that is, water has an activation energy of zero (Appendix 3.2 of the CH-TRU Payload Appendices). The temperature-corrected effective G value as a function of temperature is given in equation (1) of Table 6.9-1.

2. Hydrogen Release Rate through a Drum Filter: The diffusion of hydrogen through the drum filter varies directly as the 1.75 power of the absolute temperature.[1] Equation (2) of Table 6.9-1 defines the temperature dependence of this hydrogen release rate.

3. Hydrogen Release Rate through the Punctured Rigid Drum Liner: The diffusion of hydrogen through the punctured rigid drum liner varies directly as the 1.75 power of the absolute temperature. No credit is taken for permeation through the rigid drum liner material, and the minimum rigid drum liner hydrogen release rate through the puncture hole [at -20°F (-29°C)] is used in the decay heat limit calculations. Equation (3) of Table 6.9-1 defines the hydrogen release rate through the punctured rigid drum liner used in the decay heat calculations.

4. Hydrogen Release Rate through the Liner Bags: Total hydrogen release rate through the liner bags considers both diffusion through the twist-and-tape closure and permeation through the plastic. Total release rates through liner bags were measured at three temperatures [-18°F (-28°C), 10°F (-12°C), and 57°F (14°C)] to quantify the effect of lower (than room) temperatures on these release rates (Appendix 6.8 of the CH-TRU Payload Appendices). These experiments showed that release rates at the lower end of the operating temperatures [-18°F (-28°C) and 10°F (-12°C)] are higher than would be expected from analytical consideration of permeation and diffusion alone. At temperatures at or above 10°F (-12°C), stiffening of the plastic material in the twist-and-tape closure results in a lesser restriction to the release of hydrogen. The increased release rates at the lower temperatures are not of a functional form. That is, as seen from Table 6.8-3 of Appendix 6.8 of the CH-TRU Payload Appendices, the release rates at 10°F (-12°C), and -18°F (-28°C) are nearly the same. Hence, the hydrogen release rate is not a continuously decreasing function from low temperatures to higher temperatures.

In the decay heat limit calculations, the lowest measured total hydrogen release rate is used as the release rate at all temperatures in the operating range. No credit is taken for the increased hydrogen release rate at the lower (than room) temperatures found in the experiments. No corrections for increased permeation or diffusion are made for the higher (than room) temperatures. Equation (4) of Table 6.9-1 defines the temperature dependence of this hydrogen release rate.

5. Hydrogen Release Rate through the Inner Bags: As mentioned in the summary above, no credit is taken for permeation through the inner bags in estimating the total hydrogen release rates. In the decay heat limit calculations, the release rate through the inner bags has been modeled as strict diffusion through the twist-and-tape closure (directly proportional to the 1.75 power of the absolute temperature). No credit is taken for the experimentally measured increased hydrogen release rates through the twist-and-tape closure at the lower (than room) operating temperatures. In addition, a decrease in porosity of the closure with increasing temperatures is considered in the calculations. As shown in Attachment A, the decrease in porosity at the higher (than room) temperatures is minimal. Equation (5) of Table 6.9-1 defines the temperature dependence of this release rate.

These release rates serve as inputs into the decay heat limit calculations as described below.

6.9.4 Decay Heat Limits as Functions of Temperature—Waste Types II and III

The methodology for calculating the decay heat limits is described in Appendix 2.3 of the CH-TRU Payload Appendices (with an example for shipping category I.1A2), and in Attachment A of this appendix for the shipping category II.1A4. The equations in the decay heat calculations are summarized in Table 6.9-3. As shown in Equation (3) of Table 6.9-3, the decay heat limit for a shipping category is directly proportional to the maximum allowable hydrogen generation rate and inversely proportional to the temperature-corrected effective G value. The temperature-corrected effective G value as a function of temperature is plotted in Figure 6.9-1 for the shipping category II.1A4. The maximum allowable hydrogen generation rate is equal to the hydrogen release rate (across each layer of confinement) at equilibrium. Equation (2) of Table 6.9-3 defines the maximum allowable hydrogen generation rate in terms of the release rate parameters and the number of moles of gas in the packaging ICV. This parameter (the maximum allowable hydrogen generation rate) is plotted as a function of temperature for the shipping category II.1A4 in Figure 6.9-2. The decay heat limit as a function of temperature can be calculated from the values on Figures 6.9-1 and 6.9-2 at each temperature, as defined by equation (3) of Table 6.9-3. The decay heat limits at 5 degree (^{o}F) intervals are summarized in Table 6.9-4, along with the values of the other variables that enter into the calculations. The decay heat limit as a function of temperature is plotted in Figure 6.9-3.

Table 6.9-3 — Equations For Decay Heat Calculations

1. Calculation of Effective Resistance

The resistance of a confinement layer "i" to the flow of hydrogen is the reciprocal of the total release rate from that confinement layer. Therefore,

$$r(i)\ (\text{sec/mole}) = 1/RS(i) \qquad (1)$$

The effective resistance is computed by summing the individual confinement layer resistances.

$$r_{eff} = \Sigma\, r(i) \text{ for } i = 1 \text{ to number of confinement layers}$$

2. Calculation of Maximum Allowable Hydrogen Generation Rate

The maximum allowable hydrogen generation rate per innermost confinement layer may be computed as:

$$CG\ (\text{mole/sec}) = (X_{inner})/\{r_{eff} + [(t)(n_{gen})/N_{tg}]\} \qquad (2)$$

For 14 drum payload containers

$$(t)(n_{gen})/N_{tg} = (60 \text{ days})(14 \text{ drums})(86400 \text{ sec/day})/101.56 \text{ mole}$$
$$= 714{,}612 \text{ sec/mole}$$

3. Calculation of Decay Heat Limit

The decay heat limit per innermost confinement layer, may be computed as:

$$Q_i\ (\text{watts}) = [(CG)(N_A)/(G_{eff} \text{ molecules/100eV})][1.602(10)^{-19} \text{ watt-sec/eV}] \qquad (3)$$

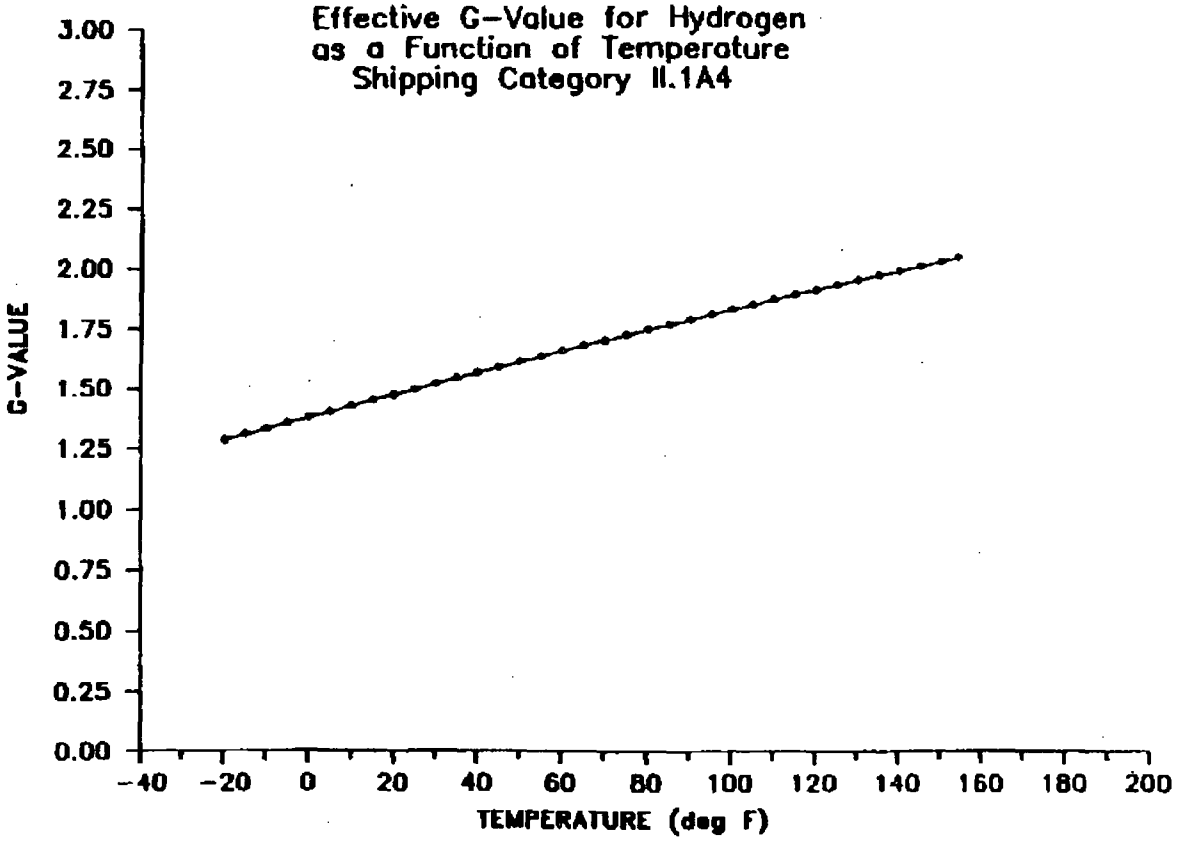

Figure 6.9-1—Effective G-Value for Hydrogen as a Function of Temperature (Shipping Category II.1A4)

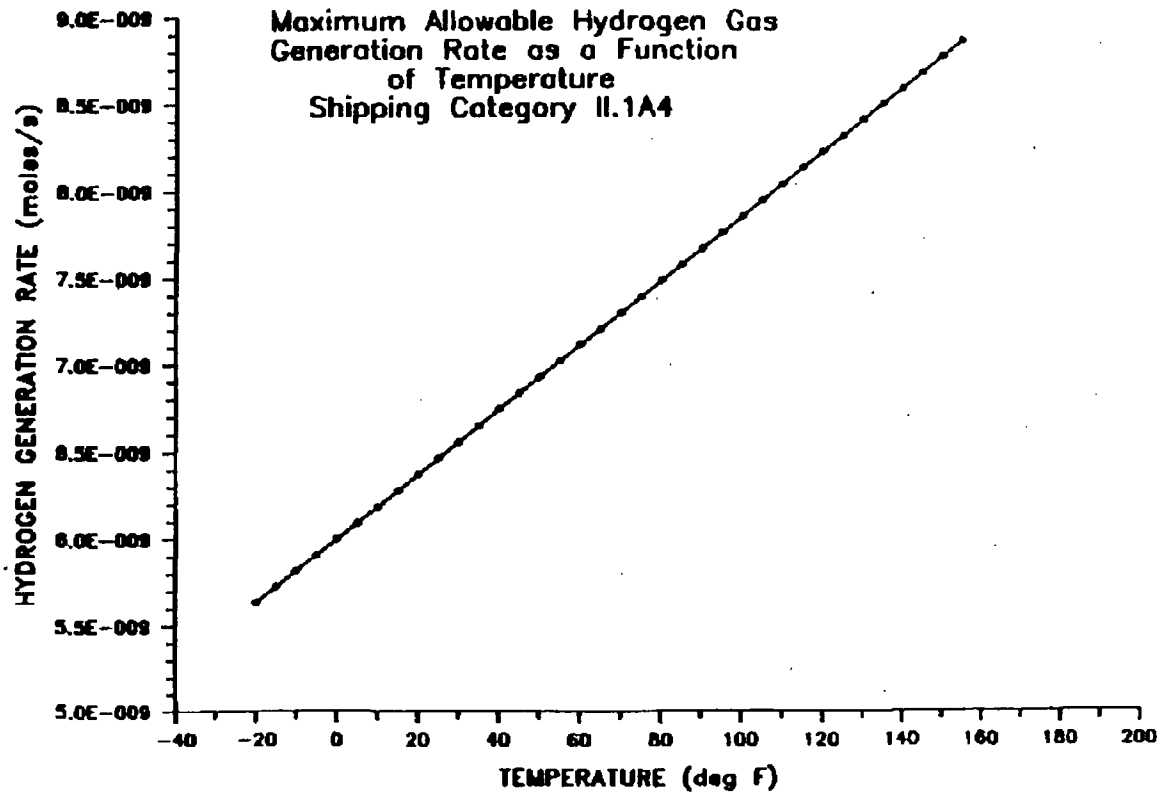

Figure 6.9-2—Maximum Allowable Hydrogen Gas Generation Rate as a Function of Temperature (Shipping Category II.1A4)

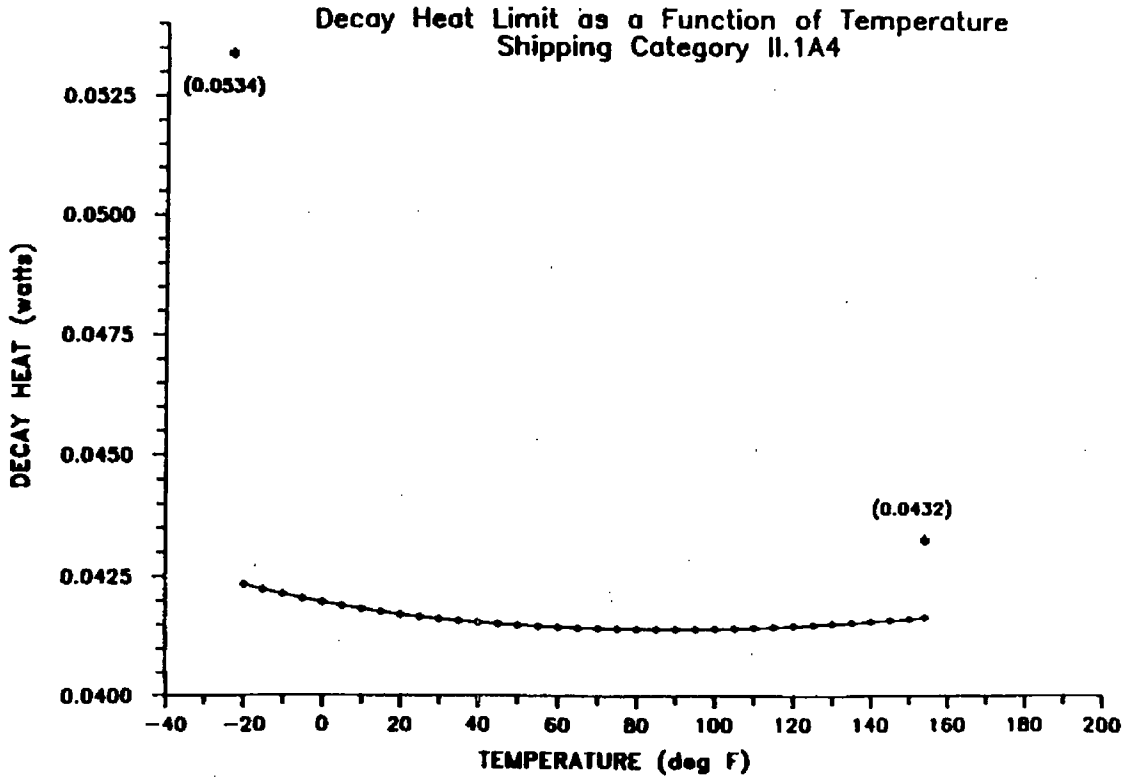

Figure 6.9-3—Decay Heat Limit as a Function of Temperature (Shipping Category II.1A4)

Table 6.9-4 — Decay Heat Parameters For Shipping Category II.1A4

Temp (F)	Temp (K)	Porosity	r(inner bag) (s/mol)	r(liner bag) (s/mol)	r(drum liner) (s/mol)	r(drum filter) (s/mol)	r(eff) (s/mol)	G(eff)	CG (mol/s)	Q_i (Watt)
-20	244	0.6934	2398864	214133	19646	729327	8159697	1.28	5.634E-09	0.0423
-15	247	0.6927	2352856	214133	19646	713896	8006243	1.31	5.733E-09	0.0422
-10	250	0.6920	2308332	214133	19646	698971	7857746	1.34	5.833E-09	0.0421
-5	253	0.6913	2265225	214133	19646	684532	7713986	1.36	5.932E-09	0.0420
0	255	0.6908	2237461	214133	19646	675164	7621325	1.38	5.998E-09	0.0420
5	258	0.6901	2196579	214133	19646	661485	7485002	1.40	6.098E-09	0.0419
10	261	0.6894	2156959	214133	19646	648237	7352894	1.43	6.198E-09	0.0418
15	264	0.6887	2118548	214133	19646	635400	7224825	1.46	6.298E-09	0.0418
20	266	0.6882	2093790	214133	19646	627064	7142214	1.47	6.364E-09	0.0417
25	269	0.6875	2057281	214133	19646	614877	7020497	1.50	6.464E-09	0.0417
30	272	0.6867	2022440	214133	19646	603058	6904158	1.52	6.563E-09	0.0416
35	275	0.6860	1988039	214133	19646	591592	6789489	1.55	6.663E-09	0.0416
40	278	0.6853	1954635	214133	19646	580465	6678148	1.57	6.763E-09	0.0415
45	280	0.6848	1933087	214133	19646	573229	6606268	1.59	6.830E-09	0.0415
50	283	0.6841	1901253	214133	19646	562637	6500176	1.61	6.930E-09	0.0415
55	286	0.6834	1870316	214133	19646	552349	6397075	1.64	7.031E-09	0.0415
60	289	0.6827	1840240	214133	19646	542354	6296852	1.66	7.131E-09	0.0414
65	291	0.6822	1820829	214133	19646	535848	6232115	1.68	7.198E-09	0.0414
70	294	0.6815	1792115	214133	19646	526316	6136440	1.70	7.298E-09	0.0414
75	297	0.6808	1764179	214133	19646	517048	6043362	1.72	7.399E-09	0.0414
80	300	0.6801	1736991	214133	19646	508033	5952787	1.75	7.499E-09	0.0414
85	303	0.6793	1711030	214133	19646	499263	5866132	1.77	7.598E-09	0.0414
90	305	0.6789	1693437	214133	19646	493548	5807639	1.79	7.666E-09	0.0414
95	308	0.6781	1668607	214133	19646	485166	5724768	1.81	7.765E-09	0.0414
100	311	0.6774	1643934	214133	19646	477006	5642587	1.83	7.865E-09	0.0414
105	314	0.6767	1619892	214133	19646	469059	5562515	1.85	7.965E-09	0.0414
110	316	0.6762	1604363	214133	19646	463876	5510745	1.87	8.032E-09	0.0414
115	319	0.6755	1581325	214133	19646	456269	5434021	1.89	8.132E-09	0.0415
120	322	0.6748	1558861	214133	19646	448856	5359219	1.91	8.232E-09	0.0415
125	325	0.6741	1536954	214133	19646	441630	5286271	1.94	8.332E-09	0.0415
130	328	0.6734	1515584	214133	19646	434585	5215116	1.96	8.432E-09	0.0415
135	330	0.6729	1501775	214133	19646	429987	5169092	1.97	8.498E-09	0.0415
140	333	0.6722	1481259	214133	19646	423231	5100786	2.00	8.598E-09	0.0416
145	336	0.6715	1461234	214133	19646	416640	5034120	2.02	8.698E-09	0.0416
150	339	0.6707	1442113	214133	19646	410209	4970327	2.04	8.795E-09	0.0416
154	341	0.6703	1429048	214133	19646	406008	4926931	2.05	8.863E-09	0.0417

Figures 6.9-1 and 6.9-2 show that both the temperature-corrected effective G value and the maximum allowable hydrogen generation rate increase with increasing temperatures. Figure 6.9-3 shows that the decay heat limits have a minimum at room temperatures and are slightly higher at both lower and higher operating temperatures. The largest difference between the lowest and the highest decay heat limit values in the operating temperature range is only 2.2%. These results show that for Waste Material Type II.1 and Waste Type III (the analysis for Waste Type III is identical to that for Waste Material Type II.1), the minimum decay heat limits are obtained assuming room temperature conditions.

In Figure 6.9-3, points are shown above the decay heat limit curve at each end of the operating temperature range. These decay heat limits would result at the two temperatures shown if the following more realistic assumptions for the hydrogen release rates through the inner bags and the liner bags are made:

- Credit is taken for increased hydrogen release through the liner bags at higher (than room) temperatures due to increased permeation and diffusion.
- Credit is taken for the experimental results (Appendices 6.7 and 6.8 of the CH-TRU Payload Appendices) at lower (than room) temperatures in order to use a constant value (measured at room temperatures) for the release rate through the inner bags.

Attachment B of this appendix provides the derivation of the decay heat limits with these assumptions. The two additional points have been provided in Figure 6.9-3 for illustrative purposes to demonstrate an added margin of safety in the analysis for the decay heat limits.

6.9.5 Decay Heat Limits as Functions of Temperature—Waste Type I and Waste Material Type II.3

For Waste Type I and Waste Material Type II.3, the effective G value does not change with temperature, while the maximum allowable hydrogen generation rate is an increasing function of temperature. Figures 6.9-4 and 6.9-5 are plots of the G value and the maximum allowable hydrogen generation rate as functions of temperature for the shipping category I.1A3. Table 6.9-5 presents the decay heat limit and related variables at 5 °F intervals through the operating temperature range. The decay heat limit as a function of temperature is plotted in Figure 6.9-6. Due to the constant values for the effective G values for waste material types in Waste Type I and Waste Material Type II.3, the decay heat limits are an increasing function of temperature, and are a minimum at the minimum operating temperature of -20°F.

In Figure 6.9-6, points are shown above the decay heat limit curve at each end of the operating temperature range. These decay heat limits would result at the two temperatures shown if the more realistic assumptions are made as listed above for the hydrogen release rates through the inner bags and the liner bags. Attachment B of this appendix provides the derivation of the decay heat limits with these assumptions. These assumptions have not been used in the decay heat limit calculations, and the conservative decay heat limits obtained at the minimum operating temperature have been used for shipping categories in Waste Type I and Waste Material Type II.3.

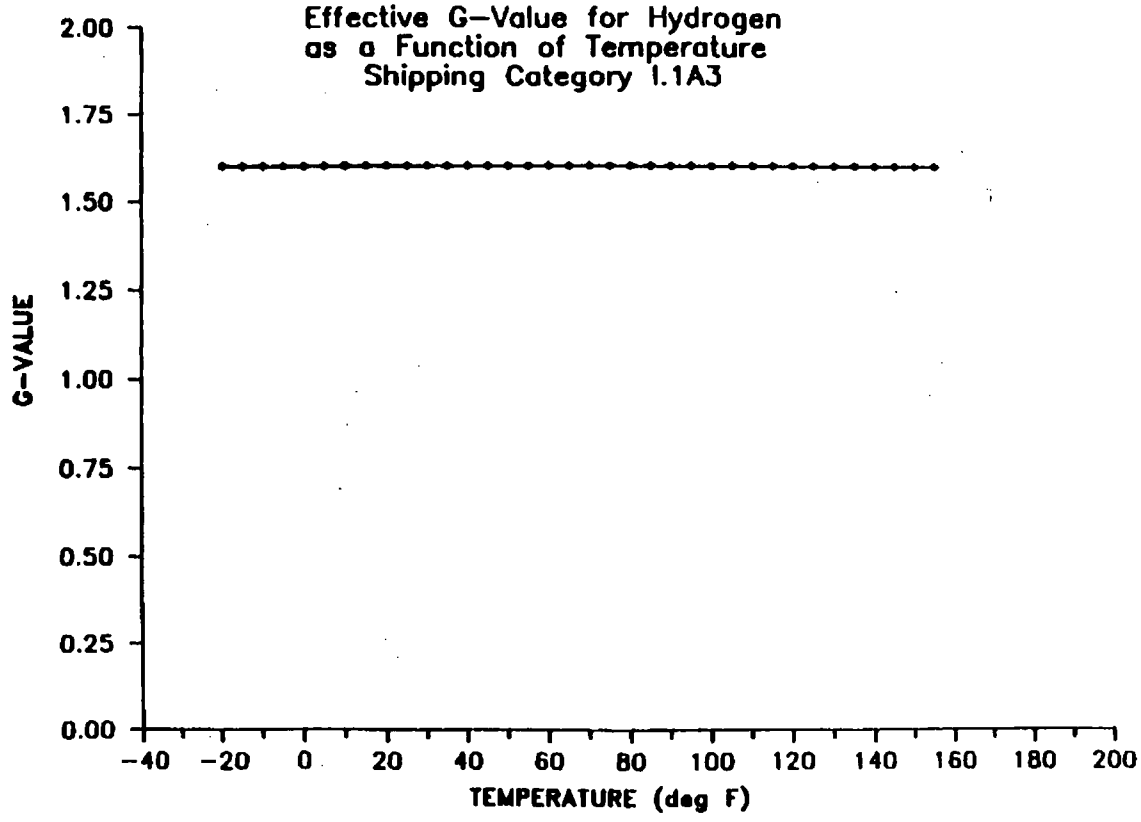

Figure 6.9-4— Effective G-Value for Hydrogen as a Function of Temperature (Shipping Category I.1A3)

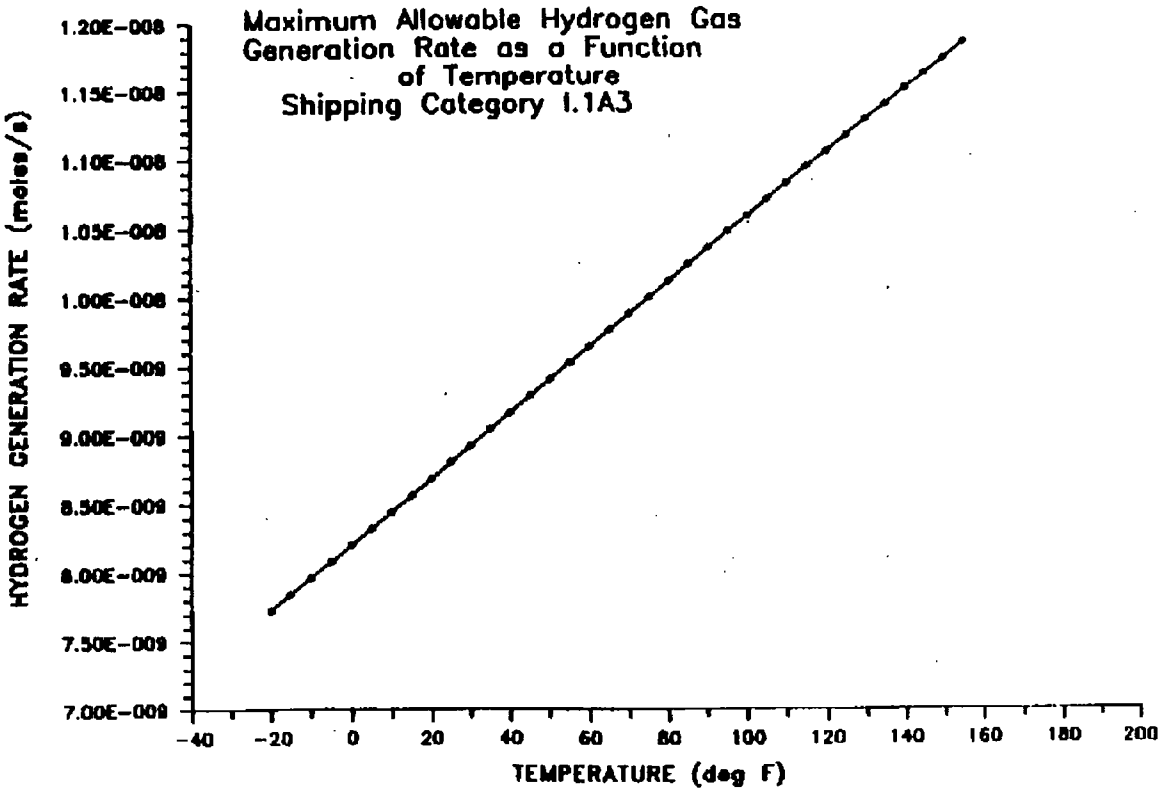

Figure 6.9-5— Maximum Allowable Hydrogen Gas Generation Rate as a Function of Temperature (Shipping Category I.1A3)

Table 6.9-5 — Decay Heat Parameters For Shipping Category I.1A3

Temp (F)	Temp (K)	Porosity	r(inner bag) (s/mol)	r(liner bag) (s/mol)	r(drum liner) (s/mol)	r(drum filter) (s/mol)	r(eff) (s/mol)	G(eff)	CG (mol/s)	Q_i (Watt)
-20	244	0.6934	2398864	214133	19646	729327	5760833	1.60	7.721E-09	0.0466
-15	247	0.6927	2352856	214133	19646	713896	5653387	1.60	7.852E-09	0.0474
-10	250	0.6920	2308332	214133	19646	698971	5549414	1.60	7.982E-09	0.0481
-5	253	0.6913	2265225	214133	19646	684532	5448761	1.60	8.112E-09	0.0489
0	255	0.6908	2237461	214133	19646	675164	5383864	1.60	8.199E-09	0.0494
5	258	0.6901	2196579	214133	19646	661485	5288422	1.60	8.329E-09	0.0502
10	261	0.6894	2156959	214133	19646	648237	5195934	1.60	8.459E-09	0.0510
15	264	0.6887	2118548	214133	19646	635400	5106276	1.60	8.590E-09	0.0518
20	266	0.6882	2093790	214133	19646	627064	5048424	1.60	8.676E-09	0.0523
25	269	0.6875	2057281	214133	19646	614877	4963217	1.60	8.806E-09	0.0531
30	272	0.6867	2022440	214133	19646	603058	4881718	1.60	8.934E-09	0.0539
35	275	0.6860	1988039	214133	19646	591592	4801450	1.60	9.064E-09	0.0547
40	278	0.6853	1954635	214133	19646	580465	4723513	1.60	9.194E-09	0.0554
45	280	0.6848	1933087	214133	19646	573229	4673181	1.60	9.280E-09	0.0560
50	283	0.6841	1901253	214133	19646	562637	4598922	1.60	9.410E-09	0.0567
55	286	0.6834	1870316	214133	19646	552349	4526760	1.60	9.539E-09	0.0575
60	289	0.6827	1840240	214133	19646	542354	4456613	1.60	9.669E-09	0.0583
65	291	0.6822	1820829	214133	19646	535848	4411286	1.60	9.754E-09	0.0588
70	294	0.6815	1792115	214133	19646	526316	4344325	1.60	9.883E-09	0.0596
75	297	0.6808	1764179	214133	19646	517048	4279184	1.60	1.001E-08	0.0604
80	300	0.6801	1736991	214133	19646	508033	4215795	1.60	1.014E-08	0.0612
85	303	0.6793	1711030	214133	19646	499263	4155102	1.60	1.027E-08	0.0619
90	305	0.6789	1693437	214133	19646	493548	4114202	1.60	1.035E-08	0.0624
95	308	0.6781	1668607	214133	19646	485166	4056160	1.60	1.048E-08	0.0632
100	311	0.6774	1643934	214133	19646	477006	3998653	1.60	1.061E-08	0.0640
105	314	0.6767	1619892	214133	19646	469059	3942623	1.60	1.074E-08	0.0647
110	316	0.6762	1604363	214133	19646	463876	3906382	1.60	1.082E-08	0.0653
115	319	0.6755	1581325	214133	19646	456269	3852697	1.60	1.095E-08	0.0660
120	322	0.6748	1558861	214133	19646	448856	3800357	1.60	1.107E-08	0.0668
125	325	0.6741	1536954	214133	19646	441630	3749317	1.60	1.120E-08	0.0675
130	328	0.6734	1515584	214133	19646	434585	3699532	1.60	1.133E-08	0.0683
135	330	0.6729	1501775	214133	19646	429987	3667316	1.60	1.141E-08	0.0688
140	333	0.6722	1481259	214133	19646	423231	3619528	1.60	1.154E-08	0.0696
145	336	0.6715	1461234	214133	19646	416640	3572886	1.60	1.166E-08	0.0703
150	339	0.6707	1442113	214133	19646	410209	3528214	1.60	1.178E-08	0.0711
154	341	0.6703	1429048	214133	19646	406008	3497883	1.60	1.187E-08	0.0716

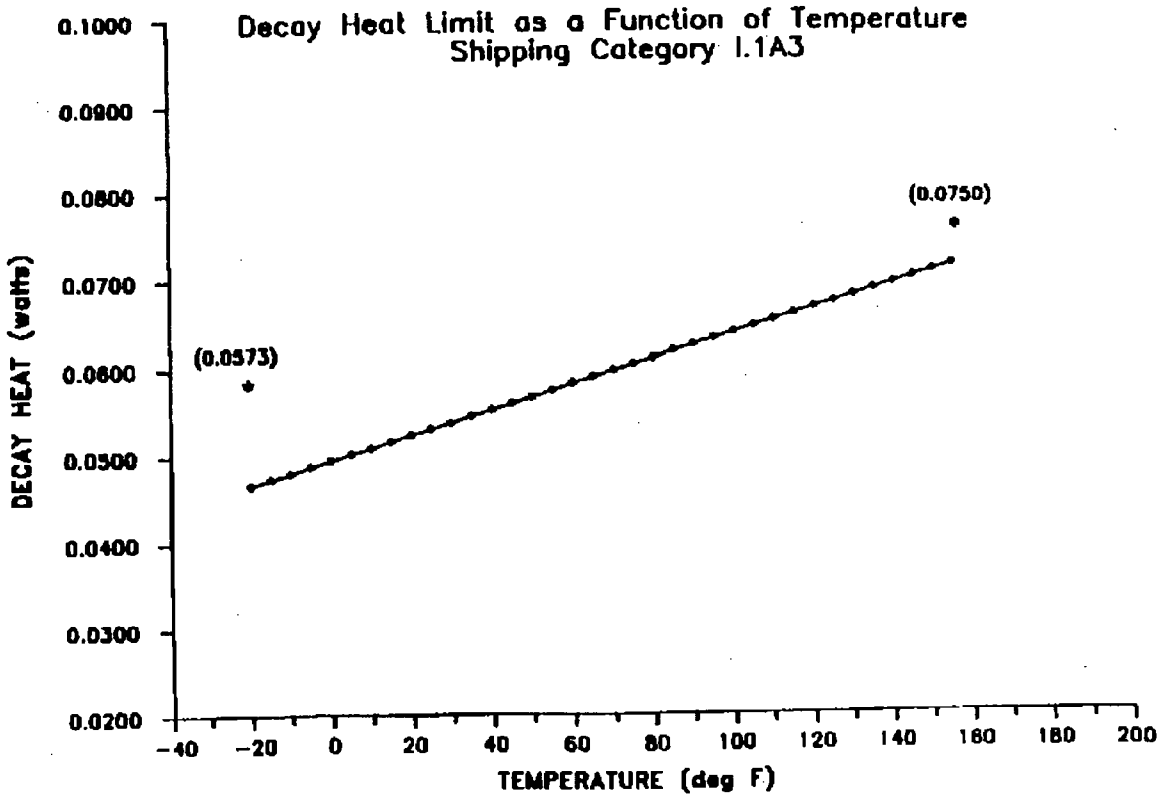

Figure 6.9-6—Decay Heat Limit as a Function of Temperature (Shipping Category I.1A3)

6.9.6 Conclusions

Hydrogen generation and release rates determined at room temperatures provide the most conservative decay heat limits for shipping categories in Waste Material Type II.1 and Waste Type III. Hydrogen generation and release rates determined at the minimum operating temperature provide the most conservative decay heat limits for shipping categories in Waste Type I and Waste Material Type II.3. This is because the effective G value for hydrogen for Waste Type I and Waste Material Type II.3 remains constant with temperature, while the hydrogen release rates are conservatively assumed to be lower than that for room temperatures.

ATTACHMENT A

DECAY HEAT LIMIT AT THE MAXIMUM OPERATING TEMPERATURE SHIPPING CATEGORY II.1A4

A1.0 Introduction

This attachment presents the steps for obtaining the decay heat limit for any shipping category at any temperature. The shipping category II.1A4 at the maximum operating temperature is used as an example for the calculations. The analysis presented here also shows that porosity effects on the twist-and-tape closure are negligible in calculating a decay heat limit.

The following is a list of assumptions that will be used in the calculation for the decay heat limit:

- A temperature of 154°F (68°C) will be assumed.
- All bags are assumed to be made of polyethylene. This will result in the highest effective G value for hydrogen at 68°C.
- The total moles of gas in the ICV cavity will remain constant during a 60-day shipping period and will be equal to 101.56 moles based on a void volume of 2,450 liters for a 14-drum payload assembly and conditions inside the ICV when the ICV is sealed for transport [70°F, and 1 atm pressure].

Other assumptions are listed in the appropriate subsections of this attachment.

A2.0 Release Rates at Maximum Temperature

The release rate of hydrogen through the bag closures is governed by the effective diffusion coefficient of hydrogen through each bag closure, which is a function of the binary diffusion coefficient of hydrogen in air and the porosity of the closure.[1] The release rate by molecular diffusion is directly proportional to temperature raised to the 1.75 power.[2] The porosity of the closure may be evaluated from the geometry of the closure. The resistance of a bag layer (to the release of hydrogen) is the reciprocal of the release rate. That is, while the release rate increases with temperature, the resistance decreases with temperature. The resistances of each of the different confinement layers at 154°F (68°C) are computed below.

[1] Smith, J.M., 1981, "Chemical Engineering Kinetics," 3rd Edition, McGraw-Hill Book Company, New York, New York, pp. 462-467.

[2] Perry, R.H., D.W. Green, and J.O. Maloney, 1984, "Perry's Chemical Engineers' Handbook," 6th Edition, McGraw-Hill Book Company, New York, New York.

A2.1 Resistance of Inner Bags

The Random-Pore Model of gaseous diffusion in porous media[1] predicts that the effective diffusion coefficient is equal to the product of effective binary diffusion coefficient of the hydrogen in air system and the square of the porosity.

Therefore,

$$D_e = D_{Hydrogen\text{-}Air} \quad \epsilon^2 \tag{1}$$

where,

D_e = effective diffusion coefficient of hydrogen through closure (mole/sec)

$D_{Hydrogen\text{-}Air}$ = binary diffusion coefficient of hydrogen in air (mole/sec)

ϵ = porosity of the closure.

Since the binary diffusion coefficient varies with temperature raised to the 1.75 power[2], the effective diffusion coefficient of hydrogen through the closure (the release rate) at temperature T_2 may be computed from the release rate at temperature T_1 using the relationship:

$$D_{e2} = D_{e1} \, (T_2/T_1)^{1.75} \quad (\epsilon_2/\epsilon_1)^2 \tag{2}$$

where,

D_{e2} = release rate of hydrogen through closure at temperature T_2 (mole/sec)

D_{e1} = release rate of hydrogen through closure at temperature T_1 (mole/sec)

ϵ_2 = porosity of closure at temperature T_2

ϵ_1 = porosity of closure at temperature T_1

T = absolute temperature (K).

By definition the porosity is the volume of voids per total volume. The volume of the bag material in the closure may be computed as:

$$V_m = 2lhw \tag{3}$$

where,

V_m = volume of the bag material in the closure

l = length of bag comprising closure, 5.5 inches (see Spurgeon[3])

h = width of bag comprising closure, 10.0 inches (Appendix 6.8 of the CH-TRU Payload Appendices)

w = thickness of bag material, 14 mil or 0.014 inch (Appendix 6.8 of the CH-TRU Payload Appendices)

V_m = 2(5.5 inches)(10.0 inches)(0.014 inch) = 1.540 in^3.

The total volume of the closure is evaluated as:

$$V_T = \pi r^2 l \quad (4)$$

where,

V_T = total volume of the closure

r = radius of the closure, average of 0.529 inches (see Spurgeon[3])

V_T = $\pi(0.529 \text{ inches})^2(5.5 \text{ inches}) = 4.835 \text{ in}^3$.

The porosity of the closure at 21°C, ϵ_1, is then computed as:

$$\epsilon_1 = (V_T - V_m(21^\circ C))/V_T = (4.835 - 1.540)/4.835 = 0.6815$$

The volumetric expansion of the bag material due to thermal stress induced by a temperature increase may be derived from Sears and Zemansky (1963)[4] as:

$$\Delta V_m = 3\alpha V_m \Delta T \quad (5)$$

where,

ΔV_m = volumetric expansion of bag material due to thermal stress (in^3)

α = linear coefficient of thermal expansion of the bag material (K^{-1})

ΔT = $T_2 - T_1$ = temperature increase (K)

[3] Spurgeon, B., Personal Communication, PN Services, Inc., Richland, Washington, July 1989.

[4] Sears, F.W., and M.W. Zemansky, 1963, "University Physics," 3rd Edition, Addison-Wesley Publishing Company, Inc., Reading Massachusetts, p. 347.

The highest reported linear coefficient of thermal expansion for polymers of $25(10)^{-5}$ K^{-1} will be used in the calculation.[5] This is a conservative assumption since it will provide the maximum reduction in closure porosity with temperature.

$\Delta V_m = 3(25(10)^{-5}\ K^{-1})(1.540\ in^3)(341K - 294K)$

$\Delta V_m = 0.054\ in^3$

The volume of the bag material in the closure at temperature T_2 (68°C) will then be:

$V_m(68°C) = V_m(21°C) + \Delta V_m = 1.540\ in^3 + 0.054\ in^3$

$V_m(68°C) = 1.594\ in^3$

The porosity of the closure at 68°C, ϵ_2, is then computed as:

$\epsilon_2 = (V_T - V_m(68°C))/V_T = (4.835 - 1.594)/4.835 = 0.6703$

The release rate of hydrogen from the closure at 21°C, D_{e1}, is $5.58(10)^{-7}$ mole/sec.

The release rate from the closure at 68°C, D_{e2} is then computed from equation (2) as:

$D_{e2} = 5.58(10)^{-7}$ mole/sec $(341K / 294K)^{1.75}$ $(0.6703 / 0.6815)^2$

$D_{e2} = 7.00(10)^{-7}$ mole/sec

The resistance of the inner bag to the release of hydrogen at 68°C, r(inner bag, 68°C), is then:

$$\begin{aligned} r(\text{inner bag, } 68°C) &= 1/D_{e2} \\ &= 1 / (7.00(10)^{-7}\ \text{mole/sec}) \\ &= 1{,}429{,}048\ \text{sec/mole} \end{aligned}$$

For comparison purposes,

r(inner bag, 21°C) = 1,792,115 sec/mole

A2.2 Resistance of Liner Bags

The release rate from a large liner bag at 68°C is assumed to be the lowest measured total release. No credit is taken for increased release through the liner bags at the higher temperature due to increased permeation and diffusion.

[5] Rodriguez, F., 1982, "Principles of Polymer Systems," 2nd Edition, McGraw-Hill Book Company, New York, New York, pp. 532-537.

The resistance of the liner bag, r(liner bag) is from Appendix 6.7 of the CH-TRU Payload Appendices,

r(liner bag) = $1/(29.15(10)^{-6}$ mole/sec) = 34,303 sec/mole.

A2.3 Resistance of Filter

The mechanism of release through the filter is also by diffusion; therefore, using the minimum measured diffusion coefficient of $1.9(10)^{-6}$ mole/sec at 70°F (21°C) (Appendix 6.7 of the CH-TRU Payload Appendices), the resistance at 154°F (68°C) is:

r(drum filter) = $1/(1.9(10)^{-6})$mole/sec x $(294/341)^{1.75}$
= 406,008 sec/mole

A2.4 Resistance of Drum Liner

The diffusion through a 0.3 inch diameter hole at -20°F (-29°C) is used to determine the total release rate (see Appendix 6.7 of the CH-TRU Payload Appendices). No credit is taken for permeation through the liner material or for increased diffusion through the hole at the higher temperature. Therefore, the resistance of the liner is: (Appendix 6.7 of the CH-TRU Payload Appendices)

r(drum liner) = 19,646 sec/mole

A2.5 Effective Resistance

The effective resistance for the layers of confinement in a payload container in the payload shipping category II.1A4 is the sum of the individual resistances of each layer. There are 3 inner bags, 1 liner bag, the punctured rigid drum liner and the drum filter. Therefore, the effective resistance at 154°F (68°C), r_{eff}, is:

$r_{eff}(68°C)$ = 3 x r(inner bag) + r(liner bag) + r(rigid drum liner) + r(drum filter)

$r_{eff}(68°C)$ = {3(1,429,048) + 214,133 + 19,646 + 406,008} sec/mole

$r_{eff}(68°C)$ = 4,926,931 sec/mole

A2.6 Increase in G Value With Temperature

The temperature corrected effective G value for hydrogen at 154°F (68°C) is calculated using an Arrhenius type dependence on temperature (see Appendix 3.2 of the CH-TRU Payload Appendices):

$G_{eff(T2)} = G_{eff(T1)} \exp[(E_G/R)\{(T_2-T_1)/(T_2 \times T_1)\}]$,

where,

E_G = is the hydrogen generation activation energy = 0.8 kcal/g-mole for polyethylene (see Appendix 3.2 of the CH-TRU Payload Appendices).

R = gas law constant = $1.987(10)^{-3}$ kcal/g-mole.

T_1 = Temperature which provides the basis for the effective G values 70°F (21°C).

T_2 = Maximum temperature in the ICV during transport of payload 154°F (68°C).

$G_{eff(T1)}$ = Effective G value for hydrogen for Waste Material Type II.1 = 1.70 at 70°F (21°C) (see Appendix 3.2 of the CH-TRU Payload Appendices).

$G_{eff(T2)}$ = Temperature corrected effective G value for hydrogen for Waste Material Type II.1 at 154°F (68°C).

Substituting the above values in the Arrhenius equation for the temperature corrected effective G value for hydrogen:

$G_{eff(T2)} = 1.70 \exp[\{(0.8 \text{ kcal/g-mole})/1.987(10)^{-3} \text{ kcal/g-mole}\} \times (341 - 294)/(341 \times 294)\}]$

$G_{eff(T2)} = 2.05.$

A2.7 Decay Heat Limit at Maximum Temperature

The allowable hydrogen gas generation rate per innermost confinement layer is computed using equation (4) of Appendix 2.3 of the CH-TRU Payload Appendices:

$$CG = (X_{inner})/(r_{eff} + (t)(N_{gen})/N_{tg})$$

$$CG = (0.05)/\{4{,}926{,}931 \text{ sec/mole} + [(60 \text{ days})(86{,}400 \text{ sec/day})(14)/(101.56 \text{ moles})]\}$$

$$= 8.863(10)^{-9} \text{ mole/sec.}$$

For shipping category II.1A4, the temperature corrected effective G value for hydrogen at 154°F (68°C) is 2.05. Therefore, the decay heat limit per innermost confinement layer, Q_i, is:

$$Q_i = [8.863(10)^{-9} \text{ mole/sec}][6.023(10)^{23} \text{ molecules/mole}] \times [1.602(10)^{-19} \text{ watt-sec/eV}]/[2.05 \text{ molecules/100 eV}]$$
$$= 0.0417 \text{ watt.}$$

The computed decay heat of 0.0417 watt at 154°F (68°C) is higher than the decay heat of 0.0414 watt that was calculated assuming a temperature of 70°F (21°C).

The sample calculation above demonstrates that the decay heat limit would be higher for the maximum operating temperature than at room temperatures even when the increase in the effective G value and possible closure restriction effects are considered.

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ATTACHMENT B

DECAY HEAT LIMITS USING MORE REALISTIC RELEASE RATES

B1.0 Introduction

This attachment presents the derivation of decay heat limits using more realistic hydrogen release rate assumptions than those used to obtain the decay heat limits in the CH-TRAMPAC (assumptions listed in Attachment A of this appendix). The limits indicated as single points in Figures 6.9-3 and 6.9-6 of this appendix would be applicable at each end of the operating temperature range. This attachment is provided for illustrative purposes to demonstrate the added margin of safety included in the analysis for the decay heat limits that are applicable to each payload shipping category.

The following is a list of assumptions that will be used in the calculations:

- For small inner bags (excluding the drum liner bags), only the diffusion through the twist-and-tape closure is used in determining the total release rate. No credit is taken for permeation through the bag material. As indicated by actual experimental measurements (Appendix 6.8 of the CH-TRU Payload Appendices), the release rate through the inner bags is not decreased at the lower operating temperatures. At temperatures above room temperature, the release rate (by diffusion) from the inner bags is a function of temperature raised to the 1.75 power and the square of porosity.

- For the drum liner bags, the sum of diffusion through the bag closure and permeation of the bag material is used in determining the total release rate. The lowest measured total release rate at three different test temperatures (Appendix 6.8 of the CH-TRU Payload Appendices) will be used for the release rate from a liner bag at temperatures below 70°F (21°C). Credit is taken for increased release through the liner bags at the higher temperature end due to increased permeation and diffusion.

- For the rigid drum liner, the diffusion through a 0.3" diameter hole will vary with the 1.75 power of temperature. No credit was taken for permeation through the liner material.

- For the filter vent in the payload containers, the lowest measured diffusion coefficient was used to determine the total release rate (Appendix 6.7 of the CH-TRU Payload Appendices) at room temperature. The release rate from the filter by diffusion will vary with the 1.75 power of temperature.

B2.0 Quantification of Confinement Layer Resistances at Minimum and Maximum Temperatures

The resistances of each of the different confinement layers at -20°F (-29°C) and at 154°F (68°C) are computed below based on the aforementioned assumptions. The resistance of a confinement layer to the release of hydrogen is the reciprocal of the hydrogen release rate from that layer.

B2.1 Resistance of Drum Liner

The drum liner resistance at -20°F, r(drum liner, -20°F) is 19,646 sec/mole. The resistance at 154°F (68°F) will be computed using equation (5) of Table 6.9-1 of this document.

r(drum liner 154°F) $= 19{,}646 \text{ sec/mole} \times (244/341)^{1.75}$
$= 10{,}937 \text{ sec/mole.}$

B2.2 Resistance of Filter

The mechanism of release through the filter is by diffusion, with a temperature dependence described by equation (2) in Table 6.9-1 of this document. The resistance of the filter at the minimum and maximum temperatures are:

r(drum filter, -20°F) $= 1/1.9(10)^{-6} \text{ sec/mole} \times (294/244)^{1.75}$
r(drum filter, -20°F) = 729,327 sec/mole

r(drum filter, 154°F) $= 1/1.9(10)^{-6} \text{ sec/mole} \times (294/341)^{1.75}$
r(drum filter, 154°F) = 406,008 sec/mole.

B2.3 Resistance of Inner Bags

The release rate through the inner bags is not decreased at lower operating temperatures, therefore:

r(inner bag, -20°F) = r(inner bag, 70°F) = 1,792,115 sec/mole

At 154°F (68°C), equation (5) of this document is used for the dependence of the hydrogen release rate from the inner bag with temperature. The porosities values were computed in Attachment A of this appendix.

r(inner bag, 154°F) $= 1/1.58(10)^{-7}(T_1/T_2)^{1.75} \quad (\epsilon_1/\epsilon_2)^2$
r(inner bag, 154°F) $= 1{,}792{,}115 \text{ sec/mole} \times (294/341)^{1.75}(0.6815/0.6703)^2$
r(inner bag, 154°F) = 1,429,048 sec/mole

B2.4 Resistance of Liner Bags

The lowest measured total release rate at three different test temperatures (Appendix 6.8 of the CH-TRU Payload Appendices) will be used for the release rate from a liner bag at temperatures below 70°F (21°C). Therefore:

r(liner bag, -20°F) = r(liner bag, 70°F) = 214,133 sec/mole

The hydrogen release rate from a large liner bag at 154°F (68°C) will be calculated as the sum of the following three terms:

a. the total release rate (sum of the diffusion through the bag closure and bag permeation) from a large liner bag at 70°F (21°C)

   = $4.67(10)^{-6}$ mole/sec (Appendix 6.7 of the CH-TRU Payload Appendices)

b. the increase in the diffusion rate from the bag closure due to increased temperature. This value is taken to be the same as for the increase seen in the small bag closure

   = (1/1,429,048 - 1/1,792,115)
   = $1.4(10)^{-7}$ mole/sec

c. the increase in the release rate due to higher permeation rates (P) as a result of the increase in temperature

   = P(154°F) - P(70°F).

   The rate of release by permeation at 154°F (68°C) will be computed from the release rate dependence on temperature in an Arrhenius function (Appendix 6.7 of the CH-TRU Payload Appendices) as

$$P(154^{\circ}F) = P(70^{\circ}F)\exp\{(E_p/R) \times (T_2 - T_1)/(T_2 \times T_1)\}$$

where,

E_p = activation energy for hydrogen permeation through polyethylene.
= [8.2 kcal/g-mole] (Appendix 6.7 of the CH-TRU Payload Appendices)

P(21°C) is the difference between the total release and the bag closure release.

P(21°C) = $4.67(10)^{-6}$ mole/sec - $5.58(10)^{-7}$ mole/sec
= $4.11(10)^{-6}$ mole/sec

Substituting for these values:
P(68°C) - P(21°C) = $24.34(10)^{-6}$ mole/sec

Therefore the hydrogen release rate from a large liner bag at 154°F (68°C) is:

$= 4.67(10)^{-6} + 1.4(10)^{-7} + 24.34(10)^{-6}$ mole/sec
$= 29.15(10)^{-6}$ mole/sec

The resistance of the liner bag, r(liner bag) is the reciprocal of the release rate,

r(liner bag) = $1/29.15(10)^{-6}$ sec/ mole = 34,305 sec/mole

B3.0 G Values at Minimum and Maximum Temperatures

The temperature corrected effective G value for hydrogen at both -20°F (-29°C) and at 154°F (68°C) for shipping category II.1A4 were computed as

G_{eff} (II.1A4 at -20°F) = 1.28

G_{eff} (II.1A4 at 154°F) = 2.05

For Waste Type I, the G value does not change with temperature (Appendix 3.2 of the CH-TRU Payload Appendices), therefore,

G_{eff} (I.1A3 at 70°F) = G_{eff} (I.1A3 at -20°F) = G_{eff} (I.1A3 at 154°F) = 1.60

B4.0 Decay Heat Limit At Minimum Normal Operating Temperature For Shipping Category I.1A3

The effective resistance for shipping category I.1A3 is the sum of the individual resistances. There are 2 inner bags, 1 liner bag, the punctured rigid drum liner, and the drum filter. Therefore, the effective resistance, r_{eff} is

$r_{eff(I.1A3,-20°F)}$ = 2 x r(inner bag) + r(liner bag) + r(drum liner) + r(drum filter)

$r_{eff(I.1A3,-20°F)}$ = {2(1,792,115) + 214,133 + 19,646 + 729,327} sec/mole

$r_{eff(I.1A3,-20°F)}$ = 4,547,336 sec/mole.

The maximum allowable hydrogen generation rate is computed from equation (2) of Table 6.9-3 as:

CG (I.1A3, -20°F) = 0.05/(4,547,336 + 714,612) mole/sec
CG (I.1A3, -20°F) = $9.502(10)^{-9}$ mole/sec

The decay heat limit is computed from equation (3) of Table 6.9-3 as:

Q_i(I.1A3 at -20°F) = [9.502(10)$^{-9}$ mole/sec][6.023(10)^{23} molecules/mole] x [1.602(10)$^{-19}$ watt-sec/eV]/(1.60 molecules/100 eV]

Q_i(I.1A3 at -20°F) = 0.0573 watt.

B5.0 Decay Heat Limit At Minimum Normal Operating Temperature for Shipping Category II.1A4

The effective resistance for shipping category II.1A4 is the sum of the individual resistances. There are 3 inner bags, 1 liner bag, the punctured drum liner, and the drum filter. Therefore, the effective resistance, r_{eff} is

$r_{eff(II.1A4,-20°F)}$ = 3 x r(inner bag) + r(liner bag) + r(drum liner) + r(drum filter)

$r_{eff(II.1A4,-20°F)}$ = {3(1,792,115) + 214,133 + 19,646 + 729,327} sec/mole

$r_{eff(II.1A4,-20°F)}$ = 6,339,451 sec/mole

The maximum allowable hydrogen generation rate is computed from equation (2) of Table 6.9-3 as:

CG (II.1A4, -20°F) = 0.05/(6,339,451 + 714,612) mole/sec

CG (II.1A4, -20°F) = 7.088(10)$^{-9}$ mole/sec

The decay heat limit is computed from equation (3) of Table 6.9-3 as:

Q_i (II.1A4 at -20°F) = [7.088(10)$^{-9}$ mole/sec] [6.023(10)^{23} molecules/mole] x [1.602(10)$^{-19}$ watt-sec/eV]/(1.28 molecules/100 eV]

Q_i(II.1A4 at -20°F) = 0.0534 watt.

B6.0 Decay Heat Limit at Maximum Normal Operating Temperature for Shipping Category I.1A3

The effective resistance for shipping category I.1A3 at 154°F (68°C) is evaluated using the resistances computed above as:

$r_{eff(I.1A3,154°F)}$ = {2(1,429,048) + 34,305 + 10,937 + 406,008} sec/mole

$r_{eff(I.1A3,154°F)}$ = 3,309,346 sec/mole

The maximum allowable hydrogen generation rate is computed from equation (2) of Table 6.9-3 as:

CG (I.1A3, 154°F) = 0.05/(3,309,364 + 714,612) mole/sec
CG (I.1A3, 154°F) = $1.243(10)^{-8}$ mole/sec

The decay heat limit is computed from equation (3) of Table 6.9-3 as:

Q_i (I.1A3 at 154°F) = [$1.243(10)^{-8}$ mole/sec] [$6.023(10)^{23}$ molecules/mole] x [$1.602(10)^{-19}$ watt-sec/eV]/(1.60 molecules/100 eV]

Q_i(I.1A3 at -20°F) = 0.0750 watt.

B7.0 Decay Heat Limit at Maximum Normal Operating Temperature for Shipping Category II.1A4

The effective resistance for shipping category II.1A4 at 154°F (68°C) is evaluated using the resistances computed above as:

$r_{eff(II.1A4,154°F)}$ = {3(1,429,048) + 34,305 + 10,937 + 406,008} sec/mole

$r_{eff(II.1A4,154°F)}$ = 4,738,394 sec/mole

The maximum allowable hydrogen generation rate is computed from equation (2) of Table 6.9-3 as:

CG (II.1A4, 154°F) = 0.05/(4,738,394 + 714,612) mole/sec
CG (II.1A4, 154°F) = $9.169(10)^{-9}$ mole/sec

The decay heat limit is computed from equation (3) of Table 6.9-3 as:

Q_i (II.1A4 at 154°F) = [$9.169(10)^{-9}$ mole/sec] [$6.023(10)^{23}$ molecules/mole] x [$1.602(10)^{-19}$ watt-sec/eV]/(2.05 molecules/100 eV]

Q_i(II.1A4 at 154°F) = 0.0432 watt.

The four decay heat limits derived above in Sections B4.0, B5.0, B6.0 and B7.0 of this attachment are the points marked in Figures 6.9-3 and 6.9-6 of this appendix. The use of the assumptions outlined in this Attachment provides decay heat limits at each end of the operating temperature range that are higher than the limits applied to each shipping category, as shown in the two figures.

APPENDIX 6.10

EFFECT ON DECAY HEAT LIMITS OF OVERPACKING PAYLOAD CONTAINERS

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6.10 Effect on Decay Heat Limits of Overpacking Payload Containers

6.10.1 Summary

The ten-drum overpack (TDOP) and standard waste box (SWB) are containers that will be primarily used to overpack other payload containers. One of the transportation parameters that could be affected as a result of this overpacking is the allowable decay heat limit per each payload container. The analyses presented in this appendix show that overpacking payload containers in a TDOP fitted with nine filters (total hydrogen diffusivity of 3.33E-5 moles per second per mole fraction [m/s/mf]) or an SWB fitted with four filters (total hydrogen diffusivity of 1.48E-5 m/s/mf) will not decrease the allowable decay heat limits, even when payload containers are allowed to remain overpacked in a TDOP or an SWB fitted with four filters for indefinite periods of time before transport. For example, a 55-gallon drum that meets the decay heat limit for a 14-drum payload in a TRUPACT-II can also be shipped in a 10-drum configuration in a TDOP inside a TRUPACT-II or in a 4-drum configuration in an SWB (fitted with four filters) with two SWBs inside a TRUPACT-II. This is due to the following reasons:

- The TDOP is fitted with a minimum of nine filters (total hydrogen diffusivity of 3.33E-5 m/s/mf) that allow hydrogen release from the TDOP. The SWB fitted with four filters (total hydrogen diffusivity of 1.48E-5 m/s/mf) will allow hydrogen release from the SWB.

- The number of payload containers per shipment is less when overpacked in a TDOP or SWB compared to the case when containers are not overpacked in a TDOP or SWB. For example, when drums are overpacked in a TDOP, there is a 10 drum payload compared to a 14-drum payload without the overpacking. Similarly, there is only an 8-drum payload when overpacked in an SWB compared to a 14-drum payload without the overpacking. The lesser number of payload containers result in less accumulation of hydrogen in the ICV and the payload containers during shipment.

- There is a known amount of additional void volume available in payload configurations overpacked in the TDOP or SWB, which reduces overall concentrations of the hydrogen generated.

This appendix describes the mathematical analyses supporting the conclusion that no reduction in decay heat limits occurs for payload configurations overpacked in a TDOP or in an SWB fitted with four filters (total hydrogen diffusivity of 1.48E-5 m/s/mf). Decay heat limits for all other overpacked configurations can be conservatively classified into one of the existing configurations for which decay heat limits have been specified in the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) document.

6.10.2 Introduction

The TDOP is an authorized payload container in the TRUPACT-II that will be used primarily for the overpacking of other payload containers (it can also be used for the direct loading of waste). Specifications for the TDOP are given in Section 2.9 of the CH-TRAMPAC.

In addition, the SWB can be used to overpack up to four 55-gallon drums with either two or four filters installed in the SWB. It is possible that these overpacked payload configurations may be kept in interim storage for indefinite periods of time before shipment in a TRUPACT-II (i.e., it is not necessary that shipment occur immediately after overpacking in a TDOP or SWB). Decay heat limits for drums overpacked in SWBs with two filters are derived as described in the CH-TRAMPAC document. Overpacking in a TDOP or an SWB fitted with four filters could potentially affect the allowable decay heat limits for payload containers due to the following differences from equivalent configurations that are not overpacked:

- There is an additional layer of resistance to the release of hydrogen when containers are overpacked.

- The number of payload containers is less when overpacked in a TDOP or in two SWBs (e.g., 10 drums per TDOP and TRUPACT-II compared to 14 drums per TRUPACT-II when not overpacked in a TDOP; one SWB per TDOP and TRUPACT-II compared to two SWBs per TRUPACT-II when not overpacked in a TDOP). The lesser number of payload containers results in less accumulation of hydrogen in the TRUPACT-II during shipment, compared to shipments where payload containers are not overpacked.

- Due to the lesser number of containers overpacked, there is additional void volume available for gas accumulation in payload configurations using overpacking.

The purpose of this appendix is to analyze these potential impacts on decay heat limits. As shown by the mathematical analysis in the following sections, decay heat limits for payload containers are not decreased by overpacking in a TDOP or in an SWB fitted with four filters (total hydrogen diffusivity of 1.48E-5 m/s/mf), and the decay heat limits that have been calculated for the payload containers without the overpacking are applicable even in the overpacked condition in a TDOP or in an SWB fitted with four filters.

6.10.3 Assumptions and Quantification of Input Parameters

Values of the input parameters used in the analysis, with applicable assumptions, are presented in this section.

6.10.3.1 Resistances of the Confinement Layers

The resistances of the various confinement layers to the release of hydrogen are quantified in Appendix 6.7 of the CH-TRU Payload Appendices, and are summarized in Table 6.10-1. The logic for the two different values of a confinement layer resistance (one value for Waste Type I and a second value for Waste Types II and III) is provided in Appendix 6.9 of the CH-TRU

Payload Appendices. The analysis assumes the use of nine filters on the TDOP or four filters on the SWB. Each filter has a hydrogen diffusivity of 3.7E-6 m/s/mf. A lesser number of filters may be used provided the total hydrogen diffusivity is equal to or greater than 3.33E-5 m/s/mf for the TDOP and 1.48E-5 m/s/mf for the SWB.

Table 6.10-1 — Resistances of the Confinement Layers

Confinement Layer	Resistances (sec/mole)	
	Waste Type I	Waste Types II and III
Drum Filter	729,327	526,316
SWB/Bin Filter	374,519	270,270
85-Gallon Drum Filter	374,519	270,270
TDOP Filter	374,519	270,270
Inner Bag	2,398,864	1,792,115
Drum Liner Bag	214,133	214,133
SWB/Bin/TDOP Liner	125,660	125,660
Punctured Drum Liner	19,646	19,646

6.10.3.2 Void Volumes

Based on the specifications for the TDOP in Section 2.9.9 of the CH-TRAMPAC, the external volume occupied by a TDOP is 4,473 liters and the internal volume is 4,426 liters. The void volume within an empty TRUPACT-II ICV is approximately 5,750 liters. The void volume between the TDOP and the TRUPACT-II ICV is approximately 1,277 liters. The void volume inside a TDOP with a payload of 10 55-gallon drums is 2,069 liters. The volume occupied by two SWBs is approximately 4,000 liters. The net void volume for gas accumulation in the ICV is 1,750 liters for an assembly of SWBs. These void volumes serve to reduce hydrogen concentrations in the different layers of the package and payload.

6.10.3.3 Other Input Parameters

All other input parameters for the decay heat calculations are the same as those presented in Appendices 6.7 and 6.9 of the CH-TRU Payload Appendices.

6.10.4 Methodology and Mathematical Analyses

The analysis conservatively assumes that the overpacked payload containers inside the TDOP or SWB can remain inside indefinitely, i.e., steady-state conditions with the maximum gas concentrations are attained. The TDOP or SWB is then loaded into the TRUPACT-II for a 60-day shipping period. Each of the payload configurations to be overpacked is analyzed below to determine impacts on decay heat limits.

Configuration 1: 10 55-gallon Drums Overpacked in a TDOP

The analysis for the configuration of 10 55-gallon drums overpacked in a TDOP is based on modeling the buildup of flammable gas within the TRUPACT-II payload assembly during the 60-day shipping period. The first step in the analysis was the calculation of a pseudo steady-state gas generated concentrations within the TDOP as a first approximation. The following equations calculate these concentrations:

$$X_{TDOP} = C_g' (10\, r_{TDOP\ filter}/n_{TDOP})$$

$$X_{Annular} = C_g'\, r_{df} + X_{TDOP}$$

$$X_{Drum\ Liner} = C_g'\, r_{dl} + X_{Annular}$$

$$X_{Multiple\ Bag\ Void} = C_g' (r_{Inner\ Bags} + r_{liner\ bags}) + X_{Drum\ Liner}$$

where:

X_{TDOP} = mole fraction of flammable gas within the TDOP void volume

$X_{Annular}$ = mole fraction of flammable gas within the annular space between the drum liner and the drum

$X_{Drum\ Liner}$ = mole fraction of flammable gas within the drum liner void volume

$X_{Multiple\ Bag\ Void}$ = mole fraction of flammable gas within the innermost confinement layer

$r_{inner\ bags}$ = total resistance of the inner bags to the release of flammable gas (sec/mole)

$r_{liner\ bags}$ = total resistance of the liner bags to the release of flammable gas (sec/mole)

r_{dl} = resistance of the drum liner to the release of flammable gas (sec/mole)

r_{df} = resistance of the 55-gallon drum filter to the release of flammable gas (sec/mole)

$r_{TDOP\ filter}$ = resistance of a single filter on the TDOP to the release of flammable gas (sec/mole)

n_{TDOP} = number of filters on the TDOP

C_g' = first approximation for maximum allowable flammable gas generation rate (mole/sec)

For example, if pseudo-steady-state flammable gas generation rate is used as the first approximation:

$$C_g = \frac{0.05}{r_{eff} + \left(10\frac{t}{N_{tg}}\right)}$$

where

r_{eff} = effective resistance of all confinement layers of the generating container to the release of flammable gas (sec/mole)

t = maximum shipping period duration (60 days)

N_{tg} = total moles of gas inside the TRUPACT-II ICV cavity outside of the TDOP,

= $P V_{void}/RT$

where:

P = pressure inside the TRUPACT-II, assumed to be constant at 1 atm., because the amount of gas generated is much less than the total amount of air originally present in the cavity

V_{void} = void volume inside the TRUPACT-II ICV and outside of the TDOP, i.e. 1,277 liters with a TDOP inside the TRUPACT-II

R = gas constant = 0.08206 atm-liter/mole-K

T = absolute temperature = 294 K.

Equations were then developed to calculate the flammable gas concentration within the various payload assembly layers as a function of time during the shipping period. Collectively, these equations model the diffusion of flammable gas generated within the waste across the various resistance layers present in the payload assembly.

$$\frac{dX_{Multiple\ Bag\ Void}}{dt} = \frac{C_g RT}{PV_{Multiple\ Bag\ Void}} - \frac{R_{bags}}{V_{Multiple\ Bag\ Void}}\left(X_{Multiple\ Bag\ Void} - X_{Drum\ Liner}\right)$$

$$\frac{dX_{Drum\ Liner}}{dt} = \frac{R_{bags}}{V_{Drum\ Liner}}(X_{Multiple\ Bag\ Void} - X_{Drum\ Liner}) - \frac{R_{dl}}{V_{Drum\ Liner}}(X_{Drum\ Liner} - X_{Annular})$$

$$\frac{dX_{Annular}}{dt} = \frac{R_{dl}}{V_{Annular}}(X_{Drum\ Liner} - X_{Annular}) - \frac{R_{df}}{V_{Annular}}(X_{Annular} - X_{TDOP})$$

$$\frac{dX_{TDOP}}{dt} = \frac{10\ R_{df}}{V_{TDOP}}(X_{Annular} - X_{TDOP}) - \frac{nTDOP\ R_{TDOP\ filter}}{V_{TDOP}}(X_{TDOP} - X_{ICV})$$

$$\frac{dX_{ICV}}{dt} = \frac{n_{TDOP}\ R_{TDOP\ filter}}{V_{void}}(X_{TDOP} - X_{ICV})$$

where:

R_{bags} = release rate across the inner bags and liner bags of flammable gas (liters/day)

R_{dl} = release rate of flammable gas across the drum liner (liters/day)

R_{df} = release rate of flammable gas across the drum filter (liters/day)

$R_{TDOP\ filter}$ = release rate of flammable gas across one TDOP filter (liters/day)

$V_{Multiple\ Bag\ Void}$ = void volume inside bag layers (conservatively assumed to be 1 liter)

$V_{Drum\ Liner}$ = void volume inside drum liner (conservatively assumed to be 1 liter)

$V_{Annular}$ = void volume between drum liner and drum (conservatively assumed to be 1 liter)

V_{TDOP} = void volume inside the TDOP with a payload of 10 55-gallon drums (2,069 liters)

X_{ICV} = mole fraction of flammable gas within the TRUPACT-II ICV cavity

C_g = maximum allowable flammable gas generation rate (mole/sec)

This system of equations must be solved simultaneously to find the maximum flammable gas generation rate that results in a concentration of five percent in the innermost confinement layer during the 60-day shipping period. The steady-state flammable gas generation rate is used as a

first approximation of the allowable transient flammable gas generation rate. An iterative calculation process using the Runge-Kutta method was adapted to solve the system of equations.

Configuration 2: 8 55-Gallon Drums Overpacked in Two SWBs With Four Filters in Each SWB

The analysis for the configuration of eight 55-gallon drums overpacked in two SWBs fitted with four filters (total hydrogen diffusivity of 1.48E-5 m/s/mf) each is based on the modeling build-up of flammable gases within the payload assembly during the 60-day shipping period. The first step in the analysis was the calculation of a pseudo-steady-state gas generation concentration within the SWBs as a first approximation. The following equations calculate those concentrations:

$X_{SWB} = C_g' (4 r_{SWB\ Filter} / n_{SWB})$

$X_{Annular} = C_g' r_{df} + X_{SWB}$

$X_{Drum\ Liner} = C_g' r_{dl} + X_{Annular}$

$X_{Multiple\ Bag\ Void} = C_g' (r_{Inner\ Bags} + r_{Liner\ Bags}) + X_{Drum\ Liner}$

where C_g', $X_{Annular}$, r_{df}, $X_{Drum\ Liner}$, r_{dl}, $X_{Multiple\ Bag\ Void}$, $r_{Inner\ Bags}$, and $r_{Liner\ Bags}$ are defined above and where:

X_{SWB} = mole fraction of flammable gas within the SWB void volume

$r_{SWB\ Filter}$ = resistance of a single filter on the SWB to the release of flammable gas (sec/mole)

n_{SWB} = number of filters on the SWB.

As in Configuration 1, equations were developed to calculate the flammable gas concentration within the various payload assembly layers as a function of time during the shipping period.

$$\frac{dX_{Multiple\ Bag\ Void}}{dt} = \frac{C_g\ RT}{PV_{Multiple\ Bag\ Void}} - \frac{R_{Bags}}{V_{Multiple\ Bag\ Void}} (X_{Multiple\ Bag\ Void} - X_{Drum\ Liner})$$

$$\frac{dX_{Drum\ Liner}}{dt} = \frac{R_{Bags}}{V_{Drum\ Liner}} (X_{Multiple\ Bag\ Void} - X_{Drum\ Liner}) - \frac{R_{dl}}{V_{Drum\ Liner}} (X_{Drum\ Liner} - X_{Annular})$$

$$\frac{dX_{Annular}}{dt} = \frac{R_{dl}}{V_{Annular}} (X_{Drum\ Liner} - X_{Annular}) - \frac{R_{df}}{V_{Annular}} (X_{Annular} - X_{SWB})$$

$$\frac{dX_{SWB}}{dt} = \frac{4\,R_{df}}{V_{SWB}}\,(X_{Annular} - X_{SWB}) - \frac{n_{SWB}\,R_{SWB\,Filter}}{V_{SWB}}\,(X_{SWB} - X_{ICV})$$

$$\frac{dX_{ICV}}{dt} = \frac{2\,n_{SWB}\,R_{SWB\,Filter}}{V_{Void}}\,(X_{SWB} - X_{ICV})$$

where:

$R_{SWB\ Filter}$ = release rate of flammable gas across one SWB filter (liters/day)

V_{SWB} = void volume inside the SWB with a payload of four 55-gallon drums (conservatively assumed to be 10 liters).

This system of equations was again solved simultaneously to find the maximum flammable gas generation rate that results in a concentration of 5 percent in the innermost confinement layer during the 60-day shipping period.

Four different packaging configurations were considered for overpacking 55-gallon drums in the SWB. The system of equations summarized above is the same for all of the packaging configurations. These packaging configurations represent the lower and upper ends of the flammable gas generation range. The four configurations were as follows:

- Four drums of Shipping Category 10 0160 0147 per SWB fitted with four SWB filters and two SWBs per TRUPACT-II. Each drum has one low hydrogen diffusivity filter (diffusion coefficient of 1.9×10^{-6} mole/sec/mole fraction).
- Four drums of Shipping Category 30 0340 1044 per SWB fitted with four SWB filters and two SWBs per TRUPACT-II. Each drum has one low hydrogen diffusivity filter.
- Four drums of Shipping Category 10 0160 0111 per SWB fitted with four SWB filters and two SWBs per TRUPACT-II. Each drum has one high hydrogen diffusivity filter (diffusion coefficient of 3.7×10^{-6} mole/sec/mole fraction).
- Four drums of Shipping Category 30 0340 1018 per SWB fitted with four SWB filters and two SWBs per TRUPACT-II. Each drum has one high hydrogen diffusivity filter.

Configuration 3: 6 85-gallon Drums Overpacked in a TDOP

The analysis for the configuration of 6 85-gallon drums overpacked in a TDOP is based on modeling the buildup of flammable gas within the TRUPACT-II payload assembly during the 60-day shipping period. The first step in the analysis was the calculation of a pseudo steady-state gas generated concentrations within the TDOP as a first approximation. The following equations calculate these concentrations:

$$X_{TDOP} = C_g' (6\, r_{TDOP\ filter}/n_{TDOP})$$

$$X_{Annular} = C_g'\, r_{85df} + X_{TDOP}$$

$$X_{Drum\ Liner} = C_g'\, r_{dl} + X_{Annular}$$

$$X_{Multiple\ Bag\ Void} = C_g' (r_{Inner\ Bags} + r_{liner\ bags}) + X_{Drum\ Liner}$$

where:

r_{85df} = resistance of the 85-gallon drum filter to the release of flammable gas (sec/mole)

As in Configuration 1, equations were then developed to calculate the flammable gas concentration within the various payload assembly layers as a function of time during the shipping period. Collectively, these equations model the diffusion of flammable gas generated within the waste across the various resistance layers present in the payload assembly.

$$\frac{dX_{Multiple\ Bag\ Void}}{dt} = \frac{C_g RT}{PV_{Multiple\ Bag\ Void}} - \frac{R_{bags}}{V_{Multiple\ Bag\ Void}} (X_{Multiple\ Bag\ Void} - X_{Drum\ Liner})$$

$$\frac{dX_{Drum\ Liner}}{dt} = \frac{R_{bags}}{V_{Drum\ Liner}} (X_{Multiple\ Bag\ Void} - X_{Drum\ Liner}) - \frac{R_{dl}}{V_{Drum\ Liner}} (X_{Drum\ Liner} - X_{Annular})$$

$$\frac{dX_{Annular}}{dt} = \frac{R_{dl}}{V_{Annular}} (X_{Drum\ Liner} - X_{Annular}) - \frac{R_{85df}}{V_{Annular}} (X_{Annular} - X_{TDOP})$$

$$\frac{dX_{TDOP}}{dt} = \frac{6R_{85df}}{V_{TDOP}} (X_{Annular} - X_{TDOP}) - \frac{n_{TDOP}\ R_{TDOP\ filter}}{V_{TDOP}} (X_{TDOP} - X_{ICV})$$

$$\frac{dX_{ICV}}{dt} = \frac{n_{TDOP}\ R_{TDOP\ filter}}{V_{void}} (X_{TDOP} - X_{ICV})$$

where:

R_{85df} = release rate of flammable gas across the 85-gallon drum filter (liters/day)

$V_{Multiple\ Bag\ Void}$ = void volume inside bag layers (from Appendix 3.7 of the CH-TRU Payload Appendices)

$V_{Drum\ Liner}$ = void volume inside drum liner (from Appendix 3.7 of the CH-TRU Payload Appendices)

$V_{Annular}$ = void volume between drum liner and drum (from Appendix 3.7 of the CH-TRU Payload Appendices)

V_{TDOP} = void volume inside the TDOP with a payload of 6 85-gallon drums (2,210 liters)

This system of equations must be solved simultaneously to find the maximum flammable gas generation rate that results in a concentration of five percent in the innermost confinement layer during the 60-day shipping period.

Other Payload Configurations

For other payload configurations, the pseudo steady-state analysis (used as a first approximation for the 10-drum configuration) is sufficient to demonstrate that decay heat limits are not decreased by overpacking in a TDOP. No further refinement of the pseudo steady-state condition is necessary since the conservative pseudo steady-state analysis itself demonstrates that decay heat limits are not decreased.

For these configurations, an equation was developed (for each of the four additional configurations) that relates the innermost confinement layer flammable gas concentration to the sum of the resistances of the confinement layers and the allowable flammable gas generation rate. These equations are summarized below for the four configurations considered. The governing equations are the same as those used in Appendix 2.3 of the CH-TRU Payload Appendices. The equations solve for the allowable gas generation rates and decay heats when overpacked in a TDOP.

Configuration 4: 4 55-gallon Drums Overpacked in an SWB Overpacked in a TDOP

$$X_1 = C_g[r_{inner\ bags} + r_{liner\ bags} + r_{dl} + r_{df} + 4r_{SWB\ filters} + r_{TDOP\ filter}/n_{TDOP} + 4(t/N_{tg})]$$

$$X_1 = C_g[r_{eff} + 4r_{SWB\ filters} + r_{TDOP\ filter}/n_{TDOP} + 4(t/N_{tg})]$$

Configuration 5: 1 SWB Overpacked in a TDOP

$$X_1 = C_g(r_{inner\ bags} + r_{SWB\ liners} + r_{SWB\ filters} + r_{TDOP\ filter}/n_{TDOP} + t/N_{tg})$$

$X_1 = C_g(r_{eff} + r_{TDOP\ filter}/n_{TDOP} + t/N_{tg})$

Configuration 6: 1 Experimental Bin Inside an SWB Overpacked in a TDOP

$X_1 = C_g(r_{inner\ bags} + r_{bin\ liners} + r_{bin\ filters} + r_{SWB\ filters} + r_{TDOP\ filter}/n_{TDOP} + t/N_{tg})$

$X_1 = C_g(r_{eff} + r_{SWB\ filters} + r_{TDOP\ filter}/n_{TDOP} + t/N_{tg})$

Configuration 7: 6 85-Gallon Drums Overpacked in a TDOP

$X_1 = C_g[r_{inner\ bags} + r_{liner\ bags} + r_{dl} + r_{df} + r_{85df} + 6r_{TDOP\ filter}/n_{TDOP} + 6(t/N_{tg})]$

$X_1 = C_g[r_{eff} + r_{85df} + 6r_{TDOP\ filter}/n_{TDOP} + 6(t/N_{tg})]$

where:

X_1 = mole fraction flammable gas within innermost confinement layer

$r_{bin\ liners}$ = total resistance of the bin liners to the release of flammable gas (sec/mole)

$r_{SWB\ liners}$ = total resistance of the SWB liners to the release of flammable gas (sec/mole)

$r_{SWB\ filters}$ = total resistance of the SWB filters to the release of flammable gas (sec/mole)

$r_{bin\ filters}$ = total resistance of the bin filters to the release of flammable gas (sec/mole)

The resistance terms, r_{eff}, $r_{SWB\ filters}$, and r_{85df}, represent the effective resistance of all confinement layers within the TDOP to the release of flammable gas. The next resistance term in these equations represents the resistance of the filters on the TDOP to the release of flammable gas. Since these filters act in parallel, increasing the number of filters decreases the total resistance. The last resistance term in the equations, t/N_{tg}, represents the effective resistance offered by the accumulation of flammable gas within the ICV during a 60-day shipping period.

6.10.5 Discussion of Results

Tables 6.10-2 through 6.10-8 present examples of the results of the analyses for all six overpacked configurations. The decay heat limit under the Configuration column (last column of each table) is the limit that could be applied under the overpacked condition. The decay heat limit under the Base Case column is the limit for each payload container without being overpacked in a TDOP or SWB. As can be seen in all cases, the overpacked configuration decay heat numbers are higher than the numbers for the base case. Therefore, decay heat numbers are not decreased due to overpacking in a TDOP or SWB. It is conservative to use the base case decay heat limits for the overpacked configurations. The tables cover shipping categories with no bags (least resistance) to multiple bags (high resistance). Other shipping categories not included in the tables would fall within this range of shipping categories.

6.10.6 Conclusions

The analysis presented in this appendix demonstrates that overpacking payload containers in a TDOP or an SWB fitted with four filters (total hydrogen diffusivity of 1.48E-5 m/s/mf) does not decrease the allowable decay heat limits for the payload containers. The overpacked configurations can be conservatively assigned the same decay heat limits as the equivalent configurations not using the TDOP or SWB for overpacking. A payload container in a shipping category that meets the decay heat limit for shipment without being overpacked in a TDOP fitted with nine filters (total hydrogen diffusivity of 3.33E-5 m/s/mf) or an SWB fitted with four filters automatically meets the required decay heat limit when overpacked. In summary, for purposes of flammable gas generation and decay heat limits, overpacked payload configurations can be considered as follows:

Ten 55-gallon drums overpacked in a TDOP	Same as 14 55-gallon drums in a TRUPACT-II
Eight 55-gallon drums overpacked in two SWBs with four filters in each SWB	Same as 14 55-gallon drums in a TRUPACT-II
Four 55-gallon drums overpacked in an SWB overpacked in a TDOP	Same as eight 55-gallon drums overpacked in two SWBs with two filters (total hydrogen diffusivity of 7.40E-6 m/s/mf) each in a TRUPACT-II
One SWB overpacked in a TDOP	Same as two SWBs in a TRUPACT-II
One experimental bin in an SWB overpacked in a TDOP	Same as two experimental bins in two SWBs in a TRUPACT-II
Six 55-gallon drums in six 85-gallon drums overpacked in a TDOP	Same as eight 55-gallon drums overpacked in two SWBs with two filters (total hydrogen diffusivity of 7.40E-6 m/s/mf) each in a TRUPACT-II
Six 85-gallon drums overpacked in a TDOP	Same as eight 85-gallon drums in a TRUPACT-II

Table 6.10-2 — Configuration 1: 10 55-gallon Drums Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 1	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
I.1A0	10 0160 0147	3.416E-08	**0.2060**	3.474E-08	**0.2095**
I.1A1	10 0160 0168	2.980E-08	**0.1797**	3.035E-08	**0.1830**
I.1A2	10 0160 0190	2.643E-08	**0.1594**	2.687E-08	**0.1620**
I.1A3	10 0160 0648	7.721E-09	**0.0466**	7.775E-09	**0.0469**
I.2A0	10 0130 0147	3.416E-08	**0.2536**	3.474E-08	**0.2578**
I.2A1	10 0130 0168	2.980E-08	**0.2212**	3.035E-08	**0.2253**
I.2A2	10 0130 0190	2.643E-08	**0.1962**	2.687E-08	**0.1994**
I.2A3	10 0130 0648	7.721E-09	**0.0573**	7.775E-09	**0.0577**
I.2A4	10 0130 0888	5.634E-09	**0.0418**	5.667E-09	**0.0421**
I.3A0	10 0040 0147	3.416E-08	**0.8241**	3.474E-08	**0.8380**
I.3A1	10 0040 0168	2.980E-08	**0.7189**	3.035E-08	**0.7321**
I.3A2	10 0040 0190	2.643E-08	**0.6375**	2.687E-08	**0.6482**
I.3A3	10 0040 0648	7.721E-09	**0.1863**	7.775E-09	**0.1875**
I.3A4	10 0040 0888	5.634E-09	**0.1359**	5.667E-09	**0.1367**
II.1A0	20 0170 0127	3.966E-08	**0.2251**	4.368E-08	**0.2479**
II.1A1	20 0170 0148	3.390E-08	**0.1924**	3.689E-08	**0.2094**
II.1A2a	20 0170 0327	2.961E-08	**0.1680**	3.187E-08	**0.1809**
II.1A2	20 0170 0169	1.531E-08	**0.0869**	1.591E-08	**0.0903**
II.1A3	20 0170 0506	9.883E-09	**0.0561**	1.014E-08	**0.0576**
II.1A4	20 0170 0686	7.298E-09	**0.0414**	7.445E-09	**0.0423**
II.1A5	20 0170 0865	5.785E-09	**0.0328**	5.880E-09	**0.0334**
II.1A6	20 0170 1044	4.791E-09	**0.0272**	4.859E-09	**0.0276**
II.2AM	20 0000 0000	NA	**40.000**	NA	**40.000**
III.1A0	30 0340 0127	3.966E-08	**0.1126**	4.368E-08	**0.1240**
III.1A1	30 0340 0148	3.390E-08	**0.0962**	3.689E-08	**0.1047**
III.1A2a	30 0340 0327	2.961E-08	**0.0840**	3.187E-08	**0.0904**
III.1A2	30 0340 0169	1.531E-08	**0.0434**	1.591E-08	**0.0452**
III.1A3	30 0340 0506	9.883E-09	**0.0280**	1.014E-08	**0.0288**
III.1A4	30 0340 0686	7.298E-09	**0.0207**	7.445E-09	**0.0211**
III.1A5	30 0340 0865	5.785E-09	**0.0164**	5.880E-09	**0.0167**
III.1A6	30 0340 1044	4.791E-09	**0.0136**	4.859E-09	**0.0138**

* Base Case: 14 55-gallon drums (as two 7-packs) loaded directly into a TRUPACT-II

Table 6.10-3 — Configuration 2: 4 55-gallon Drums Overpacked in an SWB Fitted with Four Filters, Two SWBs per TRUPACT-II Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 2	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
I.1A0	10 0160 0147	3.416E-08	**0.2060**	3.742E-08	**0.2257**
III.1A6	30 0340 1044	4.791E-09	**0.0136**	4.996E-09	**0.0142**
—	10 0160 0111	4.505E-08	**0.2716**	4.872E-08	**0.2938**
—	30 0340 1018	4.912E-09	**0.0139**	**5.126E**-09	**0.0145**

* Base Case: 14 55-gallon drums (as two 7-packs) loaded directly into a TRUPACT-II

Table 6.10-4 – Configuration 3: 6 85-gallon Drums Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 3	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg-Gas Generation (moles/sec)	Decay Heat Limit
—	10 0160 0050	1.000E-07	**0.6031**	1.478E-07	**0.8913**
—	30 0340 0995	5.025E-09	**0.0143**	5.178E-09	**0.0147**

*Base Case: 8 85-gallon drums loaded directly into a TRUPACT-II

Table 6.10-5 — Configuration 4: 4 55-gallon Drums Overpacked in an SWB Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 4	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
I.1B0	10 0160 0207	2.416E-08	**0.1457**	2.432E-08	**0.1466**
I.1B1	10 0160 0229	2.189E-08	**0.1320**	2.202E-08	**0.1328**
I.1B2	10 0160 0250	2.002E-08	**0.1207**	2.013E-08	**0.1214**
I.1B3	10 0160 0709	7.061E-09	**0.0426**	7.074E-09	**0.0427**
I.2B0	10 0130 0207	2.416E-08	**0.1793**	2.432E-08	**0.1805**
I.2B1	10 0130 0229	2.189E-08	**0.1625**	2.202E-08	**0.1635**
I.2B2	10 0130 0250	2.002E-08	**0.1486**	2.013E-08	**0.1494**
I.2B3	10 0130 0709	7.061E-09	**0.0524**	7.074E-09	**0.0525**
I.2B4	10 0130 0949	5.274E-09	**0.0391**	5.282E-09	**0.0392**
I.3B0	10 0040 0207	2.416E-08	**0.5827**	2.432E-08	**0.5866**
I.3B1	10 0040 0229	2.189E-08	**0.5281**	2.202E-08	**0.5312**
I.3B2	10 0040 0250	2.002E-08	**0.4828**	2.013E-08	**0.4855**
I.3B3	10 0040 0709	7.061E-09	**0.1703**	7.074E-09	**0.1706**
I.3B4	10 0040 0949	5.274E-09	**0.1272**	5.282E-09	**0.1274**

Table 6.10-5 — Configuration 4: 4 55-gallon Drums Overpacked in an SWB Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case* (Concluded)

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 4	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
II.1B0	20 0170 0166	3.015E-08	**0.1711**	3.128E-08	**0.1776**
II.1B1	20 0170 0188	2.670E-08	**0.1516**	2.759E-08	**0.1566**
II.1B2	20 0170 0367	1.364E-08	**0.0774**	1.387E-08	**0.0787**
II.1B2a	20 0170 0209	2.396E-08	**0.1360**	2.467E-08	**0.1400**
II.1B3	20 0170 0546	9.163E-09	**0.0520**	9.265E-09	**0.0526**
II.1B4	20 0170 0725	6.898E-09	**0.0392**	6.955E-09	**0.0395**
II.1B5	20 0170 0905	5.530E-09	**0.0314**	5.567E-09	**0.0316**
II.1B6	20 0170 1084	4.616E-09	**0.0262**	4.641E-09	**0.0263**
II.2BM	20 0000 0000	NA	**40.0000**	NA	**40.0000**
III.1B0	30 0340 0166	3.015E-08	**0.0856**	3.128E-08	**0.0888**
III.1B1	30 0340 0188	2.670E-08	**0.0758**	2.759E-08	**0.0783**
III.1B2	30 0340 0367	1.364E-08	**0.0387**	1.387E-08	**0.0394**
III.1B2a	30 0340 0209	2.396E-08	**0.0680**	2.467E-08	**0.0700**
III.1B3	30 0340 0546	9.163E-09	**0.0260**	9.265E-09	**0.0263**
III.1B4	30 0340 0725	6.898E-09	**0.0196**	6.955E-09	**0.0197**
III.1B5	30 0340 0905	5.530E-09	**0.0157**	5.567E-09	**0.0158**
III.1B6	30 0340 1084	4.616E-09	**0.0131**	4.641E-09	**0.0132**

*Base Case: Up to 4 55-gallon drums overpacked in a Standard Waste Box.

Table 6.10-6 — Configuration 5: 1 SWB Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 5	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
I.1C0	10 0160 0034	1.514E-07	**0.9132**	1.530E-07	**0.9226**
I.1C2	10 0160 0059	8.598E-08	**0.5185**	8.649E-08	**0.5216**
I.1C2b	10 0160 0286	1.751E-08	**0.1056**	1.754E-08	**0.1057**
I.2C0	10 0130 0034	1.514E-07	**1.1239**	1.530E-07	**1.1356**
I.3C0	10 0040 0034	1.514E-07	**3.6528**	1.530E-07	**3.6906**
II.1C0	20 0170 0028	1.798E-07	**1.0206**	1.900E-07	**1.0786**
II.1C1	20 0170 0041	1.238E-07	**0.7029**	1.286E-07	**0.7300**
II.1C1f	20 0170 0034	1.501E-07	**0.8518**	1.571E-07	**0.8919**
II.1C2	20 0170 0053	9.445E-08	**0.5361**	9.720E-08	**0.5517**
II.1C2b	20 0170 0220	2.277E-08	**0.1292**	2.293E-08	**0.1301**
II.1C2f	20 0170 0039	1.288E-07	**0.7309**	1.339E-07	**0.7602**
II.1C2bf	20 0170 0043	1.173E-07	**0.6659**	1.216E-07	**0.6901**
II.1C3	20 0170 0233	2.154E-08	**0.1222**	2.168E-08	**0.1230**
II.1C3f	20 0170 0049	1.039E-07	**0.5897**	1.072E-07	**0.6086**
II.1C4	20 0170 0412	1.215E-08	**0.0690**	1.220E-08	**0.0692**
II.2CM	20 0000 0000	NA	**40.0000**	NA	**40.0000**
III.1C0	30 0340 0028	1.798E-07	**0.5103**	1.900E-07	**0.5393**
III.1C1	30 0340 0041	1.238E-07	**0.3515**	1.286E-07	**0.3650**
III.1C1f	30 0340 0034	1.501E-07	**0.4259**	1.571E-07	**0.4459**
III.1C2	30 0340 0053	9.445E-08	**0.2680**	9.720E-08	**0.2758**
III.1C2b	30 0340 0220	2.277E-08	**0.0646**	2.293E-08	**0.0651**
III.1C2f	30 0340 0039	1.288E-07	**0.3655**	1.339E-07	**0.3801**
III.1C2bf	30 0340 0043	1.173E-07	**0.3329**	1.216E-07	**0.3451**
III.1C3	30 0340 0233	2.154E-08	**0.0611**	2.168E-08	**0.0615**
III.1C3f	30 0340 0049	1.039E-07	**0.2948**	1.072E-07	**0.3043**
III.1C4	30 0340 0412	1.215E-08	**0.0345**	1.220E-08	**0.0346**

*Base Case: Direct loaded Standard Waste Box.

Table 6.10-7 — Configuration 6: 1 Experimental Bin Inside an SWB Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 6	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
II.1D2	20 0170 0067	7.524E-08	**0.4271**	7.698E-08	**0.4369**
III.1D2	30 0340 0067	7.524E-08	**0.2135**	7.698E-08	**0.2184**

*Base Case: Experimental Bin overpacked in a Standard Waste Box.

Table 6.10-8 — Configuration 7: 6 85-gallon Drum Overpacks Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case*

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 7	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
I.1B0	10 0160 0207	2.416E-08	**0.1457**	2.550E-08	**0.1538**
I.1B1	10 0160 0229	2.189E-08	**0.1320**	2.299E-08	**0.1386**
I.1B2	10 0160 0250	2.002E-08	**0.1207**	2.093E-08	**0.1262**
I.1B3	10 0160 0709	7.061E-09	**0.0426**	7.171E-09	**0.0432**
I.2B0	10 0130 0207	2.416E-08	**0.1793**	2.550E-08	**0.1893**
I.2B1	10 0130 0229	2.189E-08	**0.1625**	2.299E-08	**0.1706**
I.2B2	10 0130 0250	2.002E-08	**0.1486**	2.093E-08	**0.1553**
I.2B3	10 0130 0709	7.061E-09	**0.0524**	7.171E-09	**0.0532**
I.2B4	10 0130 0949	5.274E-09	**0.0391**	5.335E-09	**0.0396**
I.3B0	10 0040 0207	2.416E-08	**0.5827**	2.550E-08	**0.6151**
I.3B1	10 0040 0229	2.189E-08	**0.5281**	2.299E-08	**0.5546**
I.3B2	10 0040 0250	2.002E-08	**0.4828**	2.093E-08	**0.5048**
I.3B3	10 0040 0709	7.061E-09	**0.1703**	7.171E-09	**0.1730**
I.3B4	10 0040 0949	5.274E-09	**0.1272**	5.335E-09	**0.1287**
II.1B0	20 0170 0166	3.015E-08	**0.1711**	3.157E-08	**0.1792**
II.1B1	20 0170 0188	2.670E-08	**0.1516**	2.781E-08	**0.1578**
II.1B2	20 0170 0367	1.364E-08	**0.0774**	1.393E-08	**0.0790**
II.1B2a	20 0170 0209	2.396E-08	**0.1360**	2.485E-08	**0.1410**
II.1B3	20 0170 0546	9.163E-09	**0.0520**	9.290E-09	**0.0527**
II.1B4	20 0170 0725	6.898E-09	**0.0392**	6.969E-09	**0.0396**

Table 6.10-8 — Configuration 7: 6 85-gallon Drums Overpacked in a TDOP Example Comparison of Maximum Allowable Gas Generation Rates and Decay Heats with Base Case* (Concluded)

Alpha-numeric Payload Shipping Category	Numeric Payload Shipping Category	Base Case		Configuration 7	
		Cg-Gas Generation (moles/sec)	Decay Heat Limit	Cg - Gas Generation (moles/sec)	Decay Heat Limit
II.1B5	20 0170 0905	5.530E-09	**0.0314**	5.576E-09	**0.0316**
II.1B6	20 0170 1084	4.616E-09	**0.0262**	4.647E-09	**0.0264**
II.2BM	20 0000 0000	NA	**40.0000**	NA	**40.0000**
III.1B0	30 0340 0166	3.015E-08	**0.0856**	3.157E-08	**0.0896**
III.1B1	30 0340 0188	2.670E-08	**0.0758**	2.781E-08	**0.0789**
III.1B2	30 0340 0367	1.364E-08	**0.0387**	1.393E-08	**0.0395**
III.1B2a	30 0340 0209	2.396E-08	**0.0680**	2.485E-08	**0.0705**
III.1B3	30 0340 0546	9.163E-09	**0.0260**	9.290E-09	**0.0264**
III.1B4	30 0340 0725	6.898E-09	**0.0196**	6.969E-09	**0.0198**
III.1B5	30 0340 0905	5.530E-09	**0.0157**	5.576E-09	**0.0158**
III.1B6	30 0340 1084	4.616E-09	**0.0131**	4.647E-09	**0.0132**

*Base Case: 55-gallon drum overpacked in a Standard Waste Box or 85-gallon drum.

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APPENDIX 6.11

SHIPMENT OF TRITIUM-CONTAMINATED WASTE

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6.11 Shipment of Tritium-Contaminated Waste

6.11.1 General Information

The TRUPACT-II and HalfPACT shipping packages have been designed and licensed to transport contact-handled transuranic (CH-TRU) materials for the U.S. Department of Energy (DOE). The DOE - Carlsbad Field Office has been requested to make shipments of tritium-contaminated materials (e.g., solidified or bonded materials) from various national laboratories to storage and/or disposal facilities using the packagings. The purpose of this appendix is to describe and justify the addition of tritium-contaminated materials as a content condition for the TRUPACT-II and the HalfPACT.

6.11.2 Description of Contents

6.11.2.1 Adsorbed/Solidified Tritium-Contaminated Liquid Waste

A high-quality stainless steel pressure vessel (primary container) is filled with adsorbent material, water containing small quantities of tritium is added, the water is adsorbed, and the primary container is sealed. The primary container is placed inside a 55-gallon drum and surrounded by dunnage and additional adsorbent material. An example of specific details and compliance with the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) is described in Content Code SL 111, see CH-TRU Waste Content Codes (CH-TRUCON) document.[1] The content description (for this code) is as follows:

- Type and form of material—Dewatered or solidified tritium contaminated waste adsorbed onto inorganic material. The waste is sealed in a high-quality stainless steel pressure vessel. Explosives, corrosives, nonradioactive pyrophorics, free liquids and flammable organics are prohibited. The internal volume of each primary container is limited to not more than 20 liters, and the internal pressure of each primary container is limited to not more than 1 atmosphere at the time of shipment. The primary containers are overpacked in 55-gallon drums.

6.11.2.2 Titanium-Contaminated Inorganic Waste

Titanium sponge, in which some of the titanium has been previously reacted at high temperature with tritium to form TiT_2, TiHT, and TiDT, is placed in a high-quality aluminum (primary) container. The primary container is then sealed. The primary container is placed inside a 55-gallon drum and surrounded by dunnage and adsorbent material. An example of specific details and compliance with the transportation requirements is detailed in Content Code LL 111B, see CH-TRUCON document.[1] The content description (for this code) is as follows:

- Type and form of material—Solidified tritium contaminated waste in the form of titanium sponge in which some of the titanium has been previously reacted at high

[1] U.S. DOE, "CH-TRU Waste Content Codes (CH-TRUCON)," current revision, DOE/WIPP 01-3194, U.S. Department of Energy, Carlsbad Field Office, Carlsbad, New Mexico.

temperature with tritium to form TiT_2, TiHT, and TiDT. The waste is sealed in aluminum containers that are overpacked into 55-gallon drums. Explosives, corrosives, nonradioactive pyrophorics, free liquids and flammable organics are prohibited. The internal pressure of each primary container is limited to not more than 1 atmosphere at the time of shipment.

- Maximum quantity of material per package—Contents not to exceed 7,265 pounds in a TRUPACT-II or 7,600 pounds in a HalfPACT including shoring and secondary containers, with no more than 1,000 pounds per 55-gallon drum. The maximum number of 55-gallon drums per package is 14 in a TRUPACT-II or 7 in a HalfPACT as shown in Section 2.9 of the CH-TRAMPAC. Decay heat not to exceed the values given in the CH-TRAMPAC.

6.11.3 Structural Evaluation

The 55-gallon drums of tritium waste will be assembled in compliance with Section 2.9 of the CH-TRAMPAC. The maximum weights will be verified to be less than or equal to the limits specified in Section 2.3 of the CH-TRAMPAC.

The inorganic nature of the waste and limited wattage due to the small amount of tritium present inside the primary payload containers limit the potential buildup of pressure that could occur inside the TRUPACT-II or HalfPACT inner containment vessel (ICV) to less than or equal to the 50 psig design pressure during one year. Since payload containers are 55-gallon drums, there are no special structural considerations for either normal or hypothetical conditions of transport that are not already discussed in the TRUPACT-II Safety Analysis Report (SAR) and the HalfPACT SAR. In summary, there are no structural impacts to the TRUPACT-II or HalfPACT packagings resulting from the shipment of 55-gallon drums containing tritium waste.

6.11.4 Thermal Evaluation

The thermal limit for tritium shipments remains the same as discussed in Section 3.0 of both the TRUPACT-II and HalfPACT SARs—not to exceed a total of 40 thermal watts in a TRUPACT-II and 30 thermal watts in a HalfPACT. There will be no thermal impact to the TRUPACT-II or HalfPACT packagings as a result of shipping tritium waste for either normal or hypothetical accident conditions of transport.

6.11.5 Containment Evaluation

The containment criteria for tritium shipments remains the same as for other shipments using the TRUPACT-II or HalfPACT as discussed in the respective SARs. Prior to shipment, both the inner containment vessel and outer confinement vessel of the packaging will be tested in accordance with the appropriate SAR. There will be no impact on the containment capability of the TRUPACT-II or HalfPACT as a result of shipping 55-gallon drums of tritium waste for either normal or hypothetical accident conditions of transport.

6.11.6 Shielding Evaluation

Tritium is a low-energy beta particle emitter and will be shielded by the stainless steel primary container. For normal conditions of transport, the 55-gallon drums containing the solidified tritium waste may be contact handled as with other TRUPACT-II or HalfPACT authorized contents—each 55-gallon drum shall have a surface dose rate of less than or equal to 200 mrem/hr at the surface. If one assumes as a worst case that both the primary container and the payload container were damaged during a hypothetical accident, the stainless steel 1/4-inch thick ICV would provide adequate shielding. The shipment of tritium waste in the TRUPACT-II or HalfPACT poses no radiation safety impact for normal or hypothetical accident conditions of transport.

6.11.7 Criticality Evaluation

Tritium is not a fissile material and, therefore, there will be no impact on the current criticality capabilities of the transportation packaging for both normal and hypothetical accident conditions of transport.

6.11.8 Operating Procedures

The TRUPACT-II and HalfPACT will be loaded and unloaded in accordance with the standard operating procedures described in the respective SARs. Prior to transport, each transportation package will be leakage rate tested in accordance with the appropriate SAR. There are no changes to the operating procedures resulting from the handling of 55-gallon drums of tritium waste.

6.11.9 Acceptance Tests and Maintenance

There are no changes to the TRUPACT-II or HalfPACT acceptance tests and maintenance (as described in the appropriate SAR) due to the shipment of drums of tritium waste. The packaging will be in full compliance with the acceptance tests and maintenance requirements prior to transport when loaded with 55-gallon drums of tritium waste.

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APPENDIX 6.12

SHIPMENT OF HIGH-WATTAGE CH-TRU WASTE

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6.12 Shipment of High-Wattage CH-TRU Waste

6.12.1 Introduction

The purpose of this appendix is to describe the shipment of payload containers of high-wattage contact-handled transuranic (CH-TRU) waste from U.S. Department of Energy (DOE) sites as authorized contents in the TRUPACT-II or HalfPACT. This appendix defines the conditions and controls under which this waste can be shipped in the TRUPACT-II or HalfPACT. This appendix includes analyses demonstrating compliance with gas generation requirements and establishes conditions for compliance with all Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) requirements. The key elements of this appendix are as follows:

- After assembly in the inner containment vessel (ICV), the payload containers that meet all applicable limits described in this appendix undergo the application of a vacuum to remove hydrogen that may have accumulated during storage. This process is described in Section 6.12.8 of this appendix. The implementation of the vacuum application is controlled as described in Section 6.12.8.1 of this appendix. After application of the vacuum process, the ICV is backfilled with an inert gas (e.g., nitrogen or argon) as an additional margin of safety (no credit is taken for this inerting in the analysis).
- The loaded TRUPACT-II or HalfPACT is evacuated and backfilled at the site, transported from the site to the Waste Isolation Pilot Plant (WIPP) or other receiving site, and vented at WIPP or other receiving site within the applicable maximum period of time (i.e., five (5) or ten (10) days) from the completion of the vacuum process at the site. The basis for the shipping period is defined in Section 6.12.6.1 of this appendix. Administrative controls required to ensure that the shipping period is not exceeded are defined in Section 6.12.8.2 of this appendix.
- The controls defined in this appendix ensure that the maximum normal operating pressure (MNOP) for this payload is well below the packaging design pressure of 50 pounds per square inch gauge (psig), as shown in Section 6.12.6.3 of this appendix.

The operating controls and conditions to be exercised by the site and WIPP or other receiving site to ensure the safe shipment of high-wattage CH-TRU waste are identified in Section 6.12.8 of this appendix.

6.12.2 Scope

This appendix applies to payload containers of high-wattage CH-TRU waste currently stored at the DOE sites. These high-wattage payload containers contain inorganic and organic debris belonging to Waste Material Type III.1, as defined in Appendix 2.1 of the CH-TRU Payload Appendices. The payload containers and packaging configurations governed by this appendix are described by Content Codes LA 154 and SQ 154, examples of which are provided in Section 6.12.10 of this appendix. Additional payload containers and packaging configurations shall be developed as described in Section 1.5 of the CH-TRAMPAC by the WIPP CH-TRU Payload Engineer using the governing equations and methodology defined by this appendix. Compliance with all other transportation requirements of the CH-TRAMPAC document shall

also be demonstrated. The WIPP CH-TRU Payload Engineer does not have the authority to change the transportation requirements of the TRUPACT-II or the HalfPACT as specified in the CH-TRAMPAC document or this appendix without approval from the U.S. Nuclear Regulatory Commission. Only CH-TRU waste containers that belong to these content codes may be qualified for shipment under the conditions specified in this appendix.

6.12.3 Container and Physical Properties

For Content Codes LA 154 and SQ 154, the container and physical properties requirements and the associated methods of compliance are the same as those described in Section 2.0 of the CH-TRAMPAC.

6.12.4 Nuclear Properties

For Content Codes LA 154 and SQ 154, the nuclear properties requirements and the associated methods of compliance are the same as those described in Section 3.0 of the CH-TRAMPAC.

6.12.5 Chemical Properties

For Content Codes LA 154 and SQ 154, the chemical properties requirements and the associated methods of compliance are the same as those described in Section 4.0 of the CH-TRAMPAC.

6.12.6 Gas Generation

For Content Codes LA 154 and SQ 154, the gas generation requirements are the same as those described in Section 5.0 of the CH-TRAMPAC.

For Content Codes LA 154 and SQ 154, the compliance methodology associated with the gas generation requirements is summarized below and detailed in Section 6.12.9 of this appendix.

The gas generation requirements compliance methodology for Content Codes LA 154 and SQ 154 involves the use of a process with the following two objectives:

- Reduction of hydrogen gas that may have accumulated in the internal layers of confinement during storage of the payload containers
- Minimization of hydrogen gas accumulation during transport of the payload containers from the site to WIPP or other receiving site.

The first objective is achieved through the application of a vacuum to the loaded ICV prior to transportation. The application of a vacuum removes the accumulated hydrogen gas from the payload containers and internal confinement layers. This evacuation process is shown to reduce the hydrogen gas concentration to a conservative value as demonstrated in Section 6.12.9 of this appendix. An iterative procedure was used to identify the limiting operating conditions for the evacuation process and the maximum allowable decay heat for each packaging configuration of Content Codes LA 154 and SQ 154. A minimum flow rate (at ambient pressure) of 11.9 standard cubic feet per minute (scfm) and a maximum allowable ultimate vacuum pump pressure of 50 millitorr (mtorr) were used to calculate a minimum vacuum duration of 12 hours (corresponding to an ICV internal vacuum pressure of 2 torr) to achieve the required hydrogen concentration in the innermost void volume.

Following the vacuum application, an inert backfill gas (e.g., nitrogen or argon) is introduced into the evacuated ICV. The use of an inert gas as backfill provides an additional margin of safety; no credit is taken for this in the demonstration of compliance. Section 6.12.9 of this appendix presents the mathematical analysis supporting the evacuation and backfill process.

The second objective is achieved by requiring shipments of Content Codes LA 154 and SQ 154 to be completed in controlled short shipping periods as described in Section 6.12.6.1 of this appendix.

6.12.6.1 Shipping Period Analysis

6.12.6.1.1 Content Code LA 154

For payloads comprised of containers belonging to Content Code LA 154, the shipping period begins at the completion of the hydrogen evacuation process at Los Alamos National Laboratory (LANL) and ends when the ICV is vented at WIPP. Conservative time estimates for the various activities determining the shipping period for Content Code LA 154 payloads are as follows:

- **Loading Time.** Loading time begins with the completion of the vacuum application to the ICV and ends with the departure of the shipment from LANL. Activities to be completed during the loading time include backfilling, leak testing, and handling of the loaded TRUPACT-II(s)/HalfPACT(s). As directed by LANL procedures, these activities are sequenced for completion within 24 hours. If these activities are delayed beyond 24 hours, the package(s) will be vented and the vacuum re-applied at LANL in accordance with the controls described in Section 6.12.8.2 of this appendix.
- **Transport Time.** Transport time begins with the departure of the shipment from LANL and ends with the arrival of the shipment at WIPP. The transport time is dependent upon the distance between LANL and WIPP. As shown in Table 6.12-1, at an average speed of 40 miles per hour (mph) the longest travel time from LANL to WIPP is 8.8 hours. This average speed takes into account stops for vehicle inspections every two hours, fueling, meals, driver relief, and state vehicle inspections.

Table 6.12-1 – Distance Between WIPP and LANL

Distance to WIPP (miles)	Transit Time (hours)			
	40 mph	45 mph	50 mph	55 mph
352	8.8	7.8	7.0	6.4

While the expected shipment time from LANL to WIPP is approximately 8.8 hours, the transport time is conservatively estimated as 48 hours. This estimate is conservative because administrative controls imposed by LANL procedures (as outlined in Section 6.12.8.2 of this appendix) eliminate the potential for departure delays associated with holiday weekends or other scheduled facility closure periods. In addition, the use of the TRANSCOM system at WIPP provides continuous tracking of the shipment during transit from LANL to WIPP. The 352-mile distance between LANL and WIPP allows for prompt emergency response, truck maintenance, and driver or equipment replacement, if needed. With approximately 20 shipments being made to WIPP each

week, the resources exist at WIPP to expeditiously attend to any contingencies for Content Code LA 154 shipments. A 48-hour transport time accounts for any unexpected impact to the normal transit time.

- **Unloading Time**. Unloading time begins with the arrival of the shipment at WIPP and ends with the venting of the ICV. Section 6.12.8.2 of this appendix outlines controls imposed to ensure venting of the ICV within 96 hours of the shipment leaving LANL.

Based on a loading time of 24 hours, a conservatively estimated transport time of 48 hours, and an unloading time of 24 hours, the maximum shipping period for shipments of Content Code LA 154 is 4 days (96 hours). The additional contingency of a one-day (24-hour) margin of safety results in a maximum shipping period of 5 days (120 hours). Table 6.12-2 provides a summary of the activities comprising the shipping period.

Table 6.12-2– Content Code LA 154 Shipping Period Analysis Summary

Activity	Normal Expected Time (days)	Maximum Time Used in Analysis (days)
Loading Time	<1	1
Transport Time	0.37	2
Unloading Time	<1	1
Margin of Safety	—	1
Shipment Time	2.37	**5**

This analysis justifies using a 5-day period as the basis for determining compliance with gas generation requirements under rigorous operational controls during loading, transport, and unloading as specified in this appendix. Only shipments of Content Code LA 154 to WIPP are eligible for evaluation using the 5-day shipping period.

6.12.6.1.2Content Code SQ 154

Payloads comprised of containers belonging to Content Code SQ 154 shall be transported as controlled shipments (i.e., 10-day shipping period) as outlined in Appendix 3.6 of the CH-TRU Payload Appendices. In addition to the controls specified in Appendix 3.6 of the CH-TRU Payload Appendices, controls for the completion of the additional activities required for shipments of Content Code SQ 154 (i.e., evacuation and backfill of the ICV) prior to the initiation of the 24-hour loading time required for controlled shipments must be established.

For controlled shipments of Content Code SQ 154, the 24-hour loading time begins with the completion of the vacuum application to the ICV and ends with the departure of the shipment from the site. Site procedures must be implemented for controlled shipments of Content Code SQ 154 to ensure that loading, as defined herein, is completed within 24 hours. If the loading activities are delayed beyond 24 hours, the package(s) will be vented and the vacuum re-applied in accordance with the administrative controls described in Section 6.12.8.2 of this appendix.

6.12.6.2 Determination of Limits

Section 6.12.9 of this appendix documents the mathematical analysis used to arrive at the flammable gas generation limits for Content Codes LA 154 and SQ 154. The analysis is performed for the TRUPACT-II package, which bounds the HalfPACT analysis. To confirm that the TRUPACT-II analysis is conservative for the HalfPACT, the mathematical analysis was run for each of the TRUPACT-II payload configurations in Section 6.12.10 that are applicable to the HalfPACT (i.e., TDOP payloads are not applicable to the HalfPACT) using applicable HalfPACT void volumes and number of payload containers per package. All other input parameters were unchanged. The evaluation results show that the modeled HalfPACT payloads reached the evacuation vacuum pressure of 2 torr in less time than the TRUPACT-II payloads. Based on the results of this evaluation, the evacuation process for the TRUPACT-II was determined to be bounding for the HalfPACT and the same evacuation process, including vacuum pump pressures and durations, can be applied to the HalfPACT.

The derivation of flammable gas generation rate and decay heat limits for Content Codes LA 154 and SQ 154, both of which are classified as Waste Material Type III.1, Solid Organic Waste, are discussed in the following sections. The G value assigned to Content Codes LA 154 and SQ 154 (1.09) is the same as that specified in Section 5.0 of the CH-TRAMPAC for containers meeting the matrix-depletion criterion of >0.012 watt*year. The release rates for the confinement layers are the same as those specified in Appendices 2.2 and 2.3 of the CH-TRU Payload Appendices.

The initial conditions for hydrogen are established for each of the packaging configurations authorized under Content Codes LA 154 and SQ 154 by the application of the vacuum as specified in this appendix. Using these initial hydrogen conditions along with the G value and maximum shipping period associated with each content code, a flammable gas generation rate limit and decay heat limit are calculated for each packaging configuration such that the flammable gas concentration within the innermost confinement layer of a payload container at the end of the shipping period is no more than 5 percent by volume. The flammable gas generation limits for individual containers belonging to Content Codes LA 154 and SQ 154 are specified in the following sections.

In addition, all payloads comprised of containers belonging to Content Codes LA 154 and SQ 154 must meet the design limit of 40 watts per TRUPACT-II or 30 watts per HalfPACT.

Shipments of Content Codes LA 154 and SQ 154 under the test category [exceeding 500 parts per million flammable volatile organic compounds (VOCs) or the decay heat limits specified in the following sections] are as described in Section 5.2 of the CH-TRAMPAC and Section 6.12.9 of this appendix. Limits applicable under mixing of shipping categories are also described in Section 6.12.9 of this appendix. Mixing of shipping categories is allowed only within containers of a single content code (e.g., all containers comprising a payload must belong to Content Code LA 154).

6.12.6.2.1 Content Code LA 154

Assuming a Content Code LA 154 payload assembly comprised of fourteen 55-gallon drums in a TRUPACT-II or seven 55-gallon drums in a HalfPACT belonging to a single packaging configuration (e.g., either Content Code LA 154A or LA 154B), up to six 85-gallon drum overpacks in a ten-drum overpack (TDOP) in a TRUPACT-II (e.g., Content Code LA 154C), or two standard waste box (SWB) overpacks in a TRUPACT-II or one SWB overpack in a

HalfPACT (e.g., Content Code LA 154D), the maximum allowable flammable gas generation rate and decay heat limits are as specified in Table 6.12-3.

Table 6.12-3 – Content Code LA 154 Flammable Gas Generation Rate and Decay Heat Limits

Content Code	Flammable Gas Generation Rate Limit per Drum (moles per second)	Decay Heat Limit per Drum (watts)
LA 154A	2.0581E-7	1.8219
LA 154B	2.7172E-7	2.4053
LA 154C	1.8936E-7	1.6762
LA 154D	2.3173E-7	2.0513

6.12.6.2.2Content Code SQ 154

Assuming a Content Code SQ 154 payload assembly comprised of fourteen 55-gallon drums in a TRUPACT-II or seven 55-gallon drums in a HalfPACT belonging to a single packaging configuration (e.g., either Content Code SQ 154A or SQ 154B), two SWB overpacks in a TRUPACT-II or one SWB overpack in a HalfPACT belonging to a single packaging configuration (e.g., either Content Code SQ 154C or SQ 154D), two direct loaded SWBs in a TRUPACT-II or one direct loaded SWB in a HalfPACT belonging to a single packaging configuration (e.g., Content Code SQ 154E, or SQ 154F), or a TDOP overpacking up to ten 55-gallon drums in a TRUPACT-II (e.g., SQ 154G), the maximum allowable flammable gas generation rate and decay heat limits are as specified in Table 6.12-4.

Table 6.12-4 – Content Code SQ 154 Flammable Gas Generation Rate and Decay Heat Limits

Content Code	Flammable Gas Generation Rate Limit per Drum or Directly Loaded SWB (moles per second)	Decay Heat Limit per Drum or Directly Loaded SWB (watts)
SQ 154A	1.0924E-7	0.9670
SQ 154B	1.6075E-7	1.4230
SQ 154C	1.2298E-7	1.0886
SQ 154D	1.4949E-7	1.3233
SQ 154E	9.8873E-8	0.8752
SQ 154F	2.6261E-7	2.3247
SQ 154G	1.0633E-7	0.9412

6.12.6.3 Pressure Analysis

The TRUPACT-II and HalfPACT MNOPs for the Content Code LA 154 payloads and the Content Code SQ 154 payloads listed in Section 6.12.10 are calculated for the maximum shipping period of 5 days and 10 days, respectively. The administrative controls imposed on shipments of Content Codes LA 154 and SQ 154 are identified in Sections 6.12.6.1 and 6.12.8 of this appendix.

The mathematical analysis for the determination of the MNOP for shipments of Content Codes LA 154 and SQ 154 is the same as that presented in Section 3.0 of the TRUPACT-II Safety Analysis Report (SAR). Table 6.12-5 and Table 6.12-6 present the results of the pressure analyses for Content Codes LA 154 and SQ 154 for both the TRUPACT-II and HalfPACT packages. The highest pressure increase at the end of the applicable shipping period for each content code is as follows:

- For Content Code LA 154, at the end of a 5-day shipping period, the highest pressure increase is 8.17 psig (Content Code LA 154B) at a decay heat of 33.674 watts per TRUPACT-II.
- For Content Code SQ 154, at the end of a 10-day shipping period, the highest pressure increase is 7.81 psig (Content Code SQ 154B) at a decay heat of 19.922 watts per TRUPACT-II.

As shown in Table 6.12-5 and Table 6.12-6, the calculated pressures within the HalfPACT package are less than the corresponding pressures within the TRUPACT-II package; therefore, the TRUPACT-II MNOPs for Content Codes LA 154 and SQ 154 payloads are bounding. The MNOP for Content Code LA 154 and SQ 154 payloads will be well below the packaging design pressure of 50 psig. In both cases, the MNOP will be well below 50 psig even at the design limit of 40 watts per TRUPACT-II and 30 watts per HalfPACT. As shown in Table 6.12-5 and Table 6.12-6, the package design pressure is approached only after approximately 68 days for Content Code LA 154 and after approximately 126 days for Content Code SQ 154. Because shipments of Content Code LA 154 and Content Code SQ 154 are restricted to 5 days and 10 days, respectively, a large margin of safety exists with respect to compliance with the time at which the design pressure is approached.

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Table 6.12-5 – TRUPACT-II and HalfPACT Pressure Increases for Content Code LA 154

Package Pressure Increase for Content Code LA 154 at 5 days															
Content Code	Decay Heat per Drum (watts)	No. Payload Containers per Package	Decay Heat per Package (watts)	Average Contents Temperature (deg. F)	Effective G Value for Total Gas (molecules/100eV)	Activation Energy (kcal/g-mole)	Temp Corrected Effective G Value (molecules/100eV)	Radiolytic Gas Generation Rate (moles/sec)	Radiolytic Gas Generation STP at 5 days (liters)	Average ICV Gas Temperature (deg. F)	Radiolytic Gas Pressure Increase (psia)	Increased Initial Gas Pressure (psia)	Minimum ICV Wall Temperature (deg. F)	Water Vapor Pressure (psia)	Pressure Increase at 5 days (psig)
TRUPACT-II															
LA 154A	1.8219	14	25.507	149.1	8.4	2.1	12.8	3.39E-05	327.91	140.2	2.40	16.65	134.3	2.50	6.85
LA 154B	2.4053	14	33.674	156.4	8.4	2.1	13.3	4.64E-05	449.14	144.7	3.31	16.77	138.6	2.79	8.17
LA 154C	1.6762	6	10.057	135.4	8.4	2.1	11.9	1.24E-05	120.30	131.7	0.96	16.41	126.1	2.01	4.68
LA 154D	2.0513	8	16.410	173.1	8.4	2.1	14.4	2.45E-05	237.42	135.3	2.41	16.51	131.3	2.30	6.52
HalfPACT															
LA 154A	1.8219	7	12.753	138.2	8.4	2.1	12.1	1.60E-05	154.87	130.7	1.48	16.38	128.5	2.14	5.30
LA 154B	2.4053	7	16.837	145.6	8.4	2.1	12.5	2.20E-05	212.56	135.6	2.05	16.52	132.7	2.39	6.26
LA 154C	1.6762	4	6.705	127.2	8.4	2.1	11.4	7.93E-06	76.74	123.3	0.80	16.18	122.2	1.80	4.08
LA 154D	2.0513	4	8.205	173.1	8.4	2.1	14.4	1.23E-05	118.71	135.3	1.41	16.51	131.3	2.30	5.52

Time to Attain the TRUPACT-II Design Pressure Limit of 50 psig for Content Code LA 154																
Content Code	Decay Heat per Drum (watts)	No. Payload Containers per Package	Decay Heat per TRUPACT-II (watts)	Average Contents Temperature (deg. F)	Effective G Value for Total Gas (molecules/100eV)	Activation Energy (kcal/g-mole)	Temp Corrected Effective G Value (molecules/100eV)	Radiolytic Gas Generation Rate (moles/sec)	Radiolytic Gas Generation STP (liters)	Average ICV Gas Temperature (deg. F)	Radiolytic Gas Pressure Increase (psia)	Increased Initial Gas Pressure (psia)	Minimum ICV Wall Temperature (deg. F)	Water Vapor Pressure (psia)	Pressure Increase (psig)	Time (days)
LA 154A	1.8219	14	25.507	149.1	8.4	2.1	12.8	3.39E-05	6223.04	140.2	45.55	16.65	134.3	2.50	50.00	94.89
LA 154B	2.4053	14	33.674	156.4	8.4	2.1	13.3	4.64E-05	6120.95	144.7	45.14	16.77	138.6	2.79	50.00	68.14
LA 154C	1.6762	6	10.057	135.4	8.4	2.1	11.9	1.24E-05	5785.66	131.7	46.28	16.41	126.1	2.01	50.00	240.47
LA 154D	2.0513	8	16.410	173.1	8.4	2.1	14.4	2.45E-05	4515.80	135.3	45.89	16.51	131.3	2.30	50.00	95.10

Table 6.12-6 – TRUPACT-II and HalfPACT Pressure Increases for Content Code SQ 154

Package Pressure Increase for Content Code SQ 154 at 10 days															
Content Code	Decay Heat per Drum or SWB (watts)	No. Payload Containers per Package	Decay Heat per Package (watts)	Average Contents Temperature (deg. F)	Effective G Value for Total Gas (molecules/100eV)	Activation Energy (kcal/g-mole)	Temp Corrected Effective G Value (molecules/100eV)	Radiolytic Gas Generation Rate (moles/sec)	Radiolytic Gas Generation STP at 10 days (liters)	Average ICV Gas Temperature (deg. F)	Radiolytic Gas Pressure Increase (psia)	Increased Initial Gas Pressure (psia)	Minimum ICV Wall Temperature (deg. F)	Water Vapor Pressure (psia)	Pressure Increase at 10 days (psig)
TRUPACT-II															
SQ 154A	0.9670	14	13.538	138.4	8.4	2.1	12.1	1.70E-05	329.27	133.6	2.38	16.47	128.0	2.11	6.26
SQ 154B	1.4230	14	19.922	144.1	8.4	2.1	12.5	2.58E-05	499.24	137.2	3.64	16.56	131.4	2.31	7.81
SQ 154C	1.0886	8	8.709	151.7	8.4	2.1	12.9	1.17E-05	226.93	131.1	2.29	16.39	127.1	2.06	6.04
SQ 154D	1.3233	8	10.586	156.9	8.4	2.1	13.3	1.46E-05	283.19	132.1	2.86	16.42	128.1	2.12	6.70
SQ 154E	0.8752	2	1.750	132.4	8.4	2.1	11.7	2.13E-06	41.22	127.3	0.41	16.29	123.3	1.86	3.86
SQ 154F	2.3247	2	4.649	140.5	8.4	2.1	12.2	5.91E-06	114.30	128.9	1.15	16.33	124.9	1.94	4.72
SQ 154G	0.9412	10	9.412	153.7	8.4	2.1	13.1	1.28E-05	247.69	131.5	1.31	16.41	127.5	2.08	5.10
HalfPACT															
SQ 154A	0.9670	7	6.769	127.4	8.4	2.1	11.4	8.01E-06	155.04	123.4	1.46	16.18	122.3	1.80	4.74
SQ 154B	1.4230	7	9.961	133.1	8.4	2.1	11.7	1.22E-05	235.46	127.3	2.24	16.29	125.6	1.98	5.81
SQ 154C	1.0886	4	4.354	123.0	8.4	2.1	11.1	5.03E-06	97.34	120.5	1.13	16.10	119.8	1.68	4.21
SQ 154D	1.3233	4	5.293	124.7	8.4	2.1	11.2	6.17E-06	119.46	121.6	1.39	16.13	120.7	1.73	4.55
SQ 154E	0.8752	1	0.875	132.3	8.4	2.1	11.7	1.06E-06	20.60	127.3	0.24	16.29	123.3	1.86	3.69
SQ 154F	2.3247	1	2.325	140.2	8.4	2.1	12.2	2.95E-06	57.05	128.9	0.67	16.33	124.9	1.94	4.24

Time to Attain the TRUPACT-II Design Pressure Limit of 50 psig for Content Code SQ 154																
Content Code	Decay Heat per Drum or SWB (watts)	No. Payload Containers per Package	Decay Heat per TRUPACT-II (watts)	Average Contents Temperature (deg. F)	Effective G Value for Total Gas (molecules/100eV)	Activation Energy (kcal/g-mole)	Temp Corrected Effective G Value (molecules/100eV)	Radiolytic Gas Generation Rate (moles/sec)	Radiolytic Gas Generation STP (liters)	Average ICV Gas Temperature (deg. F)	Radiolytic Gas Pressure Increase (psia)	Increased Initial Gas Pressure (psia)	Minimum ICV Wall Temperature (deg. F)	Water Vapor Pressure (psia)	Pressure Increase (psig)	Time (days)
SQ 154A	0.9670	14	13.538	138.4	8.4	2.1	12.1	1.70E-05	6368.06	133.6	46.10	16.47	128.0	2.11	49.98	193.4
SQ 154B	1.4230	14	19.922	144.1	8.4	2.1	12.5	2.58E-05	6290.40	137.2	45.81	16.56	131.4	2.31	49.98	126.0
SQ 154C	1.0886	8	8.709	151.7	8.4	2.1	12.9	1.17E-05	4581.80	131.1	46.24	16.39	127.1	2.06	49.99	201.9
SQ 154D	1.3233	8	10.586	156.9	8.4	2.1	13.3	1.46E-05	4564.95	132.1	46.15	16.42	128.1	2.12	49.99	161.2
SQ 154E	0.8752	2	1.750	132.4	8.4	2.1	11.7	2.13E-06	4642.31	127.3	46.55	16.29	123.3	1.86	50.00	1126.1
SQ 154F	2.3247	2	4.649	140.5	8.4	2.1	12.2	5.91E-06	4617.85	128.9	46.43	16.33	124.9	1.94	50.00	404.0
SQ 154G	0.9412	10	9.412	153.7	8.4	2.1	13.1	1.28E-05	8748.42	131.5	46.21	16.41	127.5	2.08	50.00	353.2

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6.12.7 Payload Assembly

The payload assembly requirements specified by Section 6.1 of the CH-TRAMPAC apply to Content Code LA 154 and SQ 154 payloads. The allowed methods of compliance for these requirements are the same as those described in Section 6.2 of the CH-TRAMPAC. Because the specific methodology described in this appendix for flammable gas generation rate and decay heat limits is applicable only to payload containers belonging to Content Codes LA 154 and SQ 154, the applicable content code shall be entered as the shipping category on the Payload Container Transportation Certification Document (PCTCD) (Section 6.2.1 of the CH-TRAMPAC) and the Payload Assembly Transportation Certification Document (PATCD) (Section 6.2.2 of the CH-TRAMPAC). The applicable Content Code LA 154 or SQ 154 designation (e.g., LA 154A, etc.) will direct the evaluation of the payload container for compliance with the applicable decay heat limits.

The implementation of the controls specified in Section 6.12.8.2 of this appendix for ensuring compliance with the applicable maximum shipping period also ensures compliance with the requirements of Section 6.2.3 of the CH-TRAMPAC for shipments designated as controlled shipments. A payload container's assignment to Content Code LA 154 or SQ 154 effectively designates the container for controlled shipment, and the implementation of Section 6.12.8.2 of this appendix takes the place of the implementation of Section 6.2.3 of the CH-TRAMPAC. Therefore, entries of "Yes" shall be included on the PCTCD and the PATCD in response to the question "Container/Payload Assembly Designated for Controlled Shipment?" for containers and payloads belonging to Content Codes LA 154 or SQ 154, but Table 6.12-7 shall be substituted for the documentation required for controlled shipments.

Content Code LA 154 and SQ 154 payload containers may be assembled into payload configurations mixing containers belonging to the same content code or dunnage containers as described in Section 6.12.9.4 of this appendix.

6.12.8 Operating Controls and Conditions for Shipments of Content Codes LA 154 and SQ 154

6.12.8.1 Procedures for Loading the Package

Loading the shipping package for transport involves (1) qualification and approval of each of the payload containers and the payload assembly assigned to Content Code LA 154 or SQ 154 in accordance with this appendix, (2) loading the prepared Content Code LA 154 or SQ 154 payload containers into the shipping package, (3) applying a vacuum as specified in this appendix and backfilling with a backfill gas, and (4) leakage rate testing of the ICV. The process of loading the TRUPACT-II or HalfPACT is detailed in Section 7.1 of the TRUPACT-II SAR or HalfPACT SAR. The implementation of the vacuum application and the introduction of a backfill gas into the ICV for shipments of Content Codes LA 154 and SQ 154 are controlled using the procedures delineated in Section 7.1 of the TRUPACT-II or HalfPACT SAR with the following modifications.

6.12.8.1.1 Perform loading sequence detailed in Section 7.1 of the TRUPACT-II or HalfPACT SAR through Section 7.1.5, Step 5 (i.e., Rig an overhead crane, or equivalent, with an

appropriate lift fixture capable of handling the ICV lid. Engage the lift fixture and install the ICV lid onto the ICV body. Remove the lift fixture.).

6.12.8.1.2 Perform Section 7.1.5, Step 6 with a vacuum pump that meets the following minimum specifications: (a) minimum flow rate (at ambient pressure) of 11.9 scfm, and (b) an ultimate vacuum pump pressure of less than or equal to 50 mtorr. Note: Do not disconnect the vacuum system and equalize pressure in the ICV cavity as directed in Section 7.1.5, Step 6.

6.12.8.1.3 Continue to run the vacuum pump for a minimum of 12 hours until the ICV internal vacuum pressure is less than or equal to 2 torr.

6.12.8.1.4 Backfill the ICV with an inert gas (e.g., nitrogen or argon) while equalizing pressure (0 psig) +/- 0.5 psig in the ICV cavity, install the ICV inner vent port plug and torque to 55 – 65 lb-in, and remove the vacuum pump.

6.12.8.1.5 Perform Section 7.1.5, Step 7 [i.e., Install the three 1/2 inch lock bolts (socket head cap screws) through the cutouts in the ICV locking ring to secure the ICV locking ring in the locked position. Tighten the lock bolts to 28 – 32 lb-ft torque, lubricated.].

6.12.8.1.6 Complete loading sequence detailed in Section 7.1.5, Step 8 through the remainder of Section 7.1 of the TRUPACT-II or HalfPACT SAR.

6.12.8.2 Procedures for Required Shipping Period

Compliance with the 5-day (LA 154) or 10-day (SQ 154) shipping period is administratively controlled through the following steps. The steps must be completed by the Site Transportation Certification Official, or designee, and the designated WIPP or other receiving site operations personnel, as applicable.

Loading Time

The loading time begins with the completion of Step 6.12.8.1.3 (Section 6.12.8.1 of this appendix) and ends with the departure of the shipment from the site. The loading time is limited to a maximum of 24 hours. The following steps must be completed to ensure compliance with the 24-hour loading time:

6.12.8.2.1 Note date and time that Step 6.12.8.1.3 is completed (i.e., date and time vacuum process is completed). Record date and time on the Shipping Site Control Checklist for High-Wattage CH-TRU Waste Shipments shown in Table 6.12-7. Table 6.12-7 may be reformatted for site use provided that the same information is recorded.

6.12.8.2.2 Note date and time that the shipment containing the loaded package is scheduled to depart the site. Record date and time on the Shipping Site Control Checklist for High-Wattage CH-TRU Waste Shipments.

6.12.8.2.3 Review dates and times recorded in Steps 6.12.8.2.1 and 6.12.8.2.2 to calculate total loading time. If total loading time is less than or equal to 24 hours, proceed to Step 6.12.8.2.4. If total Loading Time exceeds 24 hours, the vacuum application portion of the loading process must be repeated by returning to Step 6.12.8.1.2 of Section 6.12.8.1 above.

6.12.8.2.4 Indicate compliance with the 24-hour loading time by signature on the Shipping Site Control Checklist for High-Wattage CH-TRU Waste Shipments.

Transport and Unloading Time

The transport and unloading time begins with the departure of the shipment from the shipping site and ends with the venting of the ICV at the WIPP or other receiving site. The maximum transport and unloading time for Content Code LA 154 is 4 days (96 hours). The maximum transport and unloading time for Content Code SQ 154 is 9 days. The following steps must be completed to document compliance:

6.12.8.2.5 Review the Shipping Site Control Checklist for High-Wattage CH-TRU Waste Shipments (Table 6.12-7) to determine the date and time that the package was scheduled to depart from the shipping site. Record this date and time on the Receiving Site Control Checklist for High-Wattage CH-TRU Waste Shipments shown in Table 6.12-8. Table 6.12-8 may be reformatted for site use provided that the same information is recorded.

6.12.8.2.6 Using the date and time recorded in Step 6.12.8.2.5, ensure that the ICV is vented within the specified time period (4 days for Content Code LA 154 shipments or 9 days for Content Code SQ 154 shipments) of the departure of the shipment from the shipping site by implementing the unloading procedures specific to Content Code LA 154 and SQ 154 shipments. Record date and time to show compliance.

6.12.8.2.7 Indicate compliance with the applicable transport and unloading time (4 days for Content Code LA 154 shipments or 9 days for Content Code SQ 154 shipments) by signature on the Receiving Site Control Checklist for High-Wattage CH-TRU Waste Shipments.

Table 6.12-7 – Shipping Site Control Checklist for High-Wattage CH-TRU Waste Shipments①

Shipment No. _____ Packaging No._____

Content Code②③: _____

To be completed by the site Transportation Certification Officer, or designee, for each package:

Appendix 6.12 Section No.	Activity	Recorded Date	Recorded Time	Completion of Activity (Indicate by checkmark [√])
6.12.8.2.1	Record date and time of completion of Appendix 6.12, Step 6.12.8.1.3 (i.e., completion of vacuum process)			
6.12.8.2.2	Record date and time the shipment containing the loaded package is scheduled to depart from site			
6.12.8.2.3	Calculate and record total **Loading Time** [Limit = 24 hours]			
	Total Loading Time ≤1 day, proceed to Step 6.12.8.2.4. *Total Loading Time > 1 day,* ***STOP****. Vent package and repeat vacuum application per Appendix 6.12, Step 6.12.8.1.2.*			
6.12.8.2.4	I certify that the above data is accurate and compliant with the Loading Time limit of 24 hours, as specified in Appendix 6.12 of the CH-TRU Payload Appendices. _____ / _____ TRANSPORTATION CERTIFICATION OFFICIAL (OR DESIGNEE) DATE			

Notes:

① Table may be reformatted for site use provided that the same information is recorded.

② Content code must be LA 154 or SQ 154.

③ Content Code LA 154 is eligible for shipments only to WIPP.

Table 6.12-8 – Receiving Site Control Checklist for High-Wattage CH-TRU Waste Shipments①

Shipment No. _____ Packaging No._____

Content Code②③: _____

To be completed by designated Receiving Site Operations Personnel for each package:

Appendix 6.12 Section No.	Activity	Recorded Date	Recorded Time	Completion of Activity (Indicate by checkmark [√])
6.12.8.2.5	Record date and time that the package was scheduled to depart from the shipping site			
6.12.8.2.6	Vent ICV within specified time of date and time recorded above and record vent date and time④			
6.12.8.2.7	I certify that the above data is accurate and compliant with the applicable Transport and Unloading Time limit, as specified in Appendix 6.12 of the CH-TRU Payload Appendices. _____ / _____ RECEIVING SITE OPERATIONS PERSONNEL DATE			

Notes:

① Table may be reformatted for site use provided that the same information is recorded.

② Content code must be LA 154 or SQ 154.

③ Content Code LA 154 is eligible for shipments only to WIPP.

④ The specified time periods for transport and unloading are:
Content Code LA 154 = 4 days
Content Code SQ 154 = 9 days.

6.12.9 Derivation of Gas Generation Limits for Content Codes LA 154 and SQ 154

This section describes the methodology and mathematical analysis used for deriving the flammable gas generation rate and decay heat limits for payload containers belonging to Content Codes LA 154 and SQ 154. The limits are defined such that all containers comply with the 5 percent limit (by volume) on hydrogen concentration in all layers of confinement during a shipping period that is administratively controlled.

Containers of Content Codes LA 154 and SQ 154 undergo the following processes:

- Reduction of hydrogen generated during storage by the application of a vacuum to the ICV after payload assembly, and backfilling with an inert gas (e.g., nitrogen or argon).
- Evacuation and backfill at the shipping site, shipment from the site to WIPP or other receiving site, and venting within a maximum 5-day (LA 154) or 10-day (SQ 154) period after evacuation at the site.

Using an extension of the methodology in Section 5.0 of the CH-TRAMPAC, decay heat limits are derived using the initial conditions after the vacuum application and a 5- or 10-day shipping period as described below.

6.12.9.1 Gas Evacuation Methodology and Transport Modeling

The application of a vacuum on the loaded ICV is designed to remove hydrogen gas that may have accumulated during storage in containers of Content Codes LA 154 and SQ 154. Subsequent introduction of a backfill gas into the evacuated ICV dilutes the remaining gases. A methodology based on the existing TRUPACT-II gas generation analysis has been developed that describes gas movement between void volumes during the application of a vacuum and the introduction of a backfill gas, and also accounts for hydrogen gas generation from the waste in the innermost layer of confinement.

6.12.9.1.1 Mathematical Analysis of Evacuation and Backfill of Gas in ICV

A system of differential equations defines the rate of accumulation of species *i* in each void volume in an ICV containing M consecutive void volumes, where the M^{th} void volume is that of the ICV. There are potentially three primary means of gas transport across each volume boundary:

- Diffusion
- Permeation (bag only)
- Convection.

As a conservative estimate, only gas transport by pressure-induced gas flow, or convection, is considered. The rate of change in species *i* within the innermost layer of confinement where radiolytic gas generation occurs is defined as:

Equation 1

$$\frac{d(n_{i,1})}{dt} = n_{g,i} - r_{c,i,1}$$

where,

$n_{i,1}$ = Moles (mol) of species *i* in innermost void volume

$n_{g,i}$ = Generation rate of species *i*, mol/second (s)

$r_{c,i,1}$ = Rate of convection of species *i* across the innermost volume boundary (mol/s).

The rate of accumulation of species *i* in the k^{th} void volume (excluding the ICV void volume) is defined as:

Equation 2

$$\frac{d(n_{i,k}')}{dt} = r_{c,i,k-1} - r_{c,i,k}$$

The rate of change of species *i* in the ICV void volume is defined as:

Equation 3

$$\frac{d(n_{i,M})}{dt} = r_{c,i,M-1} - n_{v,i}$$

where,

$n_{v,i}$ = Rate in which species *i* exits the M^{th} volume.

A negative value for $n_{v,i}$ indicates that gas enters the ICV (as during pressure equilibration after removal of the vacuum).

The rate of convection of all gases, r_c, across a volume boundary in an isothermal system is defined in terms of the pressure gradient across the volume boundary:

Equation 4

$$r_c = K_c \Delta P$$

where,

K_c = Flow coefficient across volume boundary, mol/s-atmosphere (atm)

ΔP = Pressure difference across volume boundary, atm.

The convection rate for species *i* across a volume boundary in an isothermal system is defined as:

Equation 5

$$r_{c,i} = K_c y_i^* \Delta P$$

where,

y_i^* = Mole fraction of species *i* in the void volume from which the gas flows due to a pressure gradient across the volume boundary.

In order to solve the system of equations, the rate equations are expressed in terms of the quantity of each species in each void volume. In a two-component system, the mole fraction of species *i* is defined as:

Equation 6

$$y_i = \frac{n_i}{n_1 + n_2}$$

Because there are no species-component terms (permeability or diffusion coefficients) in the rate equations, the first component is hydrogen and the second component is defined as all other gases. All other gases behave the same in a convective environment and are assumed not to be generated in significant quantities within the innermost volume.

The pressure in the k^{th} void volume can be defined in terms of the moles of gas in the volume:

Equation 7

$$P_k = \frac{(n_1 + n_2)_k RT}{V_k}$$

where,

R = Gas constant, liters (L) atm/mol Kelvin (K)

T = Absolute gas temperature, K

V_k = Volume of k^{th} void volume, L.

Substituting the equations above into the rate equations yields the following for species *i* in the k^{th} void volume:

Equation 8

$$r_{c,i,k} = K_c RT y_i^* \Delta_k \left(\frac{n_1 + n_2}{V} \right)$$

where,

$$\Delta_k\left(\frac{n_1+n_2}{V}\right) = \left(\frac{n_1+n_2}{V}\right)_k - \left(\frac{n_1+n_2}{V}\right)_{k+1}$$

$$y^*_i = \left(\frac{n_i}{n_1+n_2}\right)_k \qquad \text{when } \Delta_k\left(\frac{n_1+n_2}{V}\right) > 0$$

$$y^*_i = \left(\frac{n_i}{n_1+n_2}\right)_{k+1} \qquad \text{when } \Delta_k\left(\frac{n_1+n_2}{V}\right) < 0$$

6.12.9.2 Model Parameters

The determination of vacuum system parameter limits (ultimate vacuum pump pressure, gas flow rate, vacuum duration, ICV internal vacuum pressure, and allowable decay heat) is an iterative process that reflects parameter interactions as well as physical limits. As applicable, the values for the parameters discussed in the following subsections are the same as those used in the gas generation analysis in Section 5.0 of the CH-TRAMPAC.

6.12.9.2.1 Waste Packaging Configuration

The waste packaging configurations in Content Code LA 154 and SQ 154 payload containers are those approved in Section 5.0 of the CH-TRAMPAC. The internal packaging configurations consist of a series of layers of confinement each of which contains a volume of gas. For example, for Content Code LA 154A, waste may be placed within the innermost bag and closed by the twist-and-tape method. Each of the subsequent inner bags is placed around the waste and is closed in a similar manner. These four bag layers are then collectively placed within the first of two liner bags, each closed by the twist-and-tape method, in a 55-gallon drum.

6.12.9.2.2 Void Volumes

Estimates of the void volumes in a 55-gallon drum containing Waste Material Type III.1 (solid organic waste) are the same as those used in Appendix 6.10 of the CH-TRU Payload Appendices. The volume inside the bags is distributed within the different layers of confinement.

As specified in Appendix 2.3 of the CH-TRU Payload Appendices, the void volume in a TRUPACT-II ICV containing 14 55-gallon drums is 2,450 L. As specified in Appendix 6.10 of the CH-TRU Payload Appendices, the void volume in a TRUPACT-II ICV containing two SWBs is 1,750 L. The combined void volume in a TRUPACT-II ICV with one TDOP and in a TDOP with ten 55-gallon drums is 3,346 L. The void volume in a TDOP containing six 85-gallon drums was calculated from the information presented in Appendix 6.10 of the CH-TRU Payload Appendices to be 2,210 L.

Each bag expands during the application of a vacuum (positive pressure differential across bag) and contracts during vent conditions to ambient pressure (negative pressure differential across bag). It is assumed that each bag does not expand more than 20 percent of its original volume nor contract to a volume less than 50 percent of the original volume due to the presence of the waste. When the volume limits are reached, the bag becomes a constant-volume layer of

confinement. It is assumed that bags are not breached by expansion or contraction inside the payload container.

6.12.9.2.3 Flow Coefficients

All gases are assumed to be ideal. Gas flow across a filter vent has been measured and determined to be proportional to the pressure drop across the filter vent.[1] The sites use filter vents with the minimum diffusion characteristics specified in Section 2.5 of the CH-TRAMPAC. For example, the lowest filter hydrogen diffusion coefficient for Content Code LA 154A is 3.7E-6 mol/s/mol fraction and the associated minimum flow coefficient across the filter vent is 2.8E-2 mol/s/atm:

Equation 9

$$K_{c,vent(3.7E-6)} = \{(27-4)\,\text{slpm} / [(10-1)\,\text{psi}]\}\{14.7\,\text{psi} / (22.4\,\text{L/mol} * 60\,\text{s/min})\}$$
$$= 2.8E-2\,\text{mol/s/atm}$$

where,

psi = Pounds per square inch

slpm = Standard liters per minute

min = Minute.

The flow coefficient across the twist-and-tape closure of polymer bags is estimated by assuming that it is proportional to the hydrogen diffusivity:

Equation 10

$$K_{c.bag} = K_{c,vent}\,(K_{d,bag}/K_{d.vent})$$

where,

K_d = Hydrogen diffusion coefficient, mol/s/mol fraction

therefore,

$K_{c,sb}$ = 2.8E-2 (5.6E-7/3.7E-6) = 4.2E-3 mol/s atm

$K_{c,lb}$ = 2.8E-2 (1.0E-6/3.7E-6) = 7.6E-3 mol/s atm

$K_{c,SWBlb}$ = 2.8E-2 (8.0E-6/3.7E-6) = 6.0E-2 mol/s atm

where,

sb = Inner bag

lb = Drum liner bag

SWBlb = SWB liner bag.

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[1] S. H. Peterson, July 1988, *Determination of Hydrogen Flow and Diffusion Properties of Selected Graphite Filters*, Westinghouse R&D Center, Pittsburgh, Pennsylvania.

The twist-and-tape closure diffusion coefficients are based on the values in Appendix 6.8 of the CH-TRU Payload Appendices.

6.12.9.2.4Gas Flow Rate Across ICV

For a given amount of decay heat in the payload container, the required vacuum duration and ICV internal vacuum pressure to achieve an initial hydrogen concentration in the innermost void volume (resulting in a final concentration of less than or equal to 5 percent by the end of the shipping period) is evaluated as a function of the ultimate vacuum pressure and gas flow rate. A minimum flow rate (at ambient pressure) of 11.9 scfm is used in the evaluation based on the flow rating of the Swagelok® Quick-Connect QC-8 fitting currently used during TRUPACT-II and HalfPACT unloading/loading procedures. This fitting is considered the most restrictive point to gas flow between the pump and the ICV. The double-end shut-off fitting is rated for air at a flow rate of 81 scfm at a pressure differential of 100 psi. Assuming a linear relationship between air flow and pressure differential, at a pressure differential of 14.7 psi (assuming initial system pressure of 1 atm), the initial air flow rate at zero vacuum in the ICV, F_0, is:

Equation 11

$$F_0 = 81 \text{ scfm} \left(14.7 \text{ psi} / 100 \text{ psi}\right) = 11.9 \text{ scfm}$$

A flow coefficient across the fitting, $K_{c,fit}$, is defined in terms of the gas flow rate, F, at a particular pressure differential, ΔP:

Equation 12

$$K_{c,fit} = F / \Delta P$$

At standard temperature and pressure, 1 mole of gas occupies 22.4 L. The minimum flow coefficient for any fitting is defined in terms of the Swagelok® Quick-Connect QC-8 fitting:

Equation 13

$$K_{c,fit} = \left(81 \text{ scfm} / 100 \text{ psi}\right)\left(14.7 \text{ psi} / \text{atm}\right)\left(10^3 \text{ L} / 35.3145 \text{ ft}^3\right)\left(\text{mol} / 22.4 \text{ L}\right)\left(\text{min} / 60 \text{ s}\right)$$
$$= 0.25 \text{ mol/s atm}$$

where,

ft^3 = Cubic feet.

6.12.9.2.5Gas Generation Rate

The rate of hydrogen generation is calculated from Appendix 2.3 of the CH-TRU Payload Appendices as follows:

Equation 14

$$n_{g,H} = CG_{eff}\left(DH\right)$$

where,

C = Conversion constant = 1.0365E-7 mol (100 electron volts [eV] / molecule watt [W] s)

G_{eff} = Effective G value, molecules/100 eV emitted energy

DH = Decay heat energy, W.

It is assumed that the maximum allowable decay heat is present in each payload container and that the initial ICV pressure equals 1 atm.

6.12.9.2.6 Shipping Period

As determined in Section 6.12.6.1 of this appendix, a maximum shipping period of 5 days is applicable to Content Code LA 154; a maximum shipping period of 10 days is applicable to Content Code SQ 154.

6.12.9.2.7 Iterative Procedure to Determine Maximum Allowable Hydrogen Generation Rate

For a given amount of decay heat in the payload container and specified minimum vacuum duration and ICV internal vacuum pressure, the model can determine the hydrogen concentration within the innermost volume at the beginning of the shipping period. The initial hydrogen concentration is that which would result in a final concentration of less than or equal to 5 percent (by volume) by the end of the shipping period.

Using the system of equations defined in this section, the minimum duration of vacuum application to the loaded ICV containing payload containers with up to six confinement layers is 12 hours to reach an ICV internal vacuum pressure of 2 torr. This specification is based on the assumptions of a gas flow rate (at ambient pressure) of 11.9 scfm across the Swagelok® Quick-Connect QC-8 fitting currently used during TRUPACT-II and HalfPACT unloading/loading procedures, a vacuum pump with a minimum flow rate (at ambient pressure) of 11.9 scfm, an ultimate vacuum pump pressure of less than or equal to 50 millitorr, and no off-gassing of the waste contents during the vacuum process.

6.12.9.3 Derivation of Limits

Once the ICV has undergone vacuum application, concentrations of hydrogen in the different layers increase due to the generation of hydrogen during the shipping period. Some of the hydrogen generated during the shipping period would accumulate in the payload containers with the remainder being released into the cavity. For the purpose of establishing decay heat limits, the mole fraction of hydrogen within the innermost confinement layer is evaluated using a transient methodology to simulate the generation, accumulation, and transport processes. The ICV cavity (and/or TDOP void volume for packaging configurations using a TDOP) mole fraction of hydrogen is obtained by conservatively assuming that all of the hydrogen generated is released into the ICV cavity (and/or TDOP void volume for packaging configurations using a TDOP) at the start of the shipping period. The maximum hydrogen concentration in the innermost layer is then limited to less than or equal to 5 percent (by volume) at the end of the shipping period by suitably choosing the gas generation rate and decay heat limits. The temperature dependence of decay heat limits is discussed in Appendix 6.9 of the CH-TRU Payload Appendices. As shown in Appendix 6.9 of the CH-TRU Payload Appendices, for

Waste Material Type III.1, minimum values for decay heat limits are obtained by using the hydrogen generation and release rates at an ambient temperature of 70 degrees Fahrenheit.

The mass balance on flammable gas in a container after application of the vacuum during transport is described by the following equation:

Equation 15

$$\frac{dn_d}{dt} = C_g - \frac{y_d - y_{ICV}}{r_{eff}}$$

where,

n_d	=	Moles of flammable gas in the container, mol
t	=	Time, s
C_g	=	Flammable gas generation rate in the container, mol/s
y_d	=	Mole fraction of flammable gas within innermost confinement layer of container, dimensionless
y_{ICV}	=	Mole fraction of flammable gas in the ICV and/or TDOP (for packaging configurations using a TDOP), dimensionless
r_{eff}	=	Total effective resistance of the confinement layers to the release of flammable gas, s/mol.

From the Ideal Gas Law:

Equation 16

$$n_d = \frac{y_d P V_d}{R T}$$

where,

P	=	Pressure, atm
V_d	=	Void volume within innermost confinement layer of container, L
R	=	Gas constant, 0.082056 atm L/mol K
T	=	Temperature, K.

It is assumed that all voids (within each container and in the ICV) are isothermal and isobaric, thus, the pressure and temperature may be considered constant. Substituting the Ideal Gas Law relation in the mass balance equation and rearranging terms yields:

Equation 17

$$\frac{dy_d}{dt} = \frac{C_g R T}{P V_d} - \frac{R T}{P V_d r_{eff}}(y_d - y_{ICV})$$

Let,

Equation 18

$$\alpha = \frac{C_g R T}{P V_d}$$

and

Equation 19

$$\beta = \frac{R T}{P V_d r_{eff}}$$

Then, the mass balance for flammable gas within a single container during transport is given by the following equation:

Equation 20

$$\frac{dy_d}{dt} = \alpha - \beta (y_d - y_{ICV})$$

The concentration of flammable gas in the ICV is assumed to be constant instead of solving a separate equation for the buildup of flammable gas in the ICV. The maximum mole fraction of flammable gas in the ICV is set equal to the moles of flammable gas generated by all containers during shipment divided by the initial moles of gas in the ICV. Thus, it is assumed that a constant and maximum concentration of flammable gas exists in the ICV after vacuum application at the start of the shipping period. For a given shipping period, the allowable flammable gas generation rate to attain 5 percent (by volume) hydrogen concentration at the end of the shipping period will be a minimum. The actual allowable gas generation rate would be higher if the mass balance equation of flammable gas in the ICV is solved simultaneously with the mass balance equation for flammable gas within the container. The same conservative assumptions regarding the ICV hydrogen concentration are used in the analysis in Section 5.0 of the CH-TRAMPAC.

Let,

Equation 21

$$\gamma = \beta y_{ICV}$$

and

Equation 22

$$\lambda = \alpha + \gamma$$

Substituting the definitions of α, β, and λ into the mass balance equation yields:

Equation 23

$$\frac{dy_d}{dt} = \lambda - \beta\, y_d$$

Taking the Laplace Transform yields:

Equation 24

$$s\,\tilde{y}_d - y_d(0) = \frac{\lambda}{s} - \beta\,\tilde{y}_d$$

Letting $y_d(0) = y_{d0}$ (i.e., the initial concentration within the innermost confinement layer after vacuum application) and rearranging terms yields:

Equation 25

$$\tilde{y}_d = \frac{\frac{\lambda}{s} + y_{d0}}{s + \beta}$$

Taking the inverse Laplace Transform yields:

Equation 26

$$y_d(t) = \frac{\lambda}{\beta} + (y_{d0} - \frac{\lambda}{\beta})e^{-\beta t_t}$$

Replacing λ with $\alpha + \gamma$ gives:

Equation 27

$$y_d(t) = \frac{\alpha + \gamma}{\beta} + (y_{d0} - \frac{\alpha + \gamma}{\beta})e^{-\beta t_t}$$

and y_{ICV} in the γ term is given by the relation:

Equation 28

$$y_{ICV} = \frac{n_{gen}\, C_g\, t_t}{N_{tg}}$$

where,

n_{gen} = Number of flammable gas generators per payload

t_t = Shipping period duration, s

N_{tg} = Total moles of gas in the ICV and/or TDOP (for packaging configurations using a TDOP) void volume calculated using the Ideal Gas Law as:

Equation 29

$$N_{tg} = \frac{P\,V_{ICV}}{R\,T}$$

where,

V_{ICV} = Void volume within the ICV and/or TDOP (for packaging configurations using a TDOP).

Substitution of terms in Equation 27 and simplification results in the following equation for the concentration of flammable gas within the innermost confinement layer of a container at the end of the shipping period (t_t):

Equation 30

$$y_d(t_t) = C_g\left(r_{eff} + \frac{n_{gen}\,t_t}{N_{tg}}\right) + \left[y_{d0} - C_g\left(r_{eff} + \frac{n_{gen}\,t_t}{N_{tg}}\right)\right]\exp\{-R\,T\,t_t/(P\,V_d\,r_{eff})\}$$

Rearranging terms to solve for the flammable gas generation rate limit yields:

Equation 31

$$C_g = \frac{y_d - y_{d0}\exp\{-R\,T\,t_t/(P\,V_d\,r_{eff})\}}{\left(r_{eff} + \frac{n_{gen}\,t_t}{N_{tg}}\right)[1 - \exp\{-R\,T\,t_t/(P\,V_d\,r_{eff})\}]}$$

For an initial concentration within the innermost confinement layer after vacuum application, y_{d0}, the limit for flammable gas generation rate, C_g, is calculated with the concentration (in mole fraction units) within the innermost confinement layer of a container at the end of the shipping period, e.g., for the 5-day shipping period, $y_d(t = t_t = 5$ days) set equal to 0.05.

The decay heat limit corresponding to the flammable gas generation rate limit is then calculated through Equation (5) of Appendix 2.3 of the CH-TRU Payload Appendices as:

Equation 32

$$Q = [(C_g\,N_A)/(G\text{ molecules}/100\text{ eV})]\,[1.602E-19\text{ W s/eV}]$$

where,

Q = Decay heat limit per container, W

N_A = Avogadro's number, 6.023E+23 molecules/mol

G = G_{eff}(flam gas) = Effective G value for flammable gas.

The mathematical model of the vacuum evacuation process described earlier shows that the final concentration within the innermost confinement layer at the end of the process is a function of

the flammable gas generation rate. For example, if all 14 drums in a TRUPACT-II payload are assumed to be Content Code LA 154A (4 inner bags and 2 liner bags) and each drum has a decay heat of 1.8219 watts (corresponding to a maximum flammable gas generation rate of 2.0581E-7 mol/s), the ICV vacuum evacuation model shows that the final concentration of flammable gas within the innermost confinement layer is 1.0353 volume percent. The solution of Equation 31 with $y_d(t_t = 5 \text{ day})$ set equal to 0.05 mole fraction and y_{d0} set equal to 0.010353 yields a flammable gas generation rate limit of 2.0581E-7 mol/s. The corresponding decay heat limit is 1.8219 watts.

Parameter values used to establish flammable gas generation rate and decay heat limits are listed in Table 6.12-9 for the example Content Codes summarized in Section 6.12.10 and are the same values used in the gas generation analysis in the CH-TRAMPAC. The associated flammable gas generation rate and decay heat limit examples for Content Codes LA 154 and SQ 154 are shown in Table 6.12-3 and Table 6.12-4 of this appendix, respectively.

Table 6.12-9– Parameter Values

Parameter	Symbol	Value	Reference
Pressure	P	1 atm	Appendix 2.3, Equation 2 of the CH-TRU Payload Appendices
Temperature	T	294 K	Appendix 2.3, Equation 2 of the CH-TRU Payload Appendices
Void volume within innermost confinement layer of container (i.e., multiple bag void volume)	V_d	53.5 L	Appendix 3.7 of the CH-TRU Payload Appendices, with assumption of 50 percent void volume reduction
Resistance of inner bag	—	1,792,115 s/mol	Appendix 6.10, Table 6.10-1 of the CH-TRU Payload Appendices
Resistance of drum liner bag	—	214,133 s/mol	Appendix 6.10, Table 6.10-1 of the CH-TRU Payload Appendices
Resistance of SWB liner bag	—	125,660 s/mol	Appendix 6.10, Table 6.10-1 of the CH-TRU Payload Appendices
Resistance of punctured rigid drum liner	—	19,646 s/mol	Appendix 6.10, Table 6.10-1 of the CH-TRU Payload Appendices
Resistance of 3.7E-6 mole/sec/mole fraction diffusivity filter	—	270,270 s/mol	Appendix 6.10, Table 6.10-1 of the CH-TRU Payload Appendices
Resistance of 1.85E-5 mole/sec/mole fraction diffusivity filter (5X filter)	—	54,100 s/mol	Calculated from Section 2.5, Table 2.5-1 of CH-TRAMPAC

Parameter	Symbol	Value	Reference
Total effective resistance of the confinement layers to the release of flammable gas for content code packaging configurations	r_{eff}	As calculated	Calculated by summing the products of the number of layers of each type and the resistance of each layer
Void volume within the ICV with fourteen 55-gallon drums/TRUPACT-II	V_{ICV}	2,450 L	Appendix 2.3 of the CH-TRU Payload Appendices
Void volume within a TDOP with six 85-gallon drums	V_{ICV}	2,210 L	Calculated based on values specified in Section 6.10.3.2 of Appendix 6.10 of the CH-TRU Payload Appendices
Void volume within the ICV with two SWBs/ TRUPACT-II	V_{ICV}	1,750 L	Appendix 6.10, Section 6.10.3.2 of the CH-TRU Payload Appendices
Void volume within the ICV and within the TDOP with ten 55-gallon drums/TRUPACT-II	V_{ICV}	3,346 L	Appendix 6.10, Section 6.10.3.2 of the CH-TRU Payload Appendices
Total moles of gas in the ICV with fourteen 55-gallon drums/TRUPACT-II	N_{tg}	101.56 mol	Calculated through Ideal Gas Law
Total moles of gas in a TDOP with six 85-gallon drums/TRUPACT-II	N_{tg}	91.608 mol	Calculated through Ideal Gas Law
Total moles of gas in the ICV with two SWBs/ TRUPACT-II	N_{tg}	72.54 mol	Calculated through Ideal Gas Law
Total moles of gas in the ICV and in the TDOP with ten 55-gallon drums/ TRUPACT-II	N_{tg}	138.70 mol	Calculated through Ideal Gas Law

Parameter	Symbol	Value	Reference
Number of flammable gas generators per payload	n_{gen}	14 6 8 2 10	14 55-gallon drums/ TRUPACT-II 6 85-gallon drum overpacks/TDOP 8 55-gallon drums in 2 SWBs/TRUPACT-II 2 SWBs/TRUPACT-II 10 55-gallon drums/TDOP
Shipping period duration	t_t	432,000 s 864,000 s	5-day shipping period 10-day shipping period
Effective G value for flammable gas (molecules of hydrogen formed/100 eV) for Content Codes LA 154 and SQ 154	G	1.09 molecules/100 eV	Appendix 3.2, Table 3.2-1 of the CH-TRU Payload Appendices for Waste Material Type III.1 (watt*year > 0.012)

6.12.9.4 Mixing of Containers of Content Code LA 154 or SQ 154 for Payload Assembly

This section provides the logic and mathematical analysis for assembling a payload of containers belonging to different packaging configurations under Content Code LA 154 or SQ 154. As shown in Section 6.0 of the CH-TRAMPAC, an assembly of payload containers is approved by ensuring that each payload container does not contain a flammable mixture of gases, while accounting for the properties of each of the other payload containers in the assembly, which may include dunnage containers. Each payload container is assessed through the calculation of the flammability index (FI) for the container, which accounts for the properties of each container in the assembly. For each payload container, the FI is calculated as the ratio of the actual flammable gas generation rate to the allowable flammable gas generation rate limit multiplied by 50,000. Thus, the FI must be a non-negative number less than or equal to 50,000 for each payload container. The determination of allowable flammable gas generation rates takes into account the concentrations of flammable VOCs within the innermost layer of confinement, if present, and the void volume of dunnage containers.

The derivation of allowable flammable gas generation rates is based on the methodology established in Section 6.12.9.3 of this appendix. The following definitions are made for container *i*:

Equation 33

$$\alpha_i = \frac{C_{g,i}\, R\, T}{P\, V_d}$$

and

Equation 34

$$\beta_i = \frac{R\, T}{P\, V_d\, r_{eff,i}}$$

where,

P	=	Pressure, atm
V_d	=	Void volume within innermost confinement layer of container, L
R	=	Gas constant, 0.082056 atm L/mol K
T	=	Temperature, K
$r_{eff,i}$	=	Effective resistance to the release of flammable gas of payload container *i*, s/mol
$C_{g,i}$	=	Allowable flammable gas generation rate limit per innermost confinement layer of payload container *i*, mol/s.

The following equation is an extension of the equation for the mole fraction within the innermost layer of confinement (Equation 27) and provides an expression for the allowable flammable gas concentration (AFGC) within the innermost confinement layer of container, *i*, at the end of the

shipping period. The $AFGC_i$ is equivalent to 0.05 if the concentration of flammable VOCs in the headspace of the container is less than or equal to 500 parts per million volume. Otherwise, the AFGC value is calculated as the difference between the container mixture lower explosive limit and the sum of the flammable VOC concentrations within the innermost confinement layer.

Equation 35

$$AFGC_i(t) = \frac{\alpha_i + \beta_i\, y_{ICV}}{\beta_i} + (y_{d0,i} - \frac{\alpha_i + \beta_i\, y_{ICV}}{\beta_i})e^{-\beta_i t}$$

where,

$AFGC_i$ = Allowable flammable gas concentration in the innermost confinement layer of payload container *i*, dimensionless

t = Shipping period duration, 5 days or 432,000 s, or 10 days or 864,000 s, and

Equation 36

$$y_{ICV} = \frac{\sum_{i=1}^{nc} C_{g,i}\, t}{N_{tg}}$$

where,

nc = Number of containers in the payload, dimensionless

N_{tg} = Total moles of gas in the ICV and/or TDOP void volume calculated using the Ideal Gas Law as:

Equation 37

$$N_{tg} = \frac{P\, V_{ICV}}{R\, T}$$

where,

V_{ICV} = Void volume inside the ICV cavity and/or inside the TDOP.

Substitution of terms in Equation 35 and simplification results in the following system of equations that must be solved to obtain the allowable flammable gas generation rate limit for each container ($C_{g,i}$):

Equation 38

$$y_{d0,1}\, e^{-\beta_1 t} + \left[\left(r_{eff,1} + \frac{t}{N_{tg}}\right) C_{g,1} + \frac{t}{N_{tg}} C_{g,2} + \ldots + \frac{t}{N_{tg}} C_{g,nc}\right](1 - e^{-\beta_1 t}) = AFGC_1$$

$$y_{d0,2}\, e^{-\beta_2 t} + \left[\frac{t}{N_{tg}} C_{g,1} + \left(r_{eff,2} + \frac{t}{N_{tg}}\right) C_{g,2} + \ldots + \frac{t}{N_{tg}} C_{g,nc}\right](1 - e^{-\beta_2 t}) = AFGC_2$$

$$\bullet \quad \bullet \quad \bullet$$

$$\bullet \quad \bullet \quad \bullet$$

$$\bullet \quad \bullet \quad \bullet$$

$$y_{d0,nc}\, e^{-\beta_{nc} t} + \left[\frac{t}{N_{tg}} C_{g,1} + \frac{t}{N_{tg}} C_{g,2} + \ldots + \left(r_{eff,nc} + \frac{t}{N_{tg}}\right) C_{g,nc}\right](1 - e^{-\beta_{nc} t}) = AFGC_{nc}\ .$$

The above system of equations may be written in matrix form as:

Equation 39

$$[A]\,\{CG\} = \{b\}$$

where,

A	=	Matrix of gas generation rate coefficients and initial drum concentrations
CG	=	Column vector of allowable gas generation rates
b	=	Column vector of adjusted individual AFGC values within the innermost confinement layers. The elements are: $\left(\frac{AFGC_i - y_{d0,i}\, e^{-\beta_i t}}{1 - e^{-\beta_i t}}\right)$

The solution for the unknown allowable flammable gas generation rate for each drum is given as:

Equation 40

$$\{CG\} = [A]^{-1}\{b\}$$

where,

$[A]^{-1}$	=	Inverse of matrix A.

Dunnage containers are excluded from the system of linear equations.

The FI of each drum is then calculated as:

Equation 41

$$FI_i = \frac{C_{g,i,actual}}{C_{g,i,allowable}} \times 50{,}000$$

where,

FI_i = Flammability index of payload container, *i*

$C_{g,i,actual}$ = Actual flammable gas generation of payload container *i*, mol/s

$C_{g,i,allowable}$ = Allowable flammable gas generation rate of payload container *i*, mol/s.

For analytical category payload containers, the actual flammable gas generation rate is calculated as:

Equation 42

$$C_{g,i,actual} = \frac{Q_i\,(\text{G molecules} / 100\ \text{eV})}{N_A\,(1.602\text{E}-19\ \text{W s /eV})}$$

where,

Q_i = Decay heat of payload container, W

N_A = Avogadro's number, 6.023E+23 molecules/mol

G = G_{eff} (flam gas) = Effective G value for flammable gas.

For test category containers, the actual gas generation rate is obtained either through measurement of the flammable gas concentration in the drum or liner headspace and calculation of the rate, or through container testing pursuant to Section 5.2.5 of the CH-TRAMPAC. A payload is qualified for shipment only if the FI of each payload container is a non-negative number less than or equal to 50,000. If one or more containers fail the FI requirement, the payload shall be reconfigured until all containers satisfy this requirement. The FI determination can be performed either manually or by the use of a validated software package.

6.12.10 Example Content Codes

Example Content Codes LA 154 and SQ 154 are provided on the following pages.

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CONTENT CODE: LA 154 (See Waste Packaging Description Table)

CONTENT DESCRIPTION: Mixed Combustible/Noncombustible Waste

GENERATING SITE: Los Alamos National Laboratory (LANL)

WASTE DESCRIPTION: 55-gallon drums, some of which are overpacked in 85-gallon drums, of mixed combustible/noncombustible waste generated from plutonium processing activities at LANL. The shipment of Content Code LA 154 waste is subject to the requirements and operating controls specified in Appendix 6.12 of the CH-TRU Payload Appendices.

GENERATING SOURCES: The waste originates from plutonium processing activities at LANL.

WASTE FORM: Mixtures of combustible and noncombustible waste consist of paper, rags, plastic, rubber, absorbed organic liquids, leaded glovebox gloves, glass, motors, pumps, tools, and miscellaneous metal waste. The waste is contaminated primarily with Pu-238 and/or Pu-239.

WASTE PACKAGING: Details of the waste packaging for each code are presented in the following table:

WASTE PACKAGING DESCRIPTION TABLE

Code	Description
LA 154A	The waste is packaged in a maximum of four layers of inner plastic bags. Bagged out items are placed in a 55-gallon drum lined with a maximum of two plastic liner bags. All bag closures are by the twist and tape method, or the twist, tie, and tape method.
LA 154B	The waste is placed in a 55-gallon drum lined with a maximum of one plastic liner bag. The bag liner is closed by the twist and tape method, or the twist, tie, and tape method.
LA 154C	The waste is packaged in a maximum of four layers of inner plastic bags. Bagged out items are placed in a 55-gallon drum lined with a maximum of two plastic liner bags. All bag closures are by the twist and tape method, or the twist, tie, and tape method. The 55-gallon drum is overpacked in an 85-gallon drum. For shipment, six 85-gallon drums are overpacked in a ten-drum overpack (TDOP). No additional bags are used in the 85-gallon drum or TDOP.
LA 154D	The waste is packaged in a maximum of four layers of inner plastic bags. Bagged out items are placed in a 55-gallon drum lined with a maximum of two plastic liner bags. All bag closures are by the twist and tape method, or the twist, tie, and tape method. Four 55-gallon drums are overpacked in a standard waste box (SWB). No additional bags are used in the SWB.

ASSAY: Each drum is assayed by means of a neutron or gamma counter according to written procedures. Which instrument is used depends on the matrix and nuclide content of the drum. The results of the assay are expressed in terms of grams of each radionuclide present. Assay results are used to calculate Pu-239 fissile gram equivalent (plus 2 times the error), decay heat, and plutonium equivalent curies (plus error) (required to ensure compliance with the waste acceptance criteria for disposal at the Waste Isolation Pilot Plant [WIPP]).

RESIDUAL LIQUIDS: Each drum is examined by radiography in accordance with written procedures to ensure the total volume of residual liquid in a payload container is less than 1 volume percent of the payload container. A subset of the waste assigned to Content Code LA 154 is also subjected to visual examination for the purpose of verifying the compliance determinations made by radiography. Special emphasis during these examinations is applied to internal containers (e.g., bottles and cans) and motors and pumps to ensure compliance. Any drum containing residual liquids greater than 1 volume percent of the payload container will be set aside for mitigation activities (e.g., absorption or solidification activities) in accordance with written procedures.

EXPLOSIVES/COMPRESSED GASES: Explosives are prohibited in the LANL plutonium processing areas. Each drum is examined by radiography in accordance with written procedures to ensure the absence of explosives or compressed gases. Special emphasis during these examinations is applied to ensure the absence of any pressure vessels or spray cans that could potentially contain gases under pressure. Any drum containing explosives or compressed gases will be set aside for mitigation activities to remove the prohibited item (e.g., blocking open, puncturing, flattening, or cutting a pressurized container) in accordance with written procedures.

PYROPHORICS: No pyrophoric materials will be present as determined by radiography. Drums containing pyrophoric materials as identified during the examinations are set aside for mitigation activities in accordance with written procedures.

CORROSIVES: No corrosive materials will be present as determined by radiography in accordance with written procedures. Drums containing corrosive materials as identified during the examinations are set aside for mitigation activities (e.g., neutralization) in accordance with written procedures.

CHEMICAL COMPATIBILITY: Because the LA 154 CH-TRU waste containers belong to an approved waste material type (Waste Material Type III.1), the chemical compatibility analysis described in Appendix 6.1 of the CH-TRU Payload Appendices bounds Content Code LA 154. All waste is chemically compatible for materials in greater than trace (>1% weight) quantities. The chemicals found in this content code are restricted to the table of allowable materials for Waste Material Type III.1 in Section 4.0 of the CH-TRAMPAC.

PAYLOAD CONTAINER VENTING AND ASPIRATION: Payload containers in this content code that have been stored in an unvented condition will be vented and aspirated to comply with the requirements of Section 5.3 of the CH-TRAMPAC or through the vacuum application process described in Appendix 6.12 of the CH-TRU Payload Appendices.

ADDITIONAL CRITERIA: In accordance with Section 2.9 of the CH-TRAMPAC, for 55-gallon drums, the rigid liner (if present) contains a 0.3-inch minimum diameter hole, or filter with a hydrogen release rate equivalent to or greater than the 0.3-inch minimum diameter hole.

(LA 154A) The 55-gallon drum is filtered with a minimum total filter diffusivity of 3.70E-6 moles per second per mole fraction.

(LA 154B) The 55-gallon drum is filtered with a minimum total filter diffusivity of 1.85E-5 moles per second per mole fraction.

(LA 154C) The 55-gallon drum is filtered with a minimum total filter diffusivity of 3.70E-6 moles per second per mole fraction. Each 85-gallon drum used to overpack a 55-gallon drum (85-gallon drum overpack) is filtered with a minimum total filter diffusivity of 3.7E-6 moles per second per mole fraction. Each TDOP used to overpack 85-gallon drum overpacks is filtered with a minimum total filter diffusivity of 3.33E-5 moles per second per mole fraction.

(LA 154D) The 55-gallon drum is filtered with a minimum total filter diffusivity of 3.7E-6 moles per second per mole fraction. Each SWB used to overpack four 55-gallon drums is filtered with a minimum total filter diffusivity of 1.48E-5 moles per second per mole fraction.

All waste shipped under Content Code LA 154 must comply with the additional conditions and controls specified in Appendix 6.12 of the CH-TRU Payload Appendices. Compliance with these additional conditions and controls is documented per Appendix 6.12 of the CH-TRU Payload Appendices.

SHIPPING CATEGORY: For Content Code LA 154 payload containers, "LA 154A," "LA 154B," "LA 154C," or "LA 154D," as applicable, shall be used as the shipping category to direct the evaluation of the payload container for compliance with the applicable decay heat or flammable gas generation rate limit. Applicable decay heat limits for the packaging configurations under Content Code LA 154 are specified in Appendix 6.12 of the CH-TRU Payload Appendices.

MAXIMUM ALLOWABLE WATTAGE: The maximum allowable wattages for this waste are calculated according to the methodology specified in Appendix 6.12 of the CH-TRU Payload Appendices and are listed in Appendix 6.12 of the CH-TRU Payload Appendices.

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CONTENT CODE: SQ 154 (See Waste Packaging Description Table)

CONTENT DESCRIPTION: Mixed Combustible/Noncombustible Waste

GENERATING/STORAGE SITE: Various

WASTE DESCRIPTION: Containers of mixed combustible/noncombustible waste generated from plutonium processing activities. The shipment of Content Code SQ 154 waste is subject to the requirements and operating controls specified in Appendix 6.12 of the CH-TRU Payload Appendices.

GENERATING SOURCES: The waste originates from plutonium processing activities at the DOE sites.

WASTE FORM: Mixtures of combustible and noncombustible waste consist of paper, rags, plastic, rubber, absorbed organic liquids, leaded glovebox gloves, glass, motors, pumps, tools, and miscellaneous metal waste.

WASTE PACKAGING: Details of the waste packaging for each code are presented in the following table:

WASTE PACKAGING DESCRIPTION TABLE

Code	Description
SQ 154A	The waste is packaged in a maximum of four layers of inner plastic bags. Bagged out items are placed in a 55-gallon drum lined with a maximum of two plastic liner bags. All bag closures are by the twist and tape method.
SQ 154B	The waste is placed in a 55-gallon drum lined with a maximum of one plastic liner bag. The bag liner is closed by the twist and tape method.
SQ 154C	The waste is packaged in a maximum of four layers of inner plastic bags. Bagged out items are placed in a 55-gallon drum lined with a maximum of two plastic liner bags. All bag closures are by the twist and tape method. The 55-gallon drum is overpacked in an SWB.
SQ 154D	The waste is placed in a 55-gallon drum lined with a maximum of one plastic liner bag. All bag closures are by the twist and tape method. The 55-gallon drum is overpacked in an SWB.
SQ 154E	The waste is packaged in a maximum of five layers of inner plastic bags. Five or more such bagged out items are placed directly in an SWB lined with a maximum of one plastic SWB liner bag. All bag closures are by the twist and tape method.
SQ 154F	The waste is placed directly in an SWB lined with a maximum of one plastic SWB liner bag. All bag closures are by the twist and tape method.
SQ 154G	The waste is packaged in a maximum of four layers of inner plastic bags. Bagged out items are placed in a 55-gallon drum lined with a maximum of two plastic liner bags. All bag closures are by the twist and tape method. The 55-gallon drum is overpacked in a TDOP. No additional bags are used in the TDOP.

ASSAY: Assay for all payload containers shall be performed in accordance with the CH-TRAMPAC. The isotopic composition of the waste is determined from measurements taken on the product material during the processing at the site. The processing organizations transmit the isotopic composition information to the site waste certification organization. Therefore, the isotopic composition of the waste need not be determined by direct analysis or measurement of the waste unless process information is not available. The results of the assay are expressed in terms of grams of each radionuclide present. Assay results are used to calculate Pu-239 fissile gram equivalent (plus 2 times the error), decay heat, and plutonium equivalent curies (plus error) (required to ensure compliance with the waste acceptance criteria for disposal at the Waste Isolation Pilot Plant).

RESIDUAL LIQUIDS: Liquid waste is prohibited in the payload containers except for residual amounts in well-drained containers. The total volume of residual liquid in a payload container shall be less than 1 volume percent of the payload container. Waste packaging procedures ensure that residual liquids are less than 1 volume percent of the payload container.

EXPLOSIVES/COMPRESSED GASES: Explosives and compressed gases in the payload containers are prohibited by waste packaging procedures.

PYROPHORICS: Nonradioactive pyrophorics in the payload containers are prohibited by waste packaging procedures. Waste packaging procedures shall ensure that all pyrophoric radioactive materials are present only in small residual amounts (less than 1 weight percent) in payload containers.

CORROSIVES: Corrosives are prohibited in the payload containers. Acids and bases that are potentially corrosive shall be neutralized and rendered noncorrosive prior to being a part of the waste. The physical form of the waste and the waste generating procedures ensure that the waste is in a nonreactive form.

CHEMICAL COMPATIBILITY: Because the SQ 154 CH-TRU waste containers belong to an approved waste material type (Waste Material Type III.1), the chemical compatibility analysis described in Appendix 6.1 of the CH-TRU Payload Appendices bounds Content Code SQ 154. All waste is chemically compatible for materials in greater than trace (>1% weight) quantities. The chemicals found in this content code are restricted to the table of allowable materials for Waste Material Type III.1 in Section 4.0 of the CH-TRAMPAC.

PAYLOAD CONTAINER VENTING AND ASPIRATION: Payload containers in this content code that have been stored in an unvented condition will be vented and aspirated to comply with the requirements of Section 5.3 of the CH-TRAMPAC or through the vacuum application process described in Appendix 6.12 of the CH-TRU Payload Appendices.

ADDITIONAL CRITERIA: In accordance with Section 2.9 of the CH-TRAMPAC, for 55-gallon drums, the rigid liner (if present) contains a 0.3-inch minimum diameter hole, or filter with a hydrogen release rate equivalent to or greater than the 0.3-inch minimum diameter hole.

(SQ 154A) The 55-gallon drum is filtered with a minimum total filter diffusivity of 3.70E-6 moles per second per mole fraction.

(SQ 154B) The 55-gallon drum is filtered with a minimum total filter diffusivity of 1.85E-5 moles per second per mole fraction.

(SQ 154C) The 55-gallon drum is filtered with a minimum total filter diffusivity of 3.70E-6 moles per second per mole fraction. The SWB used to overpack up to four 55-gallon drums (SWB overpack) is filtered with a minimum total filter diffusivity of 1.48E-5 moles per second per mole fraction.

(SQ 154D) The 55-gallon drum is filtered with a minimum total filter diffusivity of 1.85E-5 moles per second per mole fraction. The SWB used to overpack up to four 55-gallon drums (SWB overpack) is filtered with a minimum total filter diffusivity of 1.48E-5 moles per second per mole fraction.

(SQ 154E, SQ 154F) The SWB is filtered with a minimum total filter diffusivity of 1.48E-5 moles per second per mole fraction.

(SQ 154G) The 55-gallon drum is filtered with a minimum total filter diffusivity of 3.70E-6 moles per second per mole fraction. The TDOP used to overpack 55-gallon drums is filtered with a minimum total filter diffusivity of 3.33E-5 moles per second per mole fraction.

All waste shipped under Content Code SQ 154 must comply with the additional conditions and controls specified in Appendix 6.12 of the CH-TRU Payload Appendices. Compliance with these additional conditions and controls is documented per Appendix 6.12 of the CH-TRU Payload Appendices.

SHIPPING CATEGORY: For Content Code SQ 154 payload containers, the content code (e.g., "SQ 154A") shall be used as the shipping category to direct the evaluation of the payload container for compliance with the applicable decay heat or flammable gas generation rate limit. Applicable decay heat limits for the packaging configurations under Content Code SQ 154 are specified in Appendix 6.12 of the CH-TRU Payload Appendices.

MAXIMUM ALLOWABLE WATTAGE: The maximum allowable wattages for this waste are calculated according to the methodology specified in Appendix 6.12 of the CH-TRU Payload Appendices and are listed in Appendix 6.12 of the CH-TRU Payload Appendices.

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APPENDIX 6.13

SHIPMENT OF CH-TRU WASTE PACKAGING CONFIGURATIONS WITH UNVENTED HEAT-SEALED BAG LAYERS

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6.13 Shipment of CH-TRU Waste Packaging Configurations with Unvented Heat-Sealed Bag Layers

6.13.1 Introduction

The purpose of this appendix is to describe the shipment of contact-handled transuranic (CH-TRU) waste packaging configurations with unvented heat-sealed bag layers, in addition to other layers of confinement, as authorized contents in the TRUPACT-II or HalfPACT. This appendix includes analyses demonstrating compliance with gas generation and all other applicable requirements, and establishes limits and conditions of compliance for this CH-TRU waste inventory. The key elements of this appendix are as follows:

- Quantifying the hydrogen release by permeation through an unvented heat-sealed bag layer and establishing the resistance factor for this confinement layer using the same methodology described in Section 5.0 of the Contact-Handled Transuranic Waste Authorized Methods for Payload Control (CH-TRAMPAC) for other authorized confinement layers.

- Authorizing contents with unvented heat-sealed bag configurations using the same methodology as for other content codes in the CH-TRU Waste Content Codes (CH-TRUCON) document.

6.13.2 Scope

This appendix applies to CH-TRU waste containers with unvented heat-sealed bags as layers of confinement. Specific content codes, describing the waste attributes, shall be developed and approved as described in Section 1.5 of the CH-TRAMPAC prior to transport of these wastes.

6.13.3 Container and Physical Properties

The container and physical properties requirements and the associated methods of compliance are the same as those described in Section 2.0 of the CH-TRAMPAC.

6.13.4 Nuclear Properties

The nuclear properties requirements and the associated methods of compliance are the same as those described in Section 3.0 of the CH-TRAMPAC.

6.13.5 Chemical Properties

The chemical properties requirements and the associated methods of compliance are the same as those described in Section 4.0 of the CH-TRAMPAC.

6.13.6 Gas Generation Properties

The gas generation requirements and the associated methods of compliance are the same as those described in Section 5.0 of the CH-TRAMPAC. The quantification of the hydrogen release rate and resistance factor for an unvented heat-sealed bag layer is described below. This release rate and the associated resistance factor shall be used for an unvented heat-sealed bag layer in determining decay heat and other gas generation related limits using the methodology defined in Section 5.0 of the CH-TRAMPAC. The methods for determination of limits and assignment of

shipping categories for specific configurations with unvented heat-sealed bag layers are provided in Appendix 2.2 of the CH-TRU Payload Appendices and Section 5.0 of the CH-TRAMPAC.

6.13.6.1 Quantification of Hydrogen Release Rate for Unvented Heat-sealed Bags

Hydrogen release rates for an unvented heat-sealed bag layer meeting the requirements of Appendix 3.8 of the CH-TRU Payload Appendices are as follows.

For an unvented heat-sealed bag, the mechanism for hydrogen release is by permeation across the available surface area of the confinement layer. As specified in Appendix 3.8, unvented heat-sealed bags shall have a minimum surface area of approximately 390 square inches (2,516 square centimeters [cm^2]).

The release rate from an unvented heat-sealed bag meeting the specifications of Appendix 3.8 can be calculated as:

$$RR = \Pi * \frac{SA}{\delta} * \frac{mole}{22.4x10^3\ cm^3\ (STP)} * \frac{76\ cm\ Hg}{1\ mole\ fraction} \quad (1)$$

where,

RR = Release rate of hydrogen [mole/second/mole fraction (m/s/mf)]

Π = Permeability of bag to hydrogen ([cm^3 at standard temperature and pressure (STP) cm]/[cm^2 s cm Hg])

SA = Surface area of the bag (cm^2)

δ = Thickness of bag (cm).

While the thickness of an unvented heat-sealed bag is typically at the low end of a range from 5-mil (0.0127 cm) to 14-mil (0.03556 cm), a maximum thickness of 14-mil has been used to calculate the hydrogen release rate from unvented heat-sealed bags.

The unvented heat-sealed bags may be made of polyethylene (PE) or polyvinyl chloride (PVC). Since the permeability of hydrogen in PVC is lower than in PE (3.6×10^{-10} [cm^3 (STP) cm] / [cm^2 s cm Hg] for PVC versus 8.6×10^{-10} [cm^3 (STP) cm] / [cm^2 s cm Hg] for PE), the more conservative value for PVC at ambient temperature (Reference 6.13.8.1) is used to calculate the release rate, similar to the release rates for other configurations of Waste Type III in Appendix 6.9 of the CH-TRU Payload Appendices. Substitution of the values for the bag surface area, bag thickness, and permeability into Equation (1) yields a hydrogen release rate of 8.64×10^{-8} m/s/mf.

As described in Appendix 2.3 of the CH-TRU Payload Appendices, the resistance of an unvented heat-sealed bag to the release of hydrogen is the reciprocal of the release rate or 11,574,074 seconds/mole. Division of the resistance by 100 yields a resistance factor for an unvented heat-

sealed bag of 115,741, which is included in Table 2.2-1 of Appendix 2.2 of the CH-TRU Payload Appendices.

6.13.6.2 Determination of Limits

An example calculation of the allowable flammable gas generation rate and decay heat limits is presented in this section for two different packaging configurations with an unvented heat-sealed bag using the methodology described in Section 5.0 of the CH-TRAMPAC. The packaging configurations have waste packaged in an unvented heat-sealed bag. The waste is then placed in up to four inner bags with twist-and-tape or fold-and-tape closures. The bagged waste is then placed either in a liner bag with a twist-and-tape or fold-and-tape closure (Packaging Configuration 1) or in a rigid liner that is filtered or punctured (Packaging Configuration 2) inside a 55-gallon (208-liter) metal drum. The drum is fitted with a filter with a minimum hydrogen diffusivity of 3.7×10^{-6} m/s/mf. The waste is classified as debris waste (i.e., Waste Material Type III.1, Solid Organic Waste). As discussed in Section 5.0 of the CH-TRAMPAC, the flammable gas effective G values are 3.40 if the dose criteria is not satisfied (i.e., watt*year $\leq$ 0.012) and 1.09 if the dose criteria is satisfied (i.e., watt*year > 0.012).

Based on the two different packaging configurations, the shipping categories are determined as per Appendix 2.2 of the CH-TRU Payload Appendices using Table 2.2-1 for the resistance terms and a resistance factor for an unvented heat-sealed bag as derived above. The individual contributions to the total resistance factor are summarized in Table 6.13-1.

Table 6.13-1 —Resistance Factors for Each Configuration with an Unvented Heat-Sealed Bag Layer

Resistance Contribution Type	Packaging Configuration 1 Total Resistance Factor	Packaging Configuration 2 Total Resistance Factor
1 Unvented Heat-Sealed Bag	115,741	115,741
4 Twist-and-Tape Inner Bag Layers	71,688	71,688
1 Twist-and-Tape Drum Liner Bag	2,142	—
Rigid Drum Liner With 0.3-inch Diameter Hole	—	197
55-Gallon Drum with 3.7×10^{-6} m/s/mf Filter	2,703	2,703
Load Type (14 55-Gallon Drums)	7,147	7,147
Total Resistance Factor Sum	199,421	197,476

As per Appendix 2.2 of the CH-TRU Payload Appendices, dividing the total resistance factor sum for each packaging configuration by 100 and rounding up to a whole number results in the four-digit Total Resistance Notation (ZZZZ) values of 1995 for Packaging Configuration 1 and 1975 for Packaging Configuration 2.

Combining the two digit Waste Type Notation (XX) value of 30 from Table 2.1-1 of Appendix 2.1 of the CH-TRU Payload Appendices with the two possible values of the four-digit

G Value Notation (YYYY) of 0340 and 0109 and the ZZZZ values results in the following four distinct shipping categories:

Packaging Configuration 1	30 0340 1995	Watt*year ≤0.012
	30 0109 1995	Watt*year >0.012
Packaging Configuration 2	30 0340 1975	Watt*year ≤0.012
	30 0109 1975	Watt*year >0.012

The maximum allowable flammable gas generation rate per drum is calculated for each shipping category using Equation (8) of Appendix 2.3 of the CH-TRU Payload Appendices as:

$$CG = \frac{0.05}{(ZZZZ * 10{,}000\ s/mole)} \tag{2}$$

where,

CG = Maximum allowable flammable gas generation rate per drum (mole/second)

ZZZZ = Four-digit total resistance notation term from the numeric payload shipping category notation form, XX YYYY ZZZZ.

The maximum allowable decay heat per drum is calculated for each shipping category using Equation (9) of Appendix 2.3 of the CH-TRU Payload Appendices as:

$$Q = \frac{4824.42\ molecules/mole * watt - s/eV}{(ZZZZ * YYYY)\ s - molecules/mole - eV)} \tag{3}$$

where,

Q = Maximum allowable decay heat limit (watt)

YYYY = Four digit G value notation term from the numeric payload shipping category notation form, XX YYYY ZZZZ.

The limits for these example shipping categories are as shown in Table 6.13-2.

Table 6.13-2 —Example Flammable Gas Generation Rate and Decay Heat Limits

Shipping Category	Allowable Flammable Gas Generation Rate Limit per Drum (moles/second)	Decay Heat Limit per Drum (watts)
30 0340 1995	2.506×10^{-9}	0.0071
30 0109 1995	2.506×10^{-9}	0.0222
30 0340 1975	2.532×10^{-9}	0.0072
30 0109 1975	2.532×10^{-9}	0.0224

Shipments of drums with unvented heat-sealed bag layers under the test category (exceeding 500 parts per million flammable volatile organic compounds [VOC] or the decay heat limits) are as described in Section 5.2.5 of the CH-TRAMPAC, with headspace gas measurement and testing as options. The requirements of Section 5.2.4 of the CH-TRAMPAC apply with respect to determining steady-state (90%) VOC concentrations from drum age criteria and prediction factors. In addition, mixing of shipping categories is subject to the requirements described in Appendix 2.4 of the CH-TRU Payload Appendices and Section 6.2.4 of the CH-TRAMPAC.

Payload containers that have been stored in an unvented condition (i.e., no filter and/or unpunctured liner) shall be aspirated for the specific length of time to ensure equilibration of any gases that may have accumulated in the closed container. The derivation of aspiration times for packaging configurations with unvented heat-sealed bag layers is as outlined in Appendix 3.7 of the CH-TRU Payload Appendices. Release rates for the confinement layers are as specified in Table 3.7-1 of Appendix 3.7 of the CH-TRU Payload Appendices, with a release rate of 8.64×10^{-8} m/s/mf to be used for an unvented heat-sealed bag as derived in Section 6.13.6.1.

In summary, this section derives the release rate and resistance factor to be used for an unvented heat-sealed bag layer meeting the requirements of Appendix 3.8 of the CH-TRU Payload Appendices. The methodology for determining compliance with gas generation limits with this confinement layer is identical to that used for other confinement layers.

6.13.7 Payload Assembly

The payload assembly requirements and compliance methods for these wastes are the same as those specified in Section 6.0 of the CH-TRAMPAC.

6.13.8 References

6.13.8.1 Perry, R.H., D.W. Green, and J.O. Maloney, 1984, *Perry's Chemical Engineers' Handbook*, Sixth Edition, McGraw-Hill Book Company, New York, New York.

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APPENDIX 6.14

TEST CATEGORY MEASUREMENT METHODOLOGY FOR ANALYTICAL CATEGORY PAYLOAD CONTAINERS CONTAINING PUCK DRUMS

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6.14 Test Category Measurement Methodology for Analytical Category Payload Containers Containing Puck Drums

6.14.1 Introduction

As defined by Section 5.2.2 of the CH-TRU Waste Authorized Methods for Payload Control (CH-TRAMPAC), analytical category payload containers containing puck drums must meet the following:

- The decay heat value for the payload container is less than or equal to the analytical decay heat limit specified per payload container based on the payload shipping category
- The total concentration of potentially flammable volatile organic compounds (VOCs) within the payload container headspace is less than or equal to 500 parts per million
- The payload container is classified as Waste Type I (10), II (20), or III (30).

The contents of the analytical category payload containers addressed by this appendix are puck drums. One or more puck drums are loaded into a single payload container. Headspace gas measurements of such payload containers have shown elevated hydrogen concentrations upon loading with puck drums for a small percentage of the payload containers qualified under the analytical category. Associated studies have shown that the elevated hydrogen values are transient and decrease exponentially with time.

This appendix establishes controls to ensure that hydrogen concentrations in analytical category payload containers containing puck drums are evaluated for compliance with flammable gas generation limits prior to TRUPACT-II or HalfPACT shipment. These controls require that all payload containers containing puck drums meeting analytical category decay heat limits additionally undergo a test category by measurement evaluation that is specific to payload containers containing puck drums. The test category by measurement methodology for payload containers containing puck drums and meeting analytical category decay heat limits consists of the following elements:

- Measurement of payload container headspace hydrogen concentration – The data package for each payload container containing puck drums must include the headspace gas sampling results for hydrogen for each payload container. If a given data package does not include headspace gas sampling data, the payload container will be rejected and may not be further evaluated for shipment until the headspace hydrogen concentration is measured and the data package is updated.
- Application of test category by measurement methodology – The payload container headspace hydrogen concentration is evaluated as the steady-state hydrogen concentration value under the CH-TRAMPAC measurement methodology delineated in Section 5.2.5.

Any payload container containing puck drums meeting analytical category decay heat limits that does not also meet test category flammable gas generation rate (FGGR) limits by the method described in this appendix is not authorized for shipment.

6.14.2 Gas Generation Methodology for Analytical Category Payload Containers Containing Puck Drums

This section details the gas generation methodology for payload containers containing puck drums meeting analytical category decay heat limits. Figure 6.14-1 presents the logic for performing the compliance evaluation for analytical category payload containers containing puck drums, which consists of the following steps:

Step 1, Payload container data package – The headspace concentration of hydrogen must be measured for each payload container. The measured hydrogen concentration shall be recorded in the data package for each payload container.

Step 2, Does data package include hydrogen headspace measurement data? – If the measured hydrogen concentration is recorded in the data package, the compliance evaluation shall proceed to Step 4, Determine flammable gas generation rate using test category by measurement methodology for analytical category payload containers containing puck drums. If the measured hydrogen concentration is not recorded in the data package, the compliance evaluation shall proceed to Step 3, Measure headspace gas and update container data package.

Step 3, Measure headspace gas and update container data package – If the measured hydrogen concentration is not recorded in the data package, the payload container will be rejected and may not be further evaluated for shipment until the headspace hydrogen concentration is measured and the data package is updated. Following the completion of headspace gas measurement and data package update, the compliance evaluation shall proceed to "Start."

Step 4, Determine flammable gas generation rate using test category by measurement methodology for analytical category payload containers containing puck drums – Using the measured headspace hydrogen concentration recorded in the data package as the steady-state hydrogen concentration value, calculate the FGGR for the payload container using the methodology described in Section 6.14.3. Compare the calculated FGGR to the FGGR limit for the payload shipping category assigned to the payload container. The FGGR limit is determined from the numeric payload shipping category per the formula specified in Section 5.2.3 of the CH-TRAMPAC or determined per Section 6.2.4 of the CH-TRAMPAC. Proceed to Step 5, Flammable gas generation rate ≤ flammable gas generation rate limit?

Step 5, Flammable gas generation rate ≤ flammable gas generation rate limit? – If the calculated FGGR is less than or equal to the FGGR limit, the compliance evaluation shall proceed to Step 7, Payload container eligible for shipment. If the calculated FGGR exceeds the FGGR limit, the compliance evaluation proceeds to Step 6, Container cannot be shipped. Mitigation measures required.

Step 6, Container cannot be shipped. Mitigation measures required. - If the calculated FGGR exceeds the FGGR limit, the payload container is not eligible for shipment and the payload container must be segregated for mitigation measures. Following the completion of mitigation measures, the compliance evaluation shall proceed to "Start."

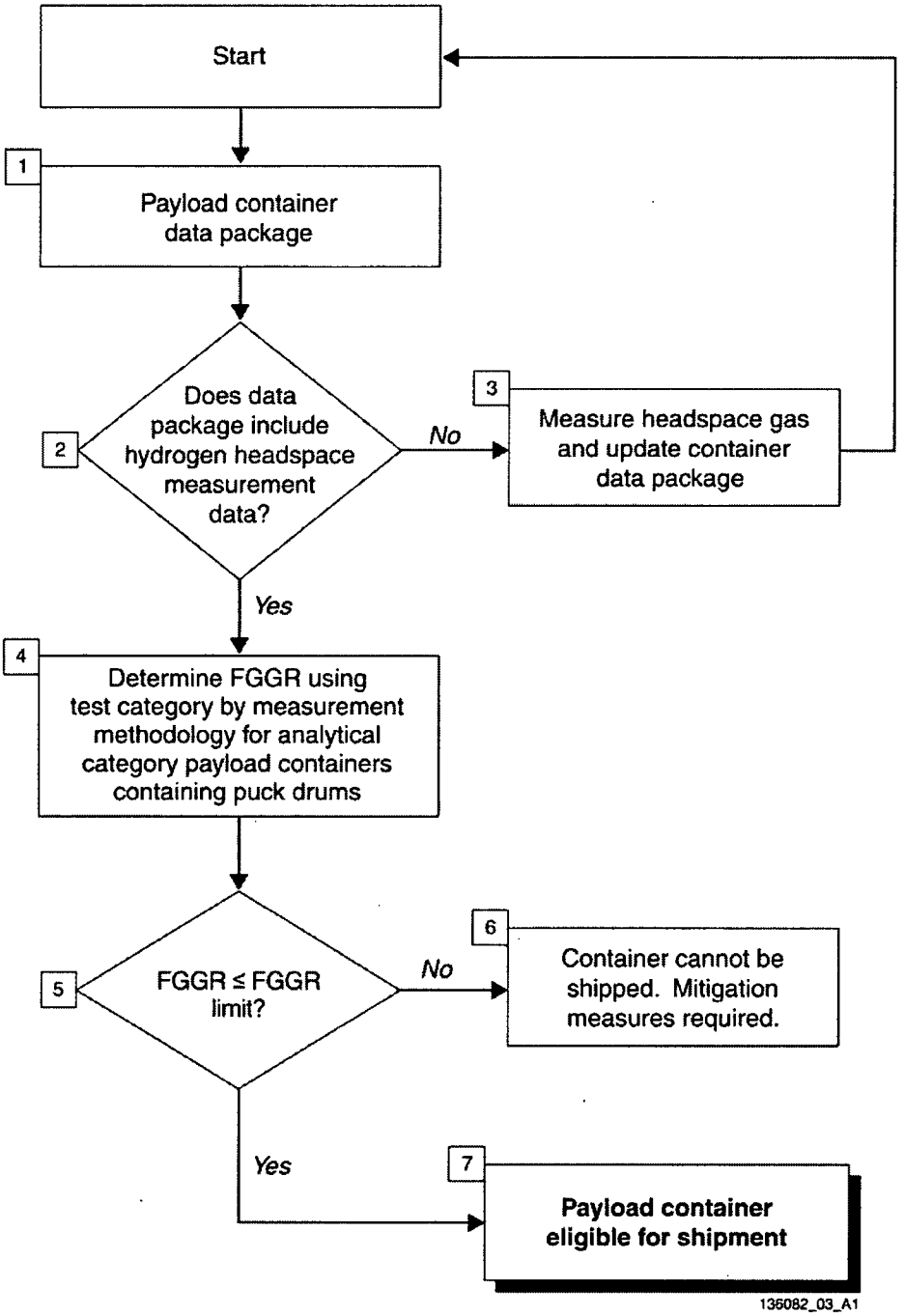

Figure 6.14-1 – Gas Generation Methodology for Analytical Category Payload Containers Containing Puck Drums

Step 7, Payload container eligible for shipment – All analytical category payload containers containing puck drums reaching this step meet the flammable (gas/VOC) limits and are eligible for shipment if all other transportation requirements are satisfied. Section 6.0 of the CH-TRAMPAC specifies the requirements for the certification of analytical category payload containers containing puck drums and for the certification of HalfPACT or TRUPACT-II payload assemblies of these payload containers.

6.14.3 Determination of Flammable Gas Generation Rate from Measured Headspace Hydrogen Concentration

The observance of initially elevated hydrogen concentration in a small percentage of the inventory of analytical category payload containers containing puck drums is a transient condition. Studies in which this percentage of the inventory was resampled showed that the initially elevated hydrogen concentration values decreased exponentially with time.[1]

For analytical category payload containers containing puck drums, the headspace hydrogen concentration at the time of payload container certification and subsequent shipment, which follow sampling, will be lower than the measured headspace hydrogen concentration at the time of sampling. As a conservative and bounding analysis, the measured headspace hydrogen concentration at the time of sampling will be used as the steady-state hydrogen concentration without credit for decay beyond the time of sampling. This steady-state concentration is used to determine the payload container FGGR based on the methodology described in CH-TRAMPAC Section 5.2.5 and Appendix 3.10 of the CH-TRU Payload Appendices[2].

As an example, based on the typical packaging configuration of 100-gallon drum payload containers containing 55-gallon puck drums (directly loaded into a 100-gallon drum with one filtered inner lid), there are two void volumes. The differential equations describing the mass balances on flammable gas for a payload container with two void volumes are provided as Equations (1) and (2) in Section 3.10.1.2, Differential Equations for a Container with Two Void Volumes, of Appendix 3.10 of the CH-TRU Payload Appendices[2]. In Equations (1) and (2), the 100-gallon drum headspace hydrogen concentration measured at the time of sampling (C_2 as a mole fraction) is assumed to be a steady-state hydrogen concentration value.

6.14.4 Summary

All analytical category payload containers containing puck drums, which by definition meet applicable analytical category decay heat limits and have total headspace flammable VOC concentrations less than or equal to 500 ppm, must also show compliance under the test category measurement methodology described in this appendix prior to TRUPACT-II or HalfPACT shipment.

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[1] Shaw Environmental, Inc., 2008, *Hydrogen Concentration Decrease Equation Fit for Resampled 100-Gallon Drums Containing 55-Gallon Puck Drums*, Shaw Environmental, Inc., Albuquerque, New Mexico.

[2] U.S. Department of Energy (DOE), *CH-TRU Payload Appendices*, U.S. Department of Energy, Carlsbad Field Office, Carlsbad, New Mexico.