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in Support of LDR/Delisting at
the WTP**

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List of Acronyms

AA	Alternative Action
AES	Atomic Emission Spectroscopy
AL	Action Level
ALARA	As Low As Reasonably Achievable
ASTM	American Society for Testing and Materials
BS	Blank Spike
CCB	Continuing Calibration Blank
CCV	Continuing Calibration Verification
CML	Composite Model for Landfills
CMTTP	Composite Model for Leachate Migration and Transformation Products
COC	Constituent of Concern
COPC	Constituent of Potential Concern
CRV	Concentrate Receipt Vessel
CVAA	Cold Vapor Atomic Absorption
DAF	Dilution/Attenuation Factor
DCP	Direct Coupled Plasma
DL	Detection Limit
DOE	United States Department of Energy
DOE-ORP	United States Department of Energy - Office of River Protection
DQO	Data Quality Objectives
DR	Decision Rule
DRAS	Delisting Risk Assessment Software
DRE	Destruction and Removal Efficiencies
DS	Decision Statement
DST	Double-Shell Tank
DTA	Differential Thermal Analysis
DWPA	Dangerous Waste Permit Application
EA	Environmental Assessment
Ecology	Washington State Department of Ecology
EPA	United States Environmental Protection Agency
EPDP	Environmental Performance Demonstration Plan

EQL	Estimated Quantitation Limit
ES&H	Environment, Safety, and Health
ETF	Effluent Treatment Facility
FLAA	Flame Atomic Absorption Spectroscopy
GC	Gas Chromatography
GEA	Gamma Energy Analysis
GFC	Glass Former Chemical
HEME	High-Efficiency Mist Eliminator
HEPA	High-Efficiency Particulate Air
HLVIT	High-Level Vitrification (refer to 40 CFR 268.42)
HLW	High-Level Waste
HQ	Hazard Quotient
HLSWAC	Hanford Site Liquid Waste Acceptance Criteria
HSSWAC	Hanford Site Solid Waste Acceptance Criteria
IC	Ion Chromatography
ICB	Initial Calibration Blank
ICP	Inductively Coupled Plasma
IHLW	Immobilized High-Level Waste
ILAW	Immobilized Low-Activity Waste
IRIS	Integrated Risk Information System
ISE	Ion Selective Electrode
LAW	Low-Activity Waste
LBGR	Lower Bound of the Gray Region
LCS	Laboratory Control Sample
LDR	Land Disposal Restrictions
LLS	Low-Level Standard
MCL	Maximum Contaminant Level
MDL	Method Detection Limit
MFPV	Melter Feed Preparation Vessel
MFV	Melter Feed Vessel
MS	Mass Spectroscopy
MSD	Matrix Spike Duplicate
MTG	Metric Tons Glass

NOS	Not Otherwise Specified
PCB	Polychlorinated Biphenyl
PB	Preparation Blank
PCT	Product Consistency Test
PFD	Process Flow Diagram
PJM	Pulse Jet Mixer
PNNL	Pacific Northwest National Laboratory
PSQ	Principal Study Question
QA	Quality Assurance
QC	Quality Control
QGCR	Qualified Glass Composition Region
R&T	Research and Technology
RCRA	Resource Conservation and Recovery Act of 1976
RFD	Reverse Flow Diverters
RPD	Relative Percent Difference
RW	Office of Civilian Radioactive Waste Management
SBS	Submerged Bed Scrubber
SEM	Scanning Electron Microscope
SRTC	Savannah River Technology Center
SST	Single-Shell Tank
SVOA	Semi-Volatile Organic Analysis
SVOC	Semi-Volatile Organic Compound
TC	Toxicity Characteristic
TCLP	Toxicity Characteristic Leaching Procedure
TIC	Total Inorganic Carbon
TIC/TOC/TC	Total Inorganic/Organic Carbon/and Total Carbon
TOC	Total Organic Carbon
TRU	Transuranic
TSD	Treatment/Storage/or Disposal
TWINS	Tank Waste Information Network System
UCL	Upper Confidence Level
UHC	Underlying Hazardous Constituents
UTS	Universal Treatment Standard

VHT	Vapor Hydration Test
VOA	Volatile Organic Analysis
VOC	Volatile Organic Compound
VSL	Vitreous State Laboratory
WAPS	Waste Acceptance Product Specification for Vitrified High-Level Waste Forms
WASRD	Waste Acceptance System Requirements Document
WCP	Waste Compliance Plan
WESP	Wet Electrostatic Precipitator
WTP	Hanford Tank Waste Treatment and Immobilization Plant
WQR	Waste Form Qualification Report

Executive Summary

The United States Department of Energy's (DOE's) Hanford Nuclear Reservation is the current home of approximately 177 million gallons of mixed waste stored in Hanford Site waste tanks. The waste is designated as a listed waste, and is subject to land disposal restrictions (LDR) in accordance with state and federal regulations. The DOE has assigned the Hanford Tank Waste Treatment and Immobilization Plant (WTP) responsibility for treating the mixed wastes by vitrification. The waste will be separated into high and low activity fractions, and vitrified into Immobilized High Level Waste (IHLW) and Immobilized Low Activity Waste (ILAW), respectively. The purpose of this document is to identify data needed to support the development of a petition to delist the IHLW, and support development of a petition for a treatability variance to establish vitrification (HLVIT) as the LDR treatment standard for both the IHLW and the ILAW. The DOE is currently evaluating alternatives to vitrification of low-activity waste. If DOE selects an alternate technology to process a portion of the low-activity waste, use of that technology will be demonstrated to comply with applicable LDRs. IHLW must be delisted to facilitate disposal in a geologic repository. Approval of a treatability variance for Hanford tank waste is needed to facilitate any land disposal pathway for the IHLW and the ILAW. This document identifies regulatory standards, establishes a compliance strategy, summarizes existing data, and identifies additional data requirements. The data needs were evaluated using the EPA 7-Step Data Quality Objective (DQO) Process. The DQO Process identifies the data needs and sampling/analysis design based on decisions, boundaries, and decision uncertainty. This summary provides an overview of the project scope, decisions, constituents of potential concern (COPCs), and recommended research and technology (R&T) data to support the delisting and LDR petitions.

Delisting is normally conditional upon demonstrating that the treated waste no longer meets the criteria that caused it to be listed, generally through analysis of the treated waste form. This approach raises concerns for the IHLW and ILAW due to radiological exposure of sampling and analytical personnel, and the practical logistics associated with sampling and analysis of the glass product. EPA and the Nuclear Regulatory Commission (NRC) have issued a joint policy that discourages unnecessary personnel exposure. WTP proposes that the appropriate method for complying with delisting requirements is to establish that the treatment process removes the hazardous constituents from the waste or immobilizes them within the waste sufficiently to allow the IHLW to be delisted. This DQO establishes the criteria for developing adequate data with acceptable data quality to support a technology-based, upfront, conditional petition for delisting IHLW.

In addition to delisting the IHLW, the treated waste forms must comply with the requirements of the LDR program for the constituents regulated through those regulations. Both the IHLW and ILAW must either meet the performance-based treatment standards for the LDR-regulated constituents, or be treated according to specified LDR treatment technologies. Some of the waste constituents do not currently have an associated treatment technology, and under normal circumstances, the treated waste would typically be sampled and analyzed for comparison to those standards, and to demonstrate compliance. WTP has determined that, because of the radiological exposures associated with the sampling and analysis required to demonstrate compliance with existing numerical standards, a performance-based standard applicable to Hanford tank wastes is inappropriate. Under the LDR program, a variance from the existing treatment standard(s) can be granted if it can be demonstrated that the existing standard(s) cannot be met or is (are) inappropriate for the waste being treated. WTP intends to petition for a treatability variance from the existing performance-based standards. The treatability variance will qualify vitrification as a specified method of treatment for Hanford tank wastes for all waste codes and hazardous constituents. This DQO

process establishes the criteria for developing adequate data with acceptable quality to support the treatability variance.

WTP is conducting an extensive research and technology R&T program to support the development of optimal glass formulations for the various waste forms. Data collection activities implemented under this DQO will be conducted under the appropriate regulatory (e.g., SW-846) quality control (QC) procedures to ensure that future results meet compliance needs. The following specific R&T activities are considered important for the petitions:

- Demonstrating the relationship between glass composition and glass performance;
- Demonstrating the means for controlling glass composition;
- Scaling development activities from small scale, through pilot scale, to production scale.

Separate lists of COPCs were established for delisting and for LDR petitions (see Table A). The selection of COPCs was conducted in a manner similar to that used for the Regulatory DQO (Wiemers, Lerchen, Miller, Meier 1998). Logic for exclusion of COPCs is based primarily on identifying compounds that were never used at Hanford, and those that are unstable in the oxidizing, caustic, and high radiation tank environment. The COPC selection process was used to identify both inorganic and organic constituents of potential concern, however, given that organic compounds will be degraded by pyrolysis during the vitrification process, there is no requirement for organics destruction testing. Evidence of organics destruction and an accompanying discussion are presented in Appendix H of this DQO.

The action limits for delisting are based on the EPA required Delisting Risk Assessment Software (DRAS). The action limits for LDR are based on minimizing threats to human health and the environment posed by land disposal of the waste and allow the project to propose alternate treatment standards. Data will be evaluated against the DRAS levels and the LDR Universal Treatment Standards (UTS). However, should the results be above the UTS and below the DRAS, the delisting standards will serve as the action level.

The sampling design is based on the two groups of COPCs:

- Metals with a low likelihood of leaching
- Metals with a higher likelihood of leaching

A research program was designed in response to this DQO that incorporates three different but increasingly complex statistical designs, depending on the TCLP response of the constituent of interest. Sample design will be based on the need to compute a 90 % upper confidence limit for the mean TCLP leachate concentration for comparison with action limit derived from the DRAS model.

In the first phase of glass testing, a small number of glasses will be spiked with all metal COPCs in order to identify those metals that can affect glass quality from a regulatory perspective. The results from this testing will support the further development of glass formulation models and determination of potential feed limiting constituents and glass former requirements. Results of TCLP analysis will be compared to the action limits, and those constituents whose leachate concentration approaches the limit will be further evaluated in a second or third phase of testing.

In the second phase of testing, the leachable metals will be spiked into a glass at multiple spiking levels to better characterize resulting TCLP leachate values as a function of metal concentrations in the feed. This information will be used to evaluate the relationship of leachate concentration with glass composition, and will provide the transition point from the first phase of testing to the third phase.

There are two situations in which a third phase of testing may be used. Testing will progress to this phase for metals where the first phase of testing has indicated an obvious potential for, or confirmed that, the constituent leaches from glass above TCLP limits. This phase of testing will also be implemented if the second phase of testing still leaves unanswered questions regarding the relationship between TCLP leachate values and COPC levels in the glass. In either case, the third phase involves simultaneously analyzing multiple glasses with multiple spiking levels of metals.

This document identifies the data requirements to support the development of delisting and LDR petitions (e.g., data collected before submission of the petitions and data generated by the R&T Program). Any additional data required during treatment will be identified via the petitioning process.

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
Organic Constituents of Potential Concern			
100-21-0	p-Phthalic acid	NID	28
100-41-4	Ethyl benzene	4.26E+01	10
100-42-5	Styrene	6.08E+00	Not UHC
10061-01-5	cis-1, 3-Dichloropropene	4.41E+06	18
10061-02-6	trans-1, 3-Dichloropropene	4.41E+06	18
101-55-3	4-Bromophenylphenyl ether	9.73E+00	15
106-46-7	1, 4-Dichlorobenzene	7.5E+00	6.0
106-93-4	Ethylene dibromide	2.40E-01	15
107-02-8	Acrolein	1.06E+03	NA
107-05-1	3-Chloropropene	ID	30
107-06-2	1, 2-Dichloroethane	1.60E-02	6.0
107-12-0	Propionitrile	NID	360
107-13-1	Acrylonitrile	7.80E-02	84
108-10-1	4-Methyl-2-pentanone (MIBK)	4.57E+01	33
108-39-4	m-Cresol	2.00E+02	Not UHC
108-88-3	Toluene	6.08E+01	10
108-90-7	Chlorobenzene	6.08E+00	6.0

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
108-95-2	Phenol	3.43E+02	6.2
109-06-8	2-Methylpyridine	ID	Not UHC
110-86-1	Pyridine	5.71E-01	16
117-81-7	Bis(2-ethylhexyl) phthalate	3.65E-01	28
117-84-0	Di-n-octylphthalate	2.80E-02	28
120-12-7	Anthracene	2.00E+01	3.4
120-82-1	1, 2, 4-Trichlorobenzene	4.26E+00	19
120-83-2	2, 4-Dichlorophenol	1.71E+00	14
122-09-8	alpha,alpha-Dimethylphenethylamine	NID	Not UHC
122-39-4	N,N-Diphenylamine	9.41E+00	13
123-91-1	1, 4-Dioxane	3.83E+00	170
126-68-1	O, O, O-Triethyl phosphorothioate	ID	Not UHC
126-98-7	2-Methyl-2-propenenitrile	5.71E-02	84
127-18-4	1, 1, 2, 2-Tetrachloroethene	3.04E-01	6.0
129-00-0	Pyrene	9.89E-01	8.2
130-15-4	1, 4-Naphthoquinone	ID	Not UHC
1319-77-3	p-Cresols (total) ^(a)	2.00E+02	Not UHC
13256-22-9	N-Nitrososarcosine	NID	Not UHC
1330-20-7	Xylene (total)	6.08E+02	30
1336-36-3	Polychlorinated biphenyls (PCBs)	2.88E-02	10
152-16-9	Octamethylpyrophosphoramidate	1.14E+00	Not UHC
156-60-5	1, 2-trans-Dichloroethene	6.08E+00	30
189-55-9	Dibenzo[a,i]pyrene	NID	Not UHC
189-64-0	Dibenzo[a,h]pyrene	NID	Not UHC
191-24-2	Benzo(ghi)perylene	ID	1.8
192-65-4	Dibenzo[a,e]pyrene	NID	NA
193-39-5	Indeno(1, 2, 3-cd)pyrene	1.23E-03	3.4
205-82-3	Benzo[j]fluoranthene	NID	Not UHC
205-99-2	Benzo(b)fluoranthene	2.33E-03	6.8

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
206-44-0	Fluoranthene	1.29E+00	3.4
207-08-9	Benzo(k)fluoranthene	3.25E-02	6.8
208-96-8	Acenaphthylene	ID	3.4
218-01-9	Chrysene	4.48E-01	3.4
224-42-0	Dibenz[a,j]acridine	NID	Not UHC
225-51-4	Benz[c]acridine	NID	Not UHC
226-36-8	Dibenz[a,h]acridine	NID	Not UHC
2303-16-4	Diallate	6.02E+03	Not UHC
25567-55-9	2, 3, 4, 6-Tetrachlorophenol, sodium salt	see 2, 3, 4, 6-Tetrachlorophenol	Not UHC
26952-23-8	Dichloropropene	See cis/trans isomers	Not UHC
297-97-2	O, O-Diethyl O-pyrazinyl phosphoro-thioate	ID	Not UHC
30402-15-4D	Pentachlorodibenzofurans	NID	Not UHC
319-84-6	alpha-BHC	7.06E+02	0.066
319-85-7	beta-BHC	2.34E-02	0.066
319-86-8	delta-BHC	NID	0.066
34465-46-8D	Hexachlorodibenzo-p-dioxins	NID	Not UHC
41903-57-5	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-) ^(b)	6.55E-09	0.001
465-73-6	Isodrin	NID	0.066
492-80-8	Auramine	NID	Not UHC
50-32-8	Benzo(a)pyrene	1.15E-02	3.4
50-55-5	Reserpine	NID	Not UHC
53535-27-6	2, 3, 4, 6-Tetrachlorophenol, potassium salt	see 2, 3, 4, 6-Tetrachlorophenol	Not UHC
53-70-3	Dibenz[a,h]anthracene	1.22E-04	8.2
541-73-1	1, 3-Dichlorobenzene	5.59E-02	6.0
56-23-5	Carbon tetrachloride	4.00E-01	6.0
56-49-5	3-Methylcholanthrene	4.83E-05	15

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
56-55-3	Benzo(a)anthracene	4.20E-03	3.4
57-97-6	7, 12-Dimethylbenz[a]anthracene	3.37E-05	Not UHC
58-89-9	gamma-BHC (Lindane)	4.00E-01	0.066
58-90-2	2, 3, 4, 6-Tetrachlorophenol	4.52E+00	7.4
59-50-7	4-Chloro-3-methylphenol	ID	14
59-89-2	N-Nitrosomorpholine	ID	2.3
60-51-5	Dimethoate	1.50E+02	Not UHC
621-64-7	N-Nitroso-di-n-propylamine	6.02E-03	14
62-75-9	N-Nitroso-N,N-dimethylamine	8.26E-04	2.3
630-20-6	1, 1, 1, 2-Tetrachloroethane	2.43E+00	6.0
6358-53-8	Citrus red No. 2	NID	Not UHC
64-18-6	Formic acid	1.14E+03	Not UHC
67-64-1	2-Propanone (Acetone)	5.71E+01	160
67-66-3	Chloroform	5.76E+00	6.0
67-72-1	Hexachloroethane	2.47E-02	30
70-30-4	Hexachlorophene	7.82E-04	Not UHC
71-43-2	Benzene	5.00E-01	10
71-55-6	1, 1, 1-Trichloroethane	1.22E+01	6.0
74-83-9	Bromomethane	3.20E+02	15
74-87-3	Chloromethane	ID	30
75-00-3	Chloroethane	1.45E+01	6.0
75-01-4	1-Chloroethene	1.22E-01	6.0
75-05-8	Acetonitrile	1.33E+02	38
75-09-2	Dichloromethane (Methylene Chloride)	2.88E-01	30
75-15-0	Carbon disulfide	5.71E+01	4.8 mg/L TCLP
75-27-4	Bromodichloromethane	6.80E-01	15
75-34-3	1, 1-Dichloroethane	3.01E+00	6.0
75-35-4	1, 1-Dichloroethene	4.04E-01	6.0
75-69-4	Trichlorofluoromethane	5.10E+01	30

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
75-71-8	Dichlorodifluoromethane	5.24E+01	7.2
78-83-1	2-Methylpropyl alcohol	1.71E+02	170
78-87-5	1, 2-Dichloropropane	5.28E-01	18
78-93-3	2-Butanone (Methyl ethyl ketone)	2.00E+02	36
79-00-5	1, 1, 2-Trichloroethane	3.04E-01	6.0
79-01-6	1, 1, 2-Trichloroethylene	3.04E-01	6.0
79-34-5	1, 1, 2, 2-Tetrachloroethane	4.39E+00	6.0
82-68-8	Pentachloronitrobenzene (PCNB)	1.09E-01	4.8
83-32-9	Acenaphthene	1.00E+01	3.4
84-66-2	Diethyl phthalate	5.53E+02	28
84-74-2	Di-n-butylphthalate	1.32E+01	28
85-01-8	Phenanthrene	ID	5.6
85-68-7	Butylbenzylphthalate	2.32E+01	28
86-73-7	Fluorene	4.44E+00	3.4
87-68-3	Hexachlorobutadiene	1.50E-02	5.6
88-06-2	2, 4, 6-Trichlorophenol	2.00E+00	7.4
88-75-5	2-Nitrophenol	ID	13
88-85-7	2-sec-Butyl-4, 6-dinitrophenol; syn Dinoseb	4.26E-01	2.5
91-20-3	Naphthalene	1.04E+00	5.6
91-58-7	2-Chloronaphthalene	9.50E+00	5.6
93-72-1	Silvex (2, 4, 5-TP)	1.00E+00	7.9
95-48-7	o-Cresol	2.86E+01	Not UHC
95-50-1	1, 2-Dichlorobenzene	3.65E+01	6.0
95-57-8	2-Chlorophenol	2.86E+00	5.7
95-95-4	2, 4, 5-Trichlorophenol	2.29E+01	7.4
98-86-2	Acetophenone	5.71E+01	9.7
98-95-3	Nitrobenzene	2.86E-01	14
99-35-4	1, 3, 5-Trinitrobenzene	1.62E+01	Not UHC

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
Inorganic Constituents of Potential Concern			
57-12-5	Cyanide (total)	1.15E+01	590
57-12-5	Cyanide (amenable)	see Cyanide (total)	30
7429-90-5	Aluminum	NID	Not UHC
7439-92-1	Lead	5.00E+00	HLVIT ^(c)
7439-97-6	Mercury	2.00E-01	HLVIT ^(c)
7440-02-0	Nickel	2.26E+01	11 mg/L TCLP
7440-09-7	Potassium	NID	Not UHC
7440-22-4	Silver	3.07E+00	HLVIT ^(c)
7440-23-5	Sodium	NID	Not UHC
7440-28-0	Thallium	2.82E-01	0.20 mg/L TCLP
7440-36-0	Antimony	6.59E-01	1.15 mg/L TCLP
7440-38-2	Arsenic	3.08E+00	HLVIT ^(c)
7440-39-3	Barium	1.00E+02	HLVIT ^(c)
7440-41-7	Beryllium	1.33E+00	1.22 mg/L TCLP
7440-43-9	Cadmium	4.80E-01	HLVIT ^(c)
7440-47-3	Chromium	5.00E+00	HLVIT ^(c)
7440-50-8	Copper	2.92E+04	Not UHC
7440-62-2	Vanadium	1.69E+01	Not UHC
7440-66-6	Zinc	2.25E+02	Not UHC
7440-70-2	Calcium	NID	Not UHC

Table A COPC Summary Table

CAS	Chemical	Delisting Level (mg/L, TCLP)	LDR Treatment Standard (mg/kg or mg/L TCLP)
7723-14-0	Phosphorus	NID	Not UHC
7782-49-2	Selenium	1.00E+00	HLVIT ^(c)

- (a) Total Cresol, CAS # 1319-77-3, represented by p-Cresol, CAS # 106-44-5 in DRAS (computed value is from p-Cresol).
- (b) Tetrachlorodibenzo-p-dioxin, CAS # 41903-57-5, represented by 2,3,7,8-Tetrachlorodibenzo-p-dioxin, CAS # 1746-01-6 in DRAS (computed value is from 2,3,7,8-Tetrachlorodibenzo-p-dioxin)
- (c) HLVIT: High-level vitrification is the current LDR technology-based standard (40 CFR 268.40) for mixed high-level radioactive waste with toxicity characteristic concentrations of the indicated constituent.

UHC - Underlying Hazardous Constituents (refer to 40 CFR 248.48)

NID - Not in DRAS

ID - Insufficient Data to calculate a DRAS Level

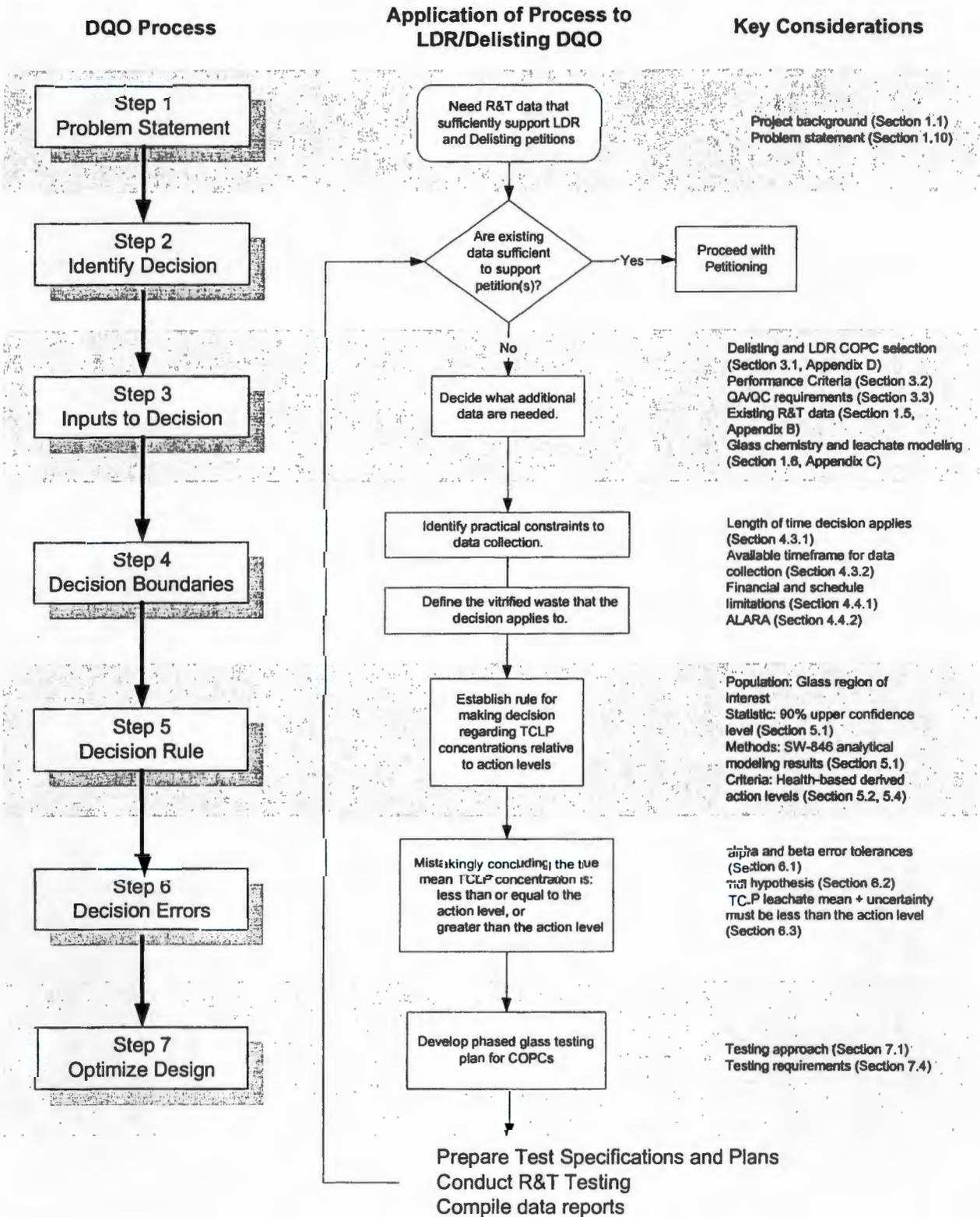
NA-Compound is a UHC but there is not non-waste water standard

Foreword

Identifying and documenting the data needed to support the LDR and delisting petitions have been lengthy and complex. Readers unfamiliar with the field of glass chemistry, or the DQO process itself, could easily be overwhelmed by the description and details provided in this document. There is, however, an overarching logical flow and structure to this document that is based on the Data Quality Objectives (DQO) guidance found in EPA QA/G-4. Figure A presents this logical structure, and is intended to provide a roadmap to guide the reader through the document. It outlines the flow of the document and highlights the main points to keep in mind while reading through the DQO. It may be helpful for readers to review Figure A in order to gain a glimpse of the overall structure of the document prior to tackling the details.

There are three columns in Figure A. The column on the left presents the seven steps of the DQO process. These are the basic steps found in many problem-solving methodologies. They are critical to the process of planning data collection because they require the investigator to think through the entire decision making process before collecting any data. The middle column illustrates how the general DQO steps apply to the LDR/Delisting DQO. Note that the flow chart presented in this middle column reflects an iterative process of conducting and refining glass testing until there is sufficient data to support LDR and delisting petitions. The right-hand column contains a list of bulleted items that are the key considerations in thinking through the associated step. These bulleted items also refer to the sections of the document that elaborate on the specific topics.

Figure A Overall LDR & Delisting DQO Logic Flowchart



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1 Step 1 - Problem Statement

The problem statement sets the context for the remainder of the data quality objectives (DQO) process. Successful project planning requires an examination of past events, identification of the appropriate technical resources, and knowledge of the basis for problem statement development. The problem to be addressed by the study must be clearly defined. This section will provide an overview of the project and processes that are the subject of this DQO process, then identify those issues that are to be resolved through the remaining steps of the DQO. The problem statement is summarized in Section 1.10.

1.1 Project Background and Scope

The United States Department of Energy (DOE) has assigned the Hanford Tank Waste Treatment and Immobilization Plant (WTP) with responsibility for treating the high-level radioactive wastes currently stored in Hanford Site waste tanks in order to prepare them for disposal. The waste materials also contain *Resource Conservation and Recovery Act of 1976* (RCRA)-regulated hazardous wastes, both listed wastes identified in 40 CFR 261.31 through 40 CFR 261.33, and constituents that are subject to the land disposal restrictions (LDR) contained in 40 CFR 268 and WAC 173-303-140. The RCRA regulated materials also are subject to management under the analogous provisions of the Washington State Dangerous Waste Regulations found in the Washington Administrative Code (WAC), Chapter 173-303. Table 1-1 provides a crosswalk between the RCRA and corresponding Dangerous Waste regulations that are used throughout this document. The reader can assume that where a citation is provided for one authority, the reference is intended to invoke the corresponding Federal or State authority, as well.

The Part A permit application for the Hanford single-shell and double-shell tanks, by which these units initially qualified for interim status, identified various listed wastes as being managed by the tank system. Issues associated with the listed wastes have been discussed in detail in a document entitled *Approach for Immobilized High Level Waste Delisting* (RPT-W375HV-EN00001, Rev. 1). The immobilized high-level waste (IHLW) is intended for disposal at the proposed geologic repository for spent nuclear fuel and high-level radioactive waste. The Federal high-level waste repository will not be permitted under Federal RCRA or corresponding State regulations, and will not accept hazardous wastes for disposal. The EPA and the State of Washington, however, have established procedures for delisting wastes that no longer meet the criteria that caused them to be listed as hazardous (e.g., 40 CFR 260.20, 40 CFR 260.22, WAC 173-303-072, EPA 1993a *Guidance on Petitions to Delist Dangerous Waste*, WA Department of Ecology, Pub. #97-434). Delisting is normally conditional upon analysis of the treated process materials demonstrating that the treated materials comply with specified performance standards. This approach raises concerns, however, due to radiological exposure of sampling and analytical personnel, and the practical logistics associated with sampling and analysis of the glass product. EPA has stated in 55 FR 22627 that, "...the Agency believes that the potential hazards associated with exposure to radioactivity during analysis of this high-level mixed waste preclude setting a concentration based treatment standard". Analytical work performed at the Savannah River Technology Center (SRTC) has confirmed this (CCN 030691).

It is possible to establish a correlation between the application of specific, approved treatment technologies and the achievement of applicable delisting criteria to minimize the need for testing of the glass product. Monitoring, in effect, is conducted on the process and critical input parameters rather than the glass itself. Because of the concerns associated with analysis of IHLW, WTP proposes that the more appropriate method for complying with delisting requirements will be to establish that the treatment

process removes the hazardous constituents from the waste or immobilizes them within the waste sufficiently to allow the IHLW to be delisted. This DQO will establish the criteria for developing adequate data with acceptable data quality to support a successful, technology-based, upfront, conditional petition for delisting IHLW, and identifies the amount and quantity of data required to demonstrate compliance with these standards.

In addition to delisting the IHLW for disposal at a deep geologic repository, the treated waste forms must comply with the requirements of the land disposal restrictions found in 40 CFR 268 and WAC 173-303-140. Treated, immobilized low-activity waste (ILAW) and immobilized high-level waste (IHLW) from the WTP must either meet the performance-based treatment standards for the LDR-regulated constituents of concern (COC), or be treated according to specified LDR treatment technologies. WTP considered the various issues associated with compliance with the LDR program in a document entitled *Approach to Immobilized Hanford Tank Waste Land Disposal Restriction Compliance* (RPT-W375LV-EN00002, Rev. 1).

Currently, the LDR treatment standard for D002 and D004-D011 for high-level radioactive wastes is a specified technology of HLVT (high-level vitrification). The treatment standards for other waste codes in the Hanford tank wastes are UTS concentration-based standards appearing in 40 CFR 268.40. That is, no specified technology treatment standard has been established for high-level wastes containing waste codes other than D002 and D004-D011. The WTP could elect to demonstrate compliance with the LDR requirements by sampling the treated glass product to show that it meets applicable universal treatment standards (UTS) criteria for the regulated constituents in the waste. The Environmental Protection Agency (EPA) has incorporated into the LDR program the ability to obtain a variance from the existing treatment standard(s), if it can be demonstrated that the existing standard(s) cannot be met or is (are) inappropriate for the waste being treated. WTP has determined that, because of the radiological and chemical exposures associated with the sampling and analysis required to demonstrate compliance with existing numerical standards, a performance-based standard applicable to Hanford tank wastes is inappropriate. Therefore, WTP has decided that a petition for a treatability variance from the existing performance-based standards is the preferred method for demonstrating compliance with LDR requirements. This DQO process must establish the criteria for developing adequate data with acceptable data quality to support the treatability variance.

Qualification activities (planned methods and documentation) conducted prior to full-scale operations will provide confidence that WTP will produce IHLW that qualifies for delisting, and IHLW and ILAW that complies with LDR criteria. WTP is conducting an extensive research and technology (R&T) program to support the development of optimal glass formulations for the various waste forms. Although much of the data that has been generated was not intended to support regulatory needs, previously generated data from the R&T program will strengthen the petitions for demonstrating compliance with delisting and LDR requirements. Ongoing data collection activities will be conducted under the appropriate quality control (QC) procedures to ensure that future results meet compliance needs. The following specific R&T activities are considered important for the petitions:

- Demonstrating the relationship between glass composition and glass performance
- Demonstrating the means for controlling glass composition
- Scaling development activities from small scale, through pilot scale, to production scale

Activities conducted to date that support these areas of interest are described below.

If the data are sufficient to support petitions for a conditional, technology-based delisting or a treatability variance, methods for verification and control of the effectiveness of the treatment process will be addressed through the petitioning process.

1.2 DQO Planning Team

This DQO effort requires the assistance of assorted technical personnel to support the decision makers with the development of this DQO process. Table 1-2 summarizes key decision making and technical personnel or organizations.

1.3 WTP Treatment Process Description

A review of the WTP treatment process is warranted in order to provide sufficient background for establishing data quality objectives in the context of a problem statement. This section summarizes the WTP treatment processes. The WTP will receive a slurry of liquids and solids stored in the Hanford Site Single-Shell (SST) and Double-Shell Tank (DST) Systems. The waste is composed of chemicals and fission products left over from the production of plutonium during the 1940's through the 1980's. The waste contains organic, inorganic, and radionuclide constituents.

The immobilized waste generated by the vitrification processes will be in the form of glass that maintains its chemical and physical integrity during long-term storage. The discussions provided below include summary descriptions of the vitrification process, and the planned approach for demonstrating compliance of the glass forms with regulatory criteria. Additional detail regarding activities within specific waste management units can be found in the WTP *Dangerous Waste Permit Application* (DWPA) (24590-WTP-DWPA-ENV-01-001) and is summarized below.

1.3.1 Process Summary

1.3.1.1 LAW and HLW Feed Envelopes

The WTP will store and treat low-activity waste (LAW) feed and high-level waste (HLW) feed from the Hanford Site DST system unit. The term "LAW feed" generally refers to the supernatant portion of the DST system unit waste, although it can include high-level waste solids. These feeds are subsets of high-level waste, which is defined in 10 CFR 72.3, and represent about 80 % of the tank waste. All the feeds have been designated as characteristic for organics and metals. LAW feed is composed of three waste feed envelopes, which are described in the contract:

- Envelope A. Cesium and technetium concentrations in this feed envelope are high enough to warrant their removal so the ILAW glass waste will meet applicable requirements.
- Envelope B. This feed envelope contains higher concentrations of cesium than Envelope A. Both cesium and technetium must be removed to comply with the ILAW specifications. This envelope also allows for concentrations of chlorine, chromium, fluorine, phosphates, and sulfates that are higher than those found in Envelope A, which may limit the rate of waste incorporation into glass.
- Envelope C. This feed envelope contains high enough concentrations of cesium, technetium, and organically complexed strontium and transuranics to require removal to meet LAW glass specifications.

The HLW feed is described below:

- Envelope D. HLW feed will be in the form of a slurry containing approximately 10 to 200 grams of unwashed solids per liter. Most of the Envelope D radionuclides are in unwashed solid form. The liquid fraction of the slurry will be composed of residues from Envelope A, B, or C waste; the solid fraction will be Envelope D waste.

Numerous sources of information documenting tank waste composition are available. The most recent version of TFCOUP (CHG 2000) should be consulted for a comprehensive description of tank waste composition. Additional data is publicly available from the Tank Waste Information Network System (TWINS) database at <http://twins.pnl.gov:8001/twins.htm>.

1.3.1.2 Pretreatment Overview

The SST and DST waste slurry will be received at the WTP Pretreatment Facility, and the LAW and HLW will be separated for vitrification at two different vitrification facilities, a LAW Vitrification Facility and a HLW Vitrification Facility. The primary function of the Pretreatment Facility is to remove excess water from the waste, separate LAW from HLW, and remove selected radionuclides and transuranics from the LAW for processing with the HLW. The WTP pretreatment process is designed to separate cesium, technetium, strontium, and transuranics from the LAW feeds, segregate solids into the HLW feed stream, and concentrate the waste fed to the melter systems. Separating LAW from HLW, and processing precipitated radionuclides and transuranics with the HLW fraction of the tank waste will ultimately reduce the volume of material requiring disposal at a geologic repository, as required by the *Nuclear Waste Policy Act*. The offgas from the treatment processes will be treated to a level that protects human health and the environment. Secondary waste streams (e.g., radioactive and dangerous solid waste, nonradioactive and nondangerous liquid effluents, and radioactive and dangerous liquid effluents) will be characterized and recycled into the treatment process, transported to permitted TSD facilities located on the Hanford Site, or transported offsite, as appropriate. After pretreatment, LAW and HLW feeds are transferred to the LAW and the HLW vitrification systems, respectively.

1.3.1.3 Overview of Vitrification

Feed concentrate (LAW or HLW solids with pretreatment intermediate waste products added) will be transferred from the pretreatment building to a concentrate receipt vessel (CRV). Batches of feed concentrate from the CRVs will then be transferred to the melter feed preparation vessel (MFPV). The feed concentrate will be blended with glass formers to ensure a uniform mixture. The melter feed slurry will then be transferred to the melter feed vessel (MFV), from which it will be fed to the melter.

The WTP will incorporate two similarly designed vitrification systems: one system will immobilize the pretreated LAW feed; the second will immobilize the pretreated HLW feed. Melters are required to convert a blended slurry of waste and glass former additives into molten glass. Figure 1-1 provides a very simplified view of a melter. Note that the partial cold cap and configuration of the melter shown in Figure 1-1 is for illustrative purposes only. Actual melter conditions will vary from those shown and are described in greater detail in WTP system descriptions and permits.

During melter operation, a mixture of glass formers and waste is added to the melter through the feed nozzles. The slurry is delivered from the MFV tank with a low-volume pump. As the slurry is fed, molten glass is formed that accumulates in the melter. When the melt level rises to a predetermined upper limit, it is discharged to a container so that a relatively constant glass pool depth is maintained throughout

the process. Air bubblers may be used to mix and agitate the molten glass. At the surface of the melt (the interface between the melt pool and plenum air), a cold cap is formed as lower temperature feed is introduced to the melt pool. The cold cap aids in melter operation by trapping heat within the melt pool. As the cold-cap heats and melts away, more feed is added to maintain cold-cap balance. During operation, feed rate, cold-cap coverage, and discharge rate are balanced to achieve the desired throughput.

In order to transfer the molten mixture of feed and glass forming materials from the melter to the product containers, the glass must be of an appropriate viscosity to allow it to be poured. This viscosity is a function of the temperature of the glass. The nominal glass melt pool temperature is 1150 °C; this temperature is measured with thermocouples in thermowells, submerged into the pool at various locations. The power to the electrodes is regulated to maintain the temperature at the nominal value.

The two HLW melters each have a nominal production rate of 1.5 metric tons of glass (MTG) per day. The average residence time in a HLW melter will be about 6 days. The two LAW melters have a combined nominal production rate of 30 MTG per day. The average residence time in each LAW melter will be about 2.5 days (24590-WTP-PL-RT-02-001). Each LAW melter will produce about two containers of ILAW a day. Melter holdup will be approximately 25 MTG (enough to fill about four containers). The high temperatures and residence times ensure that the glass can be poured into containers, and that volatiles will evaporate or decompose and be drawn off through the offgas system. Metals will generally react to form oxides and become part of the molten glass. The data collection program that will be developed as an output from this DQO process will verify the assumptions that have gone into the design of the vitrification process.

The dangerous waste constituents in the melter feed will be destroyed, removed, or immobilized in a glass matrix through the vitrification process. The ILAW and IHLW produced by the WTP will be in the form of glass sealed in stainless steel containers.

A more detailed description of the WTP process activities is provided in Appendix A.

1.3.2 Performance Standards for Melter Systems

The *Waste Acceptance Product Specification for Vitrified High-Level Waste Forms* (WAPS) establishes performance requirements for the glass in terms of durability (leach resistance). These requirements are primarily established to ensure compliance of the vitrified Hanford tank waste with the DOE/RW requirements for disposal at the Yucca Mountain geologic repository. Some of these requirements differ from those specified by environmental regulatory laws. The WAPS specifies testing related to glass durability, composition, radioactivity, spinel formation (glass crystallization), etc., as well as a requirement for compliance with hazardous waste regulations of 40 CFR 261 (WAPS Specification 1.5). These requirements are discussed in the text which follows, along with pertinent conclusions from the research activities performed to-date. Although durability tests, such as vapor hydration and the product consistency test are not adequate for demonstration of environmental compliance, the results of these tests do help to substantiate vitrification as a viable technology for treatment of Hanford tank waste. The waste form compliance strategy discussed in subsection 1.3.2.1 is presented to provide background on current strategies to ensure compliance with WAPS requirements. Subsection 1.3.2.2 discusses how the waste form compliance strategy would be applied during production. Since WAPS Specification 1.5 requires the WTP to petition for delisting IHLW, the information is relevant in that it describes the use of research data, model development and the qualified glass composition region that must be determined in order to produce a compliant glass form.

Durability is established by analysis of the glass product through the product consistency test (PCT) (7 days, 90°C test), performed according to ASTM Method C 1285. Per the WAPS, Specification 1.3, IHLW leach rates of boron, lithium, and sodium must be less than that for the environmental assessment (EA) reference glass for the disposal facility (DOE 1996). (Note: EA glass is a standard borosilicate glass formulation used as the basis for selecting vitrification as the preferred alternative for treatment of HLW in the National Environmental Policy Act EA (1969) for the Defense Waste Processing Facility. It was subsequently adopted by DOE's Office of Civilian Radioactive Waste Management as the reference for waste form performance for the proposed HLW repository.) Tests conducted on the IHLW glass product have shown that the leach rate is lower than that for standard EA glass. Tests performed on the ILAW have shown a loss rate of less than 2.0 g/m² over a 7-day test. These results are indicative that the process will result in good glass product, as evaluated by the PCT. It is important to recognize, however, that PCT is not a criterion for delisting or LDR compliance, and that there is no established correlation between PCT results and the toxicity characteristic leaching procedure (TCLP), SW-846 Method 1311 - the sample extraction method required to support compliance activities. The following discussion addresses the activities that are being performed to demonstrate that the ILAW and IHLW glass will meet compliance needs.

1.3.2.1 Waste Form Compliance

The compliance strategy for ILAW and IHLW may involve a combination of process information and sample analysis, along with possible sampling and analysis of the product (*Waste Treatment Plant Waste Analysis Plan*, 24590-WTP-RPT-ENV-01-003). The following discussion presents a generic summary of the process that will be used for monitoring the makeup of ILAW and IHLW from feed through glass formation.

Data generated through previous evaluations of vitrified waste products have shown that glass properties correlate well with the chemical composition of the glass. Studies at the West Valley and Savannah River sites have modeled the results of analysis through a wide range of glass compositions (reference Hay and Bronikowski 2000; Hay, Bronikowski, Hsu, and White 2000; West Valley 1996). These studies have included evaluations of both simulated and actual waste forms, as well as melts ranging from crucible to full-scale. The results show that 10 to 15 primary constituents make up 95 % of the glass form, and are the major players in determining the leachability of glass. Accordingly, waste form compliance sampling will be limited to that necessary to ensure product composition control (such as confirming proper assignment of glass former chemicals (GFCs) for the waste and blended pretreatment products). Analysis will be limited to the minimal parameters needed for this confirmation, namely pH, sodium molarity, specified radioisotopes, and constituents present in excess of 0.5 weight percent.

Studies and modeling activities conducted to date have been performed primarily in the context of the PCT evaluation. Ongoing studies are being conducted to establish a similar correlation model for the behavior of glass forms when subjected to the TCLP. Initial observations of the leaching behavior for toxicity characteristic (TC) metals indicate that the calculated release rates provide an accurate pattern of the actual release rate of metals subjected to TCLP. Section 1.6 and Appendix C of this DQO document provide a discussion of glass formulation chemistry and leachate modeling. The concentration of the TC metals in the waste alone, however, does not necessarily affect glass quality.

For compliance with the WAPS (DOE 1996) and the *Waste Acceptance System Requirements Document* (WASRD) (DOE 1999), the WTP project strategy is a combination of proof-of-concept demonstrations in advance of production (qualification activities), along with activities to confirm those results during

production operations (production activities). The WTP will perform the following activities for each waste type:

- Establish and populate a non-radioactive, property-composition database to develop property-composition models and corresponding uncertainty expressions. The property-composition models will be developed and validated using statistical methods.
- Develop and test non-radioactive glass formulations appropriate for possible compositions of the pretreated HLW and LAW intermediate waste products. Prepare and test radioactive glass formulations using pretreated waste treatability samples. Compare the results to non-radioactive versions of the same formulations.
- Develop a Qualified Glass Composition Region (QGCR) with appropriate glass compositions to ensure compliance with all applicable waste acceptance criteria (refer to subsection 1.3.2.2). The confidence level is discussed in Section 6 of this DQO. Property-composition models and corresponding statistical uncertainty expressions will be used to help define a QGCR. The QGCR is discussed in greater detail below.
- As new waste types are considered for treatment, their corresponding QGCRs will be developed (or an existing QGCR utilized) and reported in an addendum to the waste form qualification report (WQR). The WQR is a vehicle for reporting to DOE/RW the projected composition of IHLW glass (waste with glass formers added) to be produced from a given waste type. It will not be used for RCRA purposes.

Property-composition models and corresponding statistical uncertainty expressions will be used to help define a QGCR and to identify sub-regions within the QGCR that also satisfy processability and waste loading requirements. TCLP performance will be projected based on property-composition models relating TCLP results to chemical composition of the glass product (ILAW & IHLW). Glass compositions will be selected using formulation methods and statistical experimental design methods to adequately cover the relevant glass composition region for a given waste type. Samples of various glass compositions will be collected and analyzed during research activities, and used to refine the property-composition models and define a QGCR for each waste type. The property-composition models will be developed, evaluated, and validated using statistical regression methods (Cornell 1990, Draper and Smith 1998, and Montgomery and Peck 1992).

The projected glass composition is required to meet contract product quality requirements with high confidence, after accounting for applicable variations and uncertainties; thus, extrapolation of models beyond the region they are suited for will not be done. Additional glass formers can be added to compensate for variations in CRV composition (if needed) and produce a melter feed that is within the QGCR. During the qualification phase prior to radioactive operations, the WTP will:

- Demonstrate the ability to control the vitrification process in order to reliably produce acceptable ILAW and IHLW.
- Conduct studies to quantify the sources of variation and uncertainty affecting estimates of glass composition.

The preceding compliance activities constitute only a small portion of the activities discussed in the *Waste Form Compliance Plan for Immobilized High-Level Waste (WCP)* (24590-WTP-PL-RT-02-005). However, they are the most relevant to the development of delisting and LDR compliance strategies.

1.3.2.2 Qualified Glass Composition Region

A qualified glass composition region (QGCR) is a collection of glass compositions that are expected to satisfy all product quality requirements with high confidence after accounting for applicable variations and uncertainties. The QGCR must account for vapor hydration (ILAW only), product consistency test, and TCLP response, in addition to various other physical criteria (crystallization, thermal properties, etc.). Figure 1-2 provides a conceptual illustration of the QGCR, and how it includes these various requirements.

A QGCR is developed by combining wastes or simulated wastes with glass formers to create a variety of glasses of varying composition that meet all product quality requirements. The specific region of glass compositions covered by the QGCR depends on the chemical composition of the waste type. Concentrations of major constituents (such as aluminum, sodium, iron, and zirconium) and minor constituents (such as noble metals, RCRA metals, phosphate, and sulfate) are all considered. Possible variations and uncertainties are accounted for to provide high confidence that glass produced within the QGCR meets all applicable requirements. Variation in the waste type is accommodated during production operations by adjusting the mass and composition of glass former compounds (GFC) added. The QGCR is bound by constituent levels in the glass. It is a multi-dimensional representation of the possible permutations of glass compositions that result in a compliant waste form for a given waste type (feed envelope or sub-envelope). The QGCR is commonly referred to as "n" dimensional, where "n" is generically used to indicate the number of glass components and their acceptable range of concentration. For example, the composition for a glass composed solely of aluminum, silicon, sodium and oxygen could be plotted on a 3-dimensional graph where the acceptable concentration ranges of the 3 oxide components (Al_2O_3 , SiO_2 , Na_2O) could be illustrated. The graph could be further bound by limiting the plot to the upper and lower prediction limits of the acceptable concentration ranges (as determined from testing and modeling), and would be the equivalent of the QGCR for that glass composition. Figure 1-3 uses a dodecahedron to illustrate a QGCR in a 3-dimensional space representing the range of acceptable glass compositions (e.g. acceptable concentration ranges of the three oxide components, Al_2O_3 , SiO_2 , Na_2O) for a hypothetical glass. Note that the use of a dodecahedron is for illustrative purposes and is not intended to suggest the true shape of the QGCR in 3-dimensional space.

The glass formulation process is an iterative procedure in which glass property-composition models, knowledge, and experience are used to select glass compositions covering the range of glass components and waste constituent concentrations of interest. Data from testing programs specific to WTP, as well as production data from other vitrification plants, is used to refine the property-composition models and define a QGCR for each waste type. Multiple QGCRs are sometimes required for multiple waste types in order to optimize waste loading (e.g., maximize the waste to GFC ratio).

1.3.2.3 Process Control

The WTP will receive waste from a given feed tank in batches and process them through pretreatment to remove excess water from the waste, separate LAW from HLW, and remove selected radionuclides and transuranics from the LAW for processing with the HLW. Once pretreatment is complete, the concentrated waste will be transferred from the pretreatment plant to the feed concentrate receipt vessels (CRVs) in either the LAW vitrification facility or the HLW vitrification facility. Process control samples will be collected from the CRVs and analyzed to determine the glass former formulation. The waste will be slurried to the melter feed preparation vessel (MFPV) for blending with glass former compounds (GFCs).

The amount and specific individual GFCs needed to produce a waste product within the QGCR for the waste type will be calculated, based on the analysis of the pretreated waste. The individual GFCs that are expected to be used include silica, alumina, boric acid (or borax), calcium silicate, ferric oxide, lithium carbonate, magnesium silicate, zircon sand, zinc oxide and reductants (sugar).

Individual glass former compounds will be transferred from storage silos to individual hoppers, then to a central blending hopper, and then transferred to a GFC feed hopper in the vitrification facility. Each step of the GFC handling process will be monitored and weighed (hoppers are equipped with load cells) so that any handling loss can be identified and corrected prior to blending GFCs with the concentrated waste.

Waste from the CRV and GFCs from the GFC feed hopper will be blended together in the MFPV. Once blended, the melter feed slurry will be transferred from the MFPV to the melter feed vessel (MFV). From the MFV, the blended material is fed to the melter continuously. The dangerous waste constituents in the melter feed will be destroyed, removed, or immobilized in a glass matrix through the vitrification process. When the melt level in the melter rises to a predetermined upper limit, it is discharged to a stainless steel container, which is welded shut and decontaminated (the container exterior) and staged to await disposal.

This discussion illustrates how WTP process control is maintained through the following:

- Process characterization of the concentrated waste in the CRV
- Assignment/verification of required GFCs against the applicable QGCR
- Proper/controlled addition of the right amount of GFCs with the concentrated waste
- Vitrification of a blended waste/GFC feed that falls within the QGCR

Research, modeling, and error quantification are used in advance of processing to define the QGCR for the waste to be processed. The relationship of research, modeling, and error quantification to WTP processing is illustrated in Figure 1-4. The result is a fundamentally simple control process in which errors are controlled, identified, and corrected prior to feed ever going into the melter. Any research effort performed in support of delisting and LDR compliance must be integrated with development of the QGCR so that, in turn, it will be integrated into the WTP process control strategy.

1.4 Approach to Risk Assessment

Risk assessment is only indirectly relevant to the development of glass testing data. Risk assessment is used to calculate draft delisting levels. After testing data are developed for simulant wastes, they are compared to the risk derived levels. Based upon this statistical comparison, additional samples could be required to demonstrate compliance with the delisting levels in accordance with statistical parameters specified as part of this DQO. For an LDR treatability variance, a petition must show that the vitrification process either minimizes risk to human health and the environment, or it is inappropriate to comply with the numerical performance standards. In the WTP case, the argument is that it is inappropriate to comply with numerical performance standards because demonstrating compliance would entail exposure risks associated with sampling and analysis of active wastes.

1.5 Historical Research and Technology Results

In order to determine the effectiveness of the treatment process, WTP contracted with independent analytical laboratories to evaluate the constituents present in feed waste from tanks, simulated wastes, and treated feed materials. As noted above, considerable work has been completed on modeling and

confirming the model for preparation of glass to meet the PCT requirements. Limited work has also been completed on a similar model for TCLP metals and other leachable inorganic constituents. R&T work has also been performed to assess organic destruction across the melter system. These data will be further developed through crucible, bench, and pilot scale process testing that will be conducted using the outcome from this DQO.

The strategy for historical analyses of the waste composition has been to perform tests of glass compositions that mimic the pretreated waste from expected feed envelopes specified in the list below.

Feed Envelopes

	Envelope A			Envelope B ^(a)		Envelope C		Envelope D ^(b)	
Tank Waste Sources ^(c)	AN-105 AN-103 AP-104/ SY-101	AP-101 AW-101	AN-104	AZ-101	AZ-102	AN-107	AN-102	AZ-101 AY-102 /C-106 SY-102	AZ-102 AY-101/ C-104

^(a) Supernatant fraction of AZ-101 and AZ-102 tank waste.

^(b) Solids fraction of AZ-101 and AZ-102 tank waste.

^(c) from *Tank Farm Contractor Operations and Utilization Plan* (HNF-SD-WM-SP-012)

Formulations have been created to evaluate glass performance for these various target feed sources. Ongoing tests are being performed on simulants at the LAW pilot melter facility in Columbia, Maryland, and the HLW pilot melter at the Vitreous State Laboratory of the Catholic University of America (VSL). The results of initial testing show that spike factors of up to 500 times the UTS limits can be added before TCLP testing of the glass product results in leachate concentrations that exceed the LDR treatment standards. For example, simulated ILAW glass containing 1260 mg/kg of cadmium oxide yielded an average TCLP leachate concentration of 0.10 mg/L cadmium in duplicate TCLP analyses (see Appendix B, Table B-23). All other toxic metals tested leached at lower levels relative to UTS limits. These results are discussed in Appendix B of this document. Some non-RCRA metals, such as sodium, aluminum, boron, and iron, can drastically affect glass durability and resistance to leaching. These metals are, therefore, measured along with RCRA metals, and their affect on the glass is accounted for. This is discussed in greater detail in Appendix C, and subsequent discussions of TCLP response-model development. Additional testing will continue, and results will be used to demonstrate the performance of the glass against risk-based delisting criteria and LDR standards.

Selection of new glass formulations is guided by extensive past experience, as well as the glass-property models and database, which have been developed and are continuously updated. The development of viable glass formulations for each of the waste envelopes is an iterative process. Prospective glasses are formulated, melted in small crucible melts, and characterized to obtain the required property-composition information. The empirical data generated through each test run are used to update the glass models and formulation/property correlation, which provide the basis for the proposed approach.

Tank waste characterization data and glass product data are summarized in Appendix B. Much of the data generated through the research and technology (R&T) program was not intended to support compliance needs. Although much of the data are not supported by the necessary quality control (QC) records required for regulatory purposes, the data do, however, demonstrate the concept that vitrification is an appropriate technology for LDR treatment and waste delisting. Ongoing data collection, which will be defined through this DQO process, will be performed with the proper QC protocols developed through

the DQO process (see Section 3.3). Appendix H presents data that demonstrates the destruction of organic constituents during vitrification, and meets EPA analytical and quality protocols.

All active glass development, and much of the inactive glass development, was done on the crucible scale. In such cases, glass was formed by adding the proper glass formers to pretreated waste, or, in the case of inactive testing, a simulant made from representative oxide compositions of the waste feed. The glass composition is determined from the mass of batched chemicals, oxidation stoichiometry, and dissolution and chemical analysis. The mixture is calcified and then melted in a crucible to form glass. The calcification step mimics the plenum and cold cap reactions, and the subsequent melt is performed under temperature conditions that mimic actual melter operations. The melting process converts all components to oxides. The end-state oxide composition is independent of chemical form in the feed.

Unless indicated otherwise, the analyses described in the following subsections were performed by research laboratories to support WTP design. None of the analyses were performed according to strict SW-846 protocols and quality assurance requirements. Although the data may not be appropriate for demonstration of environmental compliance, they do provide information that can be used to establish vitrification as a viable treatment technology. Note that detection limits reported by the research laboratories are estimates based on a technical assessment of the analytical method by the analytical staff, and do not necessarily conform to SW-846 protocols. Likewise, undetected quantities do not indicate the actual absence of the compounds tested for, but do provide a reasonable lower limit for accurate quantitation of the constituent of interest for that particular analysis. Concentrations reported below the detection limit generally indicate a response on the analytical instrument below the lowest calibration standard. The values reported represent extrapolation of the calibration curve below the lower standard and are subject to great uncertainty. Appendix B should be consulted for additional detail.

The modifier "J" is commonly attached to an analytical result to indicate that the value is below the detection limit and therefore should be treated with less confidence than a result that is above the detection limit.

1.5.1 LAW Envelope A, B, and C Results

Laboratory personnel collected and analyzed samples from tank waste, intermediate feed material, and glass product from Tanks 241-AW-101, 241-AP-101, and 241-AN-103 to evaluate the makeup of the feed and effectiveness of the various process steps to remove or otherwise stabilize constituents in the Envelope A materials. As noted above, these analyses were performed to evaluate the overall performance of the process from a technical perspective. The analyses were intended to assess the quality of glass as a waste form, but were not intended to demonstrate compliance with specific regulatory criteria. Tank wastes evaluated for Envelope B included materials from Tank 241-AZ-102. Envelope C analyses were performed for feed wastes from Tanks AN-107 and AN-102.

No volatile organics, semi-volatile organics, PCBs, dioxins, or furans were detected within the limitations of the analytical method used in the glass samples from Envelope A product generated from treatment of feed from AW-101 and AN-103. No glass product analyses were available for product from AP-101. None of the TC metals analytical results exceeded TC limits. No glass product sample results are available for treated Envelope B materials. An analysis of glass product from Envelope C derived from AN-107 feed was also performed. A limited number of volatiles, semi-volatiles, PCBs, pesticides, dioxins, and furans were present at detectable concentrations in the feed materials. Analyses of glass product showed only the presence of 2-butanone (MEK) in the sample from the AN-107, at a concentration below the quantification limit, and well below the UTS for that compound. The presence of

MEK is likely the result of laboratory contamination. None of the samples from the Envelope C glass product were found to have TC metals at concentrations that exceed regulatory criteria. Consult Appendix B for specific results and references.

1.5.2 HLW Envelope D Results

Feed samples have been analyzed to characterize Envelope D wastes from Tanks C-104, C-106, AY-102, AZ-101, and AZ-102. Samples of glass product have been analyzed for treated waste from C-104 and AZ-102. No volatile compounds were detected in the glass samples within the limitations of the analytical methods used. One semi-volatile compound, bis(2-ethylhexyl)phthalate, was detected in both glass samples at concentrations less than the quantification limit (Sample 730J/110J $\mu\text{g}/\text{kg}$, quantification limit=1000 $\mu\text{g}/\text{kg}$). Bis(2-ethylhexyl)phthalate is a common plasticizer, however, and its presence may be due to contamination during sample processing. No PCBs, dioxins, or furans were detected in any of the glass samples within the limitations of the analytical methods used.

None of the TC metals results from the HLW glass samples exceeded TC limits. As indicated earlier, the results from historical tests such as this are included to demonstrate the concept that vitrification is capable of immobilizing inorganic waste constituents. The data collected as part of the implementation of this DQO will be used for compliance demonstrations. Consult Appendix B for specific results and references.

1.5.3 Simulant Testing

The Vitreous State Laboratory of the Catholic University of America performed small-scale melter tests (i.e., 10 kg glass/day production rate) on WTP non-radioactive waste simulants (LAW-A, LAW-C, and HLW-D) spiked with selected hazardous organic constituents (TRPT-W375-99-00002). The waste simulants were formed to mimic actual tank waste.

Feed samples were analyzed for spiked organic compounds, anions, and total glass formers. Each glass sample underwent complete inorganic compositional analysis, TCLP procedures for metals and organics, and organic analysis for VOCs, semi-volatile organic compounds (SVOCs), and dioxins and furans.

Appendix B presents data substantiating vitrification as a viable treatment technology for Hanford tank wastes. The data presented is research grade (e.g. not necessarily compliant with standard environmental analytical protocol and quality requirements), but it does provide evidence that organic compounds do not survive the vitrification process. All total organic results from glass samples were below quantification limits, except for small amounts of acetone, methylene chloride, chloroform, vinyl acetate, carbon disulfide, and naphthalene. Only acetone and methylene chloride were detected above reporting limits. These volatile organics are considered common laboratory contaminants that are likely in the glass sample results, due to sample handling. Other evidence that the compounds are a result of laboratory contamination include results from TCLP that are not consistent with total analyses for these compounds (the total should show $20 \times$ concentration from TCLP), and detection in the sample correlates to shipment (batch) numbers. Even if the results are taken at face value, the detected levels are below LDR limits. There were no traces of any of the spiked compounds (benzene, trichloroethene, and phenol) in any of the glass samples. No dioxins and furans were detected in glass samples.

All results for organics were well below TC limits and UTS criteria. Appendix B contains a more detailed discussion of the simulant test results.

Appendix H provides additional data demonstrating the destruction of organics in the vitrification process. The data show that even when added to the melter feed and substantially high levels, organics, and organics compound decomposition products are not retained in the glass product. With two minor exceptions (toluene and carbon disulfide), all detected organics compounds were identified as laboratory contaminants. All detected compounds were below reporting limits, and the results reflect the limits of the analytical technology. Although toluene and carbon disulfide were detected in the glass, the levels are so low that there is a clear demonstration that vitrification does destroy organics. The data presented are from analyses performed by a commercial environmental laboratory, and comply with SW-846 protocols and quality control.

The glass that is discharged from the melter is resident in the glass pool at a temperature of ~1150 °C for an average time of several hours; the residence time will be even longer for the actual WTP melters. Since the experimental glass with a shorter residence time did not contain measurable VOCs (excluding common laboratory contaminants), it is extremely unlikely that the discharged glass product would contain VOCs at concentrations that approach regulatory criteria. None of the glass analyses showed organics in amounts above the reporting level based on either TCLP or total analysis. Some common lab contaminants were found, but even these are below LDR limits and proposed delisting limits presented in Section 3. Toxicity Characteristic inorganics' concentrations were significantly below UTS limits and proposed delisting limits presented in Section 3. Refer to Appendix B, Tables B-16 through 19.

1.5.4 Glass Formulation Testing

VSL performed additional testing of LAW glass formulations developed around specific tank wastes or blends of tank wastes in order to optimize the properties of the glass for compliance with contract specifications and process requirements (Muller, Buechele, and Pegg 2001). For each RCRA metal analyte, formulations were spiked with from 100 to 10,000 times the corresponding threshold concentration listed in the UTS. Spike factors of 100 and 1,000 were used for elements for which the UTS limit is above 0.5 ppm, while factors of 1,000 and 10,000 were used for elements with a UTS limit below 0.5 ppm. TCLP analysis was used to determine the leach resistance of glass produced from these formulations. In all cases, the concentrations of the TCLP metals in the LAW glass leachate did not exceed the UTS limits.

Additional testing was conducted to evaluate the leachability of TC metals from HLW glass formulations (Gan and Pegg 2002). These formulations were not spiked, but were based primarily on best estimates of feed compositions from candidate waste tanks and LAW pretreatment products. All of the HLW glasses performed satisfactorily when compared against the TCLP limits. When compared against the UTS limits, however, the results indicate that cadmium can exceed the UTS criteria of 0.11 mg/L, especially for glass with much more than 0.5 wt% of CdO.

These types of observations have been integral to understanding the leach behavior of metals and building the TCLP leachate models. The data collected to date show that cadmium has a high intrinsic release rate from the glass. This fact, combined with the relative abundance of cadmium in some candidate feeds to the WTP, has prompted the WTP to pay close attention to cadmium to be sure the eventual glass formulations will meet the delisting criteria. A statistical model will be used to ensure an adequate margin of error is built into the QGCR.

This series of tests also included evaluations of various physical parameters of the glass. A summary of these reports is included in Appendix B.

1.6 Glass Chemistry and Leachate Modeling

Vitrification is a viable treatment technology for the tank waste because it volatilizes and destroys organic constituents, and incorporates the inorganic waste constituents directly into the final waste form through covalent and ionic chemical bonding, forming a leach resistant solid. Understanding glass structure and its resulting properties is fundamental to understanding the advantages of vitrification as a treatment technology. This section provides an summary of glass properties and describes “how” glass is used to immobilize hazardous constituents. The discussion that follows provides a general background on glass chemistry and leach behavior. A more detailed description can be found in Appendix C.

1.6.1 Basic Glass Structure and Principles

Glass is a rigid, noncrystalline material of relatively low porosity, often composed primarily of silica, alumina, and oxides of alkali and alkaline earth elements. Glasses are produced by melting previously formed glasses called frit or raw glass forming materials to produce molten glass. The molten glass is subsequently cooled to a rigid condition without crystallization, that is, without long-range molecular order (Doremus 1994). Glasses are composed of three-dimensional networks consisting primarily of tetrahedrally coordinated orthosilicate monomers (SiO_4^{4-}), each silicon atom bonded to four oxygen atoms (see Figure 1-5).

Most inorganic oxides can be incorporated into silicate glasses. Elements that can replace silicon are called network formers. Most monovalent and divalent cations, such as sodium, do not enter the network, form ionic bonds, and are called network modifiers. Boron is a valuable additive (primarily as a network former) that improves durability and is thus commonly used in waste glass.

Hazardous inorganic constituents can be immobilized in vitrification processes by two main interactions with the glass matrix: chemical bonding and encapsulation. In most waste glass, the waste constituents are chemically bonded. Certain inorganic species can be immobilized by chemically bonding covalently with oxygen or silica as network formers. Additionally, ionic bonding also incorporates inorganic constituents into the glass matrix (network modifiers); however, it changes the glass properties.

Section 7.5 provides a discussion of how testing data will be collected to demonstrate that the glass complies with LDR and delisting criteria. Appendix C provides additional information of the incorporation of network modifiers and formers into the glass matrix.

1.6.2 Glass Composition Region of Interest

There are a large number of composition variables that are relevant for waste glasses. In order to simplify this discussion, a reduced set of composition variables can be selected based on the structural roles of the underlying components in the glass matrix. The glass-melt properties will vary with the structural indicators that are employed. These variations can be illustrated graphically. Gross boundaries of glass stability or durability can be rationalized using structural information at the microscopic scale. Once these boundaries are established, the range of acceptable glass former and waste constituent concentrations are used to define a specific glass composition region of interest for glass formulation, production, and testing.

This approach has been very successful in defining the compositional constraints that are appropriate for development of composition models and glass formulations (DOE/CH9601). Testing is used to further refine the specific glass composition region of interest down to a QGCR that meets test criteria after accounting for applicable variations and uncertainties.

1.6.3 Glass Reactivity

Vitreous materials are relatively inert due to their high resistance to corrosion; however, they are subject to some chemical breakdown under severe conditions. There are two major forms of chemical attack on vitrified material: matrix dissolution and interdiffusion.

Matrix dissolution is generally caused by caustic attack (exposure to a high pH). It begins with the hydration of the silica network and liberation of water soluble alkali silicate (Na_2SiO_3), and may proceed to dissolution of the vitreous material (EPA 1992). Matrix dissolution occurs at the surface of the vitrified material.

Interdiffusion involves the ionic exchange of hydronium ions in solution for ionically bonded network modifiers in the glass. Interdiffusion generally leaves the silica structure almost intact (EPA 1992). Since the process is controlled predominantly by diffusion, the rate of leaching decreases as the thickness of the diffusion layer increases.

The effect of interdiffusion can be limited if the diffusion layer also begins to dissolve, for example, by matrix dissolution. In this case, the overall leach rate would be governed by the matrix dissolution. In other words, if there is dissolution of the outer surface of the diffusion layer, the layer will not be as thick; there will be less resistance to mass transfer by diffusion; and therefore, somewhat higher leach rates will result than without dissolution. If the rate of matrix dissolution were fast compared to interdiffusion, then a diffusion layer would never form. However, interdiffusion is generally the predominant mechanism and matrix dissolution rates are slow by comparison. This has been evident by the phenomena observed in actual tests.

The leach rates of individual constituents depend on their chemical properties and behavior under leaching conditions. However, actual leach test conditions represent a complex set of interdependent mechanisms such that they are better represented by a combination of general thermodynamic principles and data on observed behavior. These phenomena are the basis for development of leach response models like the preliminary TCLP model discussed in subsequent sections of this document. Additional discussion of these processes is provided in Appendix C. Section 7.5 provides a discussion of how testing data will be collected to demonstrate that the glass complies with LDR and delisting criteria.

1.6.4 Normalization of Data

In order to permit comparison of constituents on a common basis, data are typically normalized to glass composition. This comparison enables data users to quickly assess glass performance with regard to the degree of constituent immobilization attained for any particular waste loading and glass formulation. It also enables data users to compare the constituent release rate for glass formers, as well as constituents of concern. This approach to data reporting also makes sense as, generally, the release of element *i* depends on the amount of *i* in the glass. Normalized data are reported as a ratio of the concentration in the leachate versus that in the waste, or mass in leachate versus that in the waste. Data are presented in either a mass:mass or concentration:concentration ratio. Mass:mass is often presented as ppm in leachate versus

the weight percent in the waste. If one desires the mass:mass ratio to be in ppm, the weight percent is converted to ppm, by multiplying the weight percent by 10,000.

1.6.5 Intrinsic Release Rates

Resistance of a glass to leaching can be thought of as an intrinsic glass property. The glass inherently retards leaching because the waste constituents are covalently and ionically bonded within the matrix. The leach rate of each constituent is primarily a function of the coordination number and amount (percent oxide) of the constituent in the glass. Coordination number, for the purposes of this document, is defined as the number of neighboring atoms in the glass structure to which a given element is bonded. For simplicity, the release rate for each hazardous constituent can be compared to that of boron, the most abundant and mobile of the glass formers used in WTP glass. The following categorization of metals can be deduced from the experimental data to date (Gan and Pegg 2002).

- **Group 1: Advanced Elements** [Release=1, relative to boron release]

Barium	Manganese
Cadmium	Nickel
Calcium	Potassium
Cobalt	Silver
Copper	Strontium
Lithium	Uranium
Magnesium	Zinc

- **Group 2: Retarded Elements** [Release ~ 1/4, relative to boron release]

Antimony	Silicon
Lead	Thallium
Selenium	

- **Group 3: Slow and Irregular Elements** [Release ~ 1/10, relative to boron release]

Aluminum	Iron
Arsenic	Zirconium
Chromium	

The relevance of this categorization is that it helps to simplify overall glass response (constituent leachability) to the TCLP. Glasses with a lower boron release are intrinsically more leach-resistant. Boron leachability can be used to assess glass performance early in the testing program to determine if additional development work is warranted. These characteristics are discussed in greater detail in later sections and in Appendix C.

1.6.6 TCLP Response Models

The Vitreous State Laboratory of the Catholic University of America has conducted a series of experiments with glass formulation and TCLP leachate concentration in order to assess the performance of glass from a RCRA perspective (Gan and Pegg 2002). While only the concentrations of RCRA metals are routinely measured in the TCLP, the data used in the present work also included all of the major glass constituents. The inclusion of these elements provides valuable information on the way in which the glass dissolves under TCLP conditions. Findings from this work have shown a correlation between glass formulae (sum of waste and contributions from glass-forming chemicals) and TCLP leachate concentration.

The previous grouping of constituents into "advanced", "retarded", and "slow/irregular" elements, based on their TCLP release rates, suggest a correlation that can be incorporated into models which can be used to predict glass TCLP performance, and assess the potential performance of a theoretical glass. Essentially, for each constituent, the estimated release, plus the allowance for uncertainties, must be less than the delisting limit. For evaluation of the TCLP leaching versus the delisting levels, the leaching can be summarized as the:

$$\text{Release} = \% \text{ in glass} \times \text{Normalized release}$$

while

$$\% \text{ in glass} = \% \text{ in waste} \times \text{waste loading} \times \text{retention.}$$

and

$$\text{waste loading} = \text{wt. of feed} / (\text{wt. of feed} + \text{wt. of glass formers})$$

Retention is a factor for the likelihood that the material will be retained in the glass, versus moving into the gas phase. Volatile compounds or elements, such as mercury, that may be lost due to their volatility, will have less retention, and will result in the appearance of release; however, the release is not into the leachate, but into the melter offgas that is subsequently processed through air pollution control devices.

As previously discussed, the release rate can be assessed relative to the release of boron. Table 1-3 lists the waste tank or envelope, glass formulation as discussed in Gan and Pegg (2001), and the corresponding normalized release rate based on boron.

The relative release rate can then be used to estimate the constituent of potential concern (COPC) oxide levels that would be allowed in the glass before the delisting level would be exceeded based on TCLP leaching. The following formula shows the calculation of the COPC oxide level for inorganics.

$$\text{COPC Oxide Level} = \text{Delisting Level} \div [(\text{Group Rate}) \times (\text{Norm. B Rate}) \times (\text{Oxide Factor})]$$

where:

Norm. B Rate: Normalized boron release rate. This is the concentration of boron released to the TCLP leachate over the duration of the test, normalized by dividing the concentration of boron in the glass sample. Normalization can variously employ concentrations on a mass-per-mass or mass-per-volume basis.

Oxide Factor: For a given element, the ratio of the mass of that element in one mole of its oxide to the mass of one mole of its oxide.

1.7 Conceptual Model

To support identification of DQOs, a conceptual model describing the material to be sampled is formulated based on the background information available. The conceptual model is meant to provide a short, cohesive description of the contamination problem (in this case, vitrified glass) and the associated pathways and mechanism of COPC release. The conceptual model is helpful in defining study boundaries and focusing the problem statements and decisions on the relevant issues.

The conceptual model of the vitrified material assumes it is homogeneous, will meet the relevant health-based delisting levels or LDR requirements, and that treatment effectively mitigates the health and safety concerns associated with the listed wastes. The current assumptions, which are supported by preliminary research and technology (R&T) results, are that the organics will be removed or destroyed during the melting process. Volatile metals (for example, mercury and selenium) will either be in the offgas and appropriately trapped in scrubbers, or will be captured as oxides in the glass. Metals and other ions will be bound into the glass matrix, and will not leach in concentrations greater than levels that are acceptable for compliance with either delisting or LDR criteria.

1.8 Exposure Scenario

The following section describes the approach that was used to develop exposure scenarios consistent with the requirements for compliance with delisting and LDR program needs.

1.8.1 Delisting

A successful petition to delist the glass waste form must demonstrate that the waste form does not present a threat to human health or the environment. This demonstration will be made primarily by comparing the concentrations of hazardous constituents that could leach from the waste against health-based levels for those constituents. The EPA has incorporated the use of a computer model into their process for evaluating the concentrations of treated waste materials to determine suitability for delisting (EPA 1993b). The computer model used for delisting assumes the waste is disposed of in a solid waste landfill, and that a remote user consumes groundwater contaminated from leachate. The EPA has recently adopted a new model for delisting entitled *Delisting Risk Assessment Software* (DRAS) (EPA 2000b). This model is based on an update of the EPA Composite Model for Landfills (CML), entitled the *EPA Composite Model for Leachate Migration and Transformation Products* (EPACMTP) (EPA 1995). The new DRAS/EPA CMTP was used in the evaluation for this DQO.

Delisting levels are back calculated using the DRAS, which gives results based on the EPACMTP (EPA 2000b). Inputs include projected maximum waste generation rates, landfill lifetime, and target cancer risk and hazard quotient (HQ). Models used for delisting assume the waste is disposed in a solid waste landfill and a remote user consumes groundwater contaminated from leachate. The DRAS model contains risk assessment information used in the calculations. The model uses the oral reference dose and cancer slope factors taken from the EPA's Integrated Risk Information System (IRIS), when available, and a variety of other sources when the data are not available in IRIS (EPA 1996).

The DRAS back calculates a chemical-specific delisting level based on target cancer risk and HQs, annual volume of waste production, landfill lifetime, and chemical-specific information. The software calculates a chemical-specific dilution/attenuation factor (DAF) and delisting levels by multiple groundwater and surface exposure pathways. The following groundwater pathways are the primary exposure routes for the COPCs:

- Groundwater ingestion
- Groundwater dermal exposure for both an adult and child
- Groundwater inhalation

The DRAS model evaluates exposure via several groundwater exposures, in addition to the single groundwater exposure route (ingestion) considered previously. It also considers exposure to groundwater via dermal pathways for both adults and children (showering), and inhalation of materials volatilized from contaminated groundwater. Several of the delisting levels provided in Table 3-7 are based on child dermal exposure, and at least one (chloroform) is based on inhalation. The DRAS model also calculates maximum total concentrations that would be allowable in the waste based on runoff into surface water and subsequent ingestion of surface water, air particulate and air inhalation pathways, as well as fish and soil ingestion pathways.

A delisting level associated with each pathway is calculated and the most restrictive level is highlighted. A delisting level based on a drinking water standard (if one exists), multiplied by the chemical-specific DAF, is also calculated and reported. Additional discussion and presentation of the delisting limits, based on this approach, are presented in Section 3.2.

The EPACMTP uses a Monte Carlo (probabilistic) approach to calculating chemical specific DAFs. The inputs to the model are based on distributions of sizes of landfills, rainfall, soil conditions, distance to groundwater, distance to a drinking water source, and other factors. This approach is based on national data and the model calculates a DAF that will be more conservative than the actual situation 90 % of the time.

In some cases, the EPA's recent delistings have been based on maximum contaminant levels (MCLs) for some metals. Implicit in this approach is exposure and consumption of contaminated groundwater.

In summary, the approach to establishing a DAF and associated health-based delisting level for constituents of interest considers exposure to contaminated groundwater (via land disposal unit leachate) with varied exposure scenarios. The impact of the distinct exposure routes (groundwater dermal/groundwater ingestion) is considered in the determination of health-based delisting levels. This approach is discussed in greater detail in Section 3.2.

1.8.2 Land Disposal Restrictions

The LDR program in 40 CFR 268 prohibits the disposal of hazardous waste that has not been treated in accordance with standards specified by the EPA. Treatment standards include both performance-based requirements (numerical limits) and specified treatment technologies for identified waste forms. The regulations stipulate that the waste constituents, or constituents in treatment residues, must meet specified levels in order to dispose of the waste in a land disposal unit. A variance may be granted, however, if it can be demonstrated that it is inappropriate to require the waste to be treated to the level or by the method specified. For Hanford tank waste, the petition will be developed on the basis that compliance with LDR

through treatment to the specified level is technically inappropriate because of the human health risk associated with sampling and analysis required to demonstrate waste compliance. Furthermore, a treatment standard based on vitrification of Hanford tank waste meets the statutory requirements to:

“...substantially diminish the toxicity or substantially reduce the likelihood of migration of hazardous constituents from the waste so that short-term and long-term threats to human health and the environment are minimized.” (42 U.S.C 6924(m))

Due to the nature of LDR legislation, the development of an exposure scenario is much more relevant in the context of delisting, where the impacts of waste disposal activities are assessed as part of determining the health-based delisting levels. As such, data collected to support the health-based delisting data needs will be used to support the LDR treatability variance as well. These data will be evaluated to confirm vitrification minimizes risk to human health and the environment.

1.9 Resources and Constraints

The EPA guidance document for DQOs (EPA 2000a) recommends that project resources and constraints be considered prior to formulation of a problem statement. Such topics include project scope, budget, and schedule, as well as relevant issues. These topics are discussed in great detail in the supporting documents, *Approach to Immobilized Hanford Tank Waste Land Disposal Restrictions Compliance*, (RPT-W375LV-EN00002) and *Approach for Immobilized High Level Waste Delisting*, (RPT-W375HV-EN00001). For brevity, the reader is referred to the above referenced “approach documents” for a discussion of project resources and constraints.

1.10 Problem Statement

Current data are insufficient to support a determination that the IHLW will be suitable for delisting and the ILAW and IHLW comply with LDR criteria (that is, minimize threats to human health and the environment posed by land disposal) for a treatability variance. The data are also insufficient to verify the conceptual model, identified in Section 1.7.

The problem is to ensure that the R&T data collection approach will provide data that are adequate to support decisions for future petitions to justify vitrification as an alternative technology-based treatment standard under LDR for ILAW and IHLW, and for an upfront, conditional delisting for IHLW.

The following information provides context and support to the problem statement:

- Sampling of the treated waste forms, as required through a traditional compliance verification program, would require exposure of sampling and analytical personnel to dangerous levels of radionuclides on a consistent and ongoing basis.
- Dilution of the waste to levels that would result in acceptable exposure levels could also result in detection levels for COCs that do not allow meaningful comparison to regulatory criteria.
- For delisting, the intent will be to prepare a petition for an upfront, conditional delisting based on a technology demonstration showing that the vitrification process removes or stabilizes the COCs such that the delisting levels as determined by use of the DRAS model are met. This demonstration will be based on use of non-radioactive simulants. This approach is in contrast to the more traditional, up-front delisting, which would include collection of pre-operational data to support the delisting, followed by additional data collection from the treated glass form during operations to demonstrate

ongoing compliance. Because of the ALARA concerns associated with the treated IHLW glass, ongoing sampling of glass from operations is not practical.

- The goal for achieving compliance with the land disposal regulations will be to receive approval of a petition for a treatability variance that establishes vitrification as the specified method of treatment for Hanford tank wastes for all waste codes and hazardous constituents. The intent of the DQO process will be to identify the data needs to establish the suitability of vitrification for these wastes.
- Data generated through R&T activities will be used to determine the necessary processing requirements (e.g., QGCR, melter temperature) to ensure production of a compliant waste glass. The balance of this DQO process will establish the optimal approach for data collection to meet these needs.

Table 1-1 Regulation Crosswalk

The provisions found in the Federal RCRA regulations at:		Are contained in the analogous Washington State Dangerous Waste regulations at:		Topic
40 CFR Section	260	WAC 173-303	-010	Hazardous Waste Management System
	260.20		-910	Rulemaking Petitions - General
	260.22		-072	Petitions to exclude a waste produced at a specific facility
	261.20-.24		-090	Characteristics of Hazardous Wastes
	260.11 261.10		-110	References Test methods
	261.20(c)		-110	Sampling Methods
	No comparable provision		-100	Dangerous Waste Criteria
	261.31		-082 -9904	Hazardous Wastes from non-specific sources
	261.33		-081 -9903	Discarded Commercial Products, etc.
	268		-140*	Land Disposal Restrictions
	268.2		-140(3)*	Definitions
	268.40		-140(4)*	Applicability of Treatment Standards
	268.44		-140(6)*	Variance from a treatment standard
	268.48		*	Universal treatment standards

*Washington State has adopted by reference the provisions of the Federal LDR Program. WAC 173-303-140 contains additional requirements that apply to State-only wastes (EHW, organic/carbonaceous waste).

Table 1-2 DQO Planning Team

Organization	Company	Role
Environmental Protection Agency Region 10 (EPA)	Federal Regulator	Decision maker, regulatory authority, representation of national stakeholders
Washington State Department of Ecology (Ecology)	State Regulator	Decision maker, regulatory authority, representation of state and local stakeholders
U.S. Department of Energy, Office of River Protection (DOE-ORP)	Federal Agency	Decision maker, waste/petition owner, enforcement of DOE national policy
WTP Environmental Safety & Health (ES&H)	Bechtel National	Project lead, petition development, government contractor
WTP Research & Technology (R&T)	Bechtel National	Data development, oversight of research activities, government contractor
WTP Engineering	Bechtel National	WTP design, government contractor
WTP Statistical Support	Battelle	Statistical support, consultation, project integration with waste form qualification statistically based approach, project subcontractor
WTP Technical Support	Bechtel-SAIC	Consultation, government contractor
WTP DQO Facilitation	Environmental Quality Management Inc.	Facilitation, draft DQO document, project subcontractor

Table 1-3 Waste Tank/Envelope Glass Formulation and Normalized Release Rate Relative to Boron in the TCLP Leachate

Waste	Glass	Normalized B (ppm/wt%)
AZ-101, HLW	HLW98-31	0.20
AZ-102, HLW	HLW98-61	0.27
C106/AY-102, HLW	HLW-98-34	0.41
C-104, HLW	HLW98-51R	0.52
LAW A, B, C	Various	0.5 - 1.1

Figure 1-1 Simplified Generic Melter Diagram (Isometric Cut-Away)

(not to scale, for illustrative purposes only)

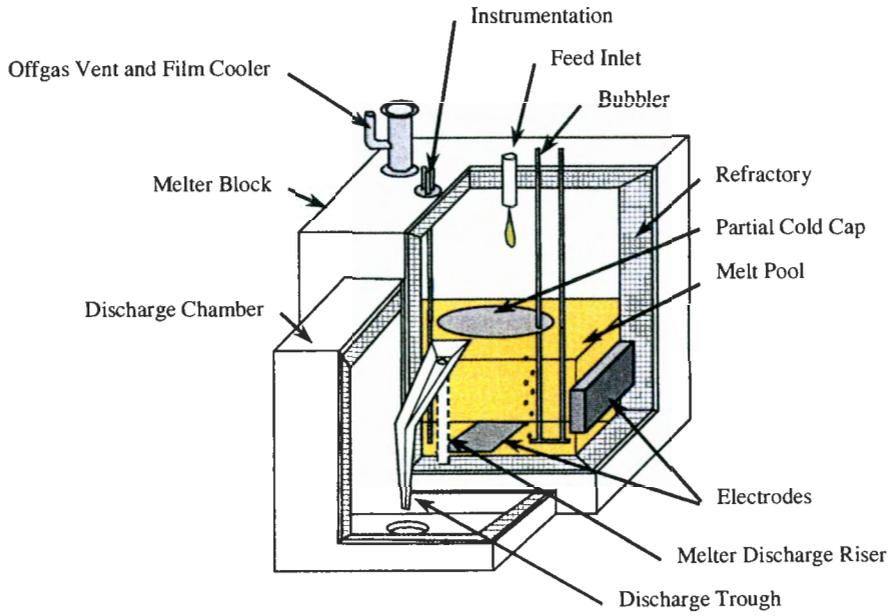


Figure 1-2 Simplified Schematic of the Qualified Glass Composition Region

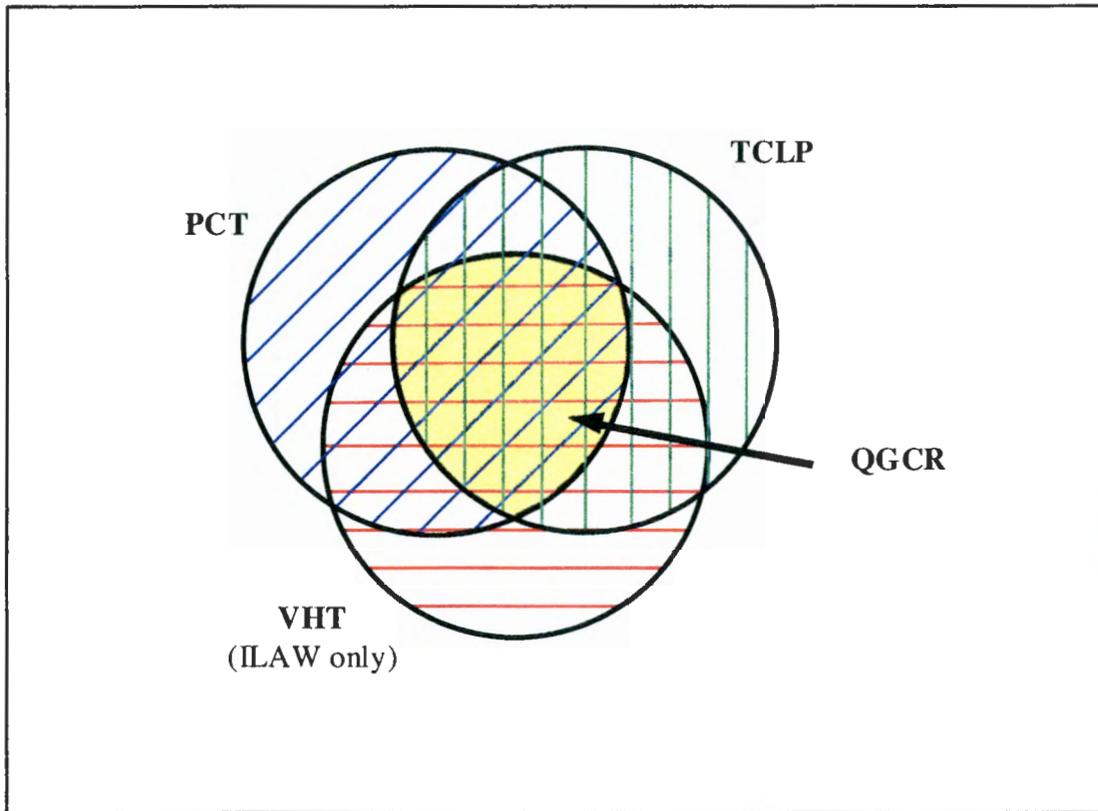


Figure 1-3 3-Dimensional Representation of Qualified Glass Composition Region for a Simple Hypothetical Glass

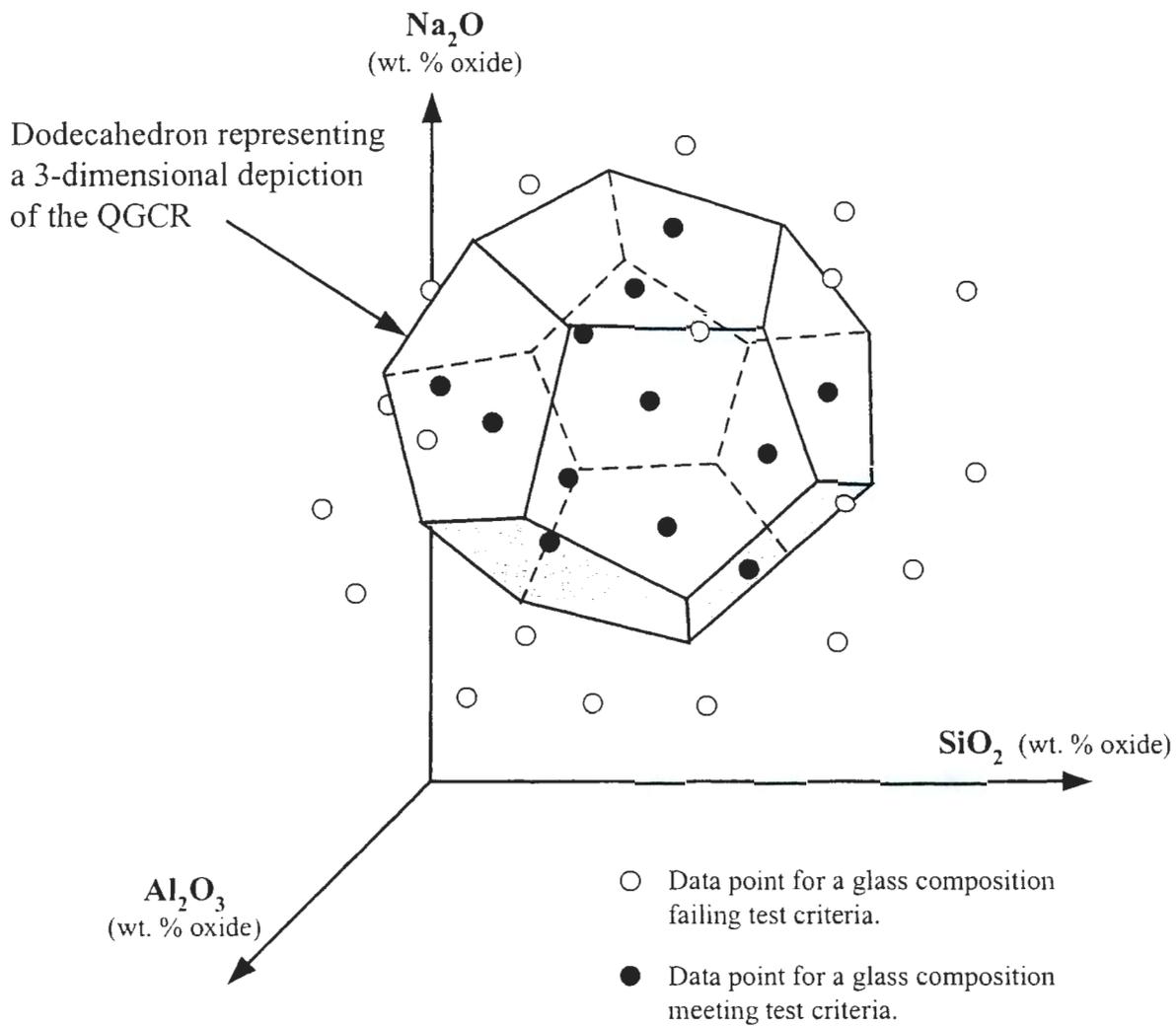


Figure 1-4 Integrated Research and Testing Program

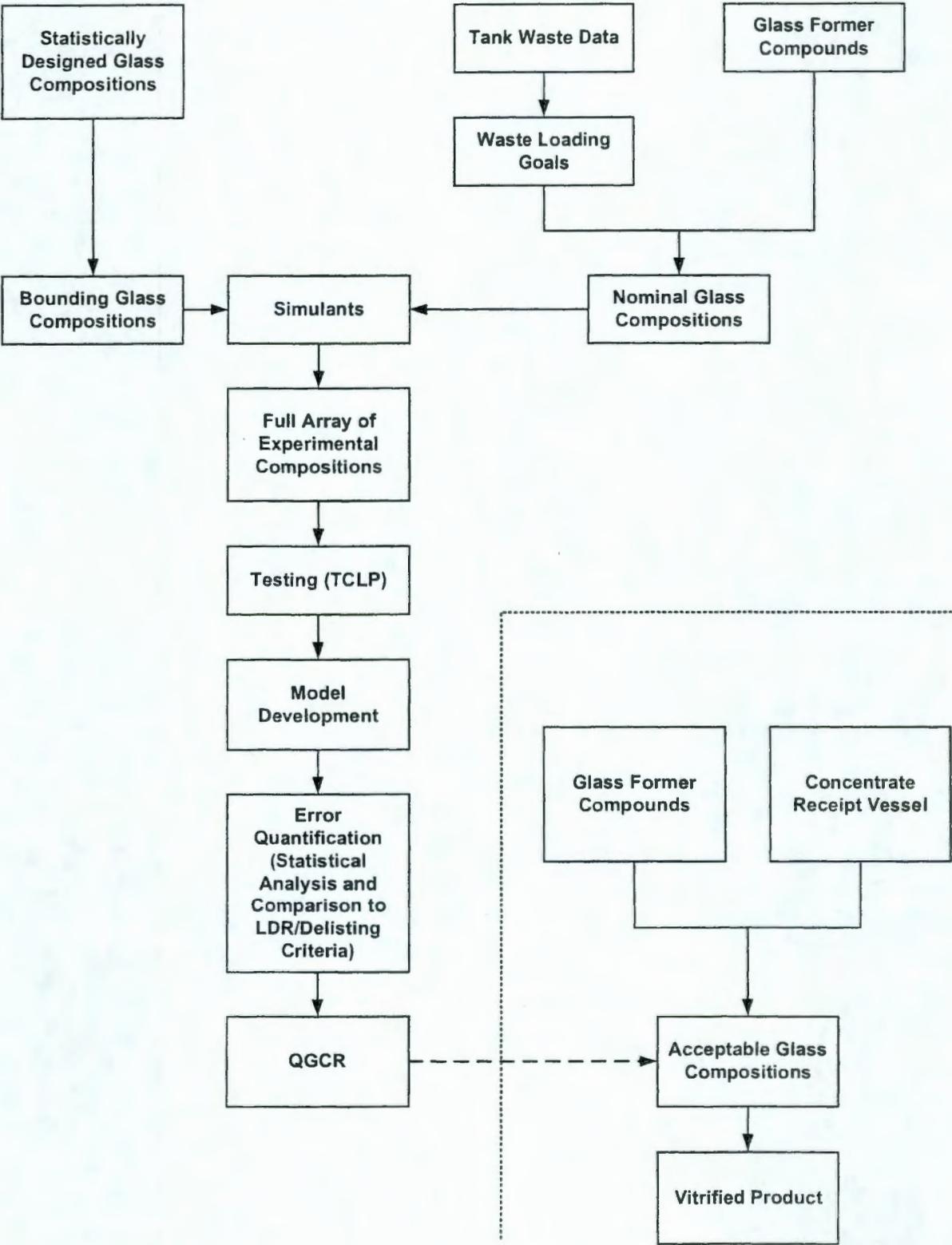
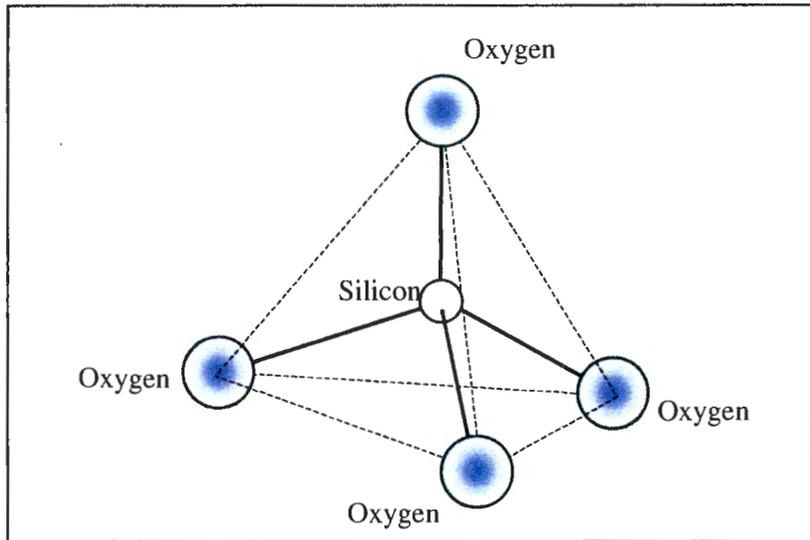


Figure 1-5 Tetrahedral Ortho-Silicate Monomer



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2 Step 2 – Decisions

The objective of DQO step 2 is to define the decision statements (DSs) to be resolved.

Principal study questions (PSQs) are derived from the problem statement. Alternative actions (AAs) are developed (including a no-action alternative, if appropriate) for each PSQ; these indicate the actions that could be taken after each PSQ is answered. For this DQO process, there are two PSQs—the first addresses issues related to the adequacy of data to support a delisting petition, and the second addresses demonstration of compliance with LDR requirements.

The PSQs and AAs were developed from the problem statement, and are listed in Table 2-1. Table 2-1 also presents the DS(s) which were developed by combining PSQs and AAs.

PSQ #1 will evaluate whether the data generated through the treatment of surrogate and actual waste are adequate to support a technology-based, up-front conditional petition to delist the HLW. If the data are adequate, the project will proceed with a petition to delist the HLW, based on the application of the technology. This petition will rely on a demonstration that vitrification will be capable of effectively treating any waste feed materials with a defined constituent makeup. The demonstration will be done primarily via upfront research and technology (R&T) testing of glass made from simulants spiked with surrogate constituents. The details of the R&T testing are key to the discussions in this DQO process. If the data do not support this approach, the project will decide whether it is more appropriate to develop an upfront petition that includes verification sampling during operations.

PSQ #2 is directed toward the decision of whether it is reasonable to move forward with a petition seeking approvals for vitrification as an LDR treatment technology for Hanford tank waste. This decision will be based on an evaluation of the results from simulated waste glasses, vitrified waste surrogates, and vitrified samples of tank waste to determine whether the treatment process (pretreatment and vitrification) treats the waste sufficiently to meet the goals of the LDR program. If the data support conclusively that the treatment process will enable the treated waste to meet LDR program criteria, then the project will move forward with a petition for a treatment technology (AA 2a). This conclusion assumes that adherence to the treatment process will inherently result in a compliant waste form. If the data are not conclusive, the project may decide to gather additional data (AA 2b). If the data cannot demonstrate that treatment will be consistently able to achieve compliance with LDR standards, then the project will demonstrate compliance through sampling of the treated glass product (AA 2c).

There are 2 scales of decision that apply to each decision statement. Decisions statements 1 and 2 must first be evaluated in the context of research data, i.e., do the research data support petition development for delisting and a treatability variance for a new LDR treatment standard? This is the focus of this DQO. The scale of the decision applies to the set of concentration boundaries that represent each envelope of waste based on the COPCs, glass formers, and modifiers.

The second scale of decision applies after the conclusion of the research program developed in response to this DQO. As described in subsequent sections of this DQO, the research will be used to determine the variety of suitable glass compositions that can be made from Hanford tank waste. In this case, “suitability” is defined by acceptable glass compositions, which produce a final waste form compliant with conditions specified by the petitions that are ultimately granted.

Table 2-1 PSQs and Associated AAs

#	PSQ	#	AA
1	Do the data support an upfront, conditional, technology-based petition for delisting treated IHLW?	1a	Yes - Proceed with an upfront, conditional, technology-based petition for delisting the IHLW.
		1b	No - Evaluate alternative strategies and identify and gather additional data to support delisting the IHLW through an upfront, conditional, technology-based approach or other means.
DS#1	Determine whether the data generated through the R&T program will support development of an upfront, conditional, technology-based delisting petition for the IHLW.		
2	Do the data support a treatability variance based on application of vitrification as a specified technology for the LDR-regulated constituents in LAW and HLW?	2a	Yes - Proceed with petition for a new treatment standard.
		2b	No - Identify and gather additional data to support an LDR treatability variance.
		2c	No - Do not proceed with petition and plan to meet existing treatment standards (for example, demonstrate compliance through WTP operations and sampling of glass product).
DS#2	Determine whether data from vitrified LAW and HLW support a treatability variance petition based on vitrification for the LDR regulated constituents in ILAW and IHLW.		

PSQ = Principal Study Question

AA = Alternative Action

DS = Decision Statement

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3 Step 3 - Identify Inputs

In order to generate responses to the principal study questions (PSQs), the members of the data quality objectives (DQO) team must evaluate available information and identify additional data needs. Critical information to consider includes the results of the research and technology (R&T) program activities that have been conducted to date and those that remain to be performed, identification of the constituents of potential concern (COPCs) that must be evaluated to determine the suitability of the glass product for compliance purposes, and the contractual and regulatory criteria that will provide the basis for this evaluation. Data that have been generated from the R&T program to date are summarized in Section 1.5 and Appendix B. Future R&T data generation needs will be determined through the balance of this DQO process.

3.1 COPCs Selection

The following sections present the logic that was used to identify the organic and inorganic COPCs for evaluation of the waste feed and its resulting glass product. Subsequent to the evaluation of analytical data generated by the R&T program, the project team will determine the appropriate list of COCs for monitoring during process activities.

Although the COPC selection process presented below results in the identification of several organic compounds as COPCs for delisting and LDR, organics are destroyed during vitrification primarily by pyrolysis or combustion (EPA 1992). There is currently no need for additional analytical data to support or verify organics destruction/volatilization during vitrification. The identification of COPCs in the sub-sections below is primarily to support the development of a delisting petition and LDR treatability variance that are complete in their consideration of all possible tank waste constituents, including underlying hazardous constituents.

3.1.1 COPCs Selection for Delisting

Figure 3-1 summarizes the approach used to identify the COPCs for delisting. The selection of COPCs for delisting has been conducted using the detailed logic in Figure 3-2 and Figure 3-3; the tables of organic compounds that are referenced in these figures are found in Appendix D, except for the final lists of COPCs that are provided in Table 3-1 and Table 3-5. All tables and queries are linked to a database and designated by a "Q" (listed in the table captions). This database was compiled to implement the Regulatory DQO (Wiemers, Lerchen, Miller, and Meier 1998). The Regulatory DQO database allows users to sort and filter data based on a number of possible queries. The text, figures, and tables provide the number of compounds that remain after each step illustrated in the flowchart. Decisions, designated by "D", are numbered for ease of discussion. A database similar to the Regulatory DQO was created to support Delisting and LDR.

The input list for the selection logic included the UTS compounds identified in 40 CFR 268.48. The constituents from the DST Part A permit application were also added. The DST Part A includes a waste code for multi-source leachate (F039) as derived from non-specific source wastes F001 through F005. Compounds that solely relate to F039 have not been considered because F039 coded waste has not been placed in the tanks. Therefore, should F039 waste codes be placed in the tanks, the LDR/Delisting DQO would need to be revisited. In addition, the Appendix VIII constituents, per 40 CFR 261, and select additional compounds identified in the EPA Delisting Guidance Manual (EPA 1993b), were added.

For many compounds, the regulatory lists present isomers or classes of compounds; an example is cresol. Although isomers and total cresol are listed in the regulations, total cresol was substituted for each isomer in the COPCs list. For general categories of dioxins that do not have a Chemical Abstracts Service (CAS) number listed in the original regulatory list, 2, 3, 7, 8 tetrachlorodibenzo(p)dioxin (TCDD) was substituted; 2, 3, 7, 8 TCDD is listed in risk databases as the most toxic of the dioxins. The Appendix VIII list presents a category of compound classes not otherwise specified (NOS). Since these classes cannot be tested, a typical compound was substituted for the NOS. This approach is consistent with the effluent treatment facility (ETF) delisting analyte selection logic (DOE-RL 1993b). For polychlorinated biphenyls (PCBs), some Aroclors are listed in the Universal Treatment Standards (UTS) list, and some are not. In this case, total PCBs were substituted for all the Aroclors.

Appendix D, Table D-1 shows the compounds that were substituted for the various categories, along with the origin of each compound in the consolidated starting list. This approach to substitutions for isomers is consistent with the Regulatory DQO and the ETF delisting approaches. Table D-1 (Appendix D) also shows the regulatory list from which each compound originated.

Following the above actions, all compound names and their CAS numbers were consolidated. This consolidation was performed because each list may use differing names for the various organic compounds and, in a few cases, incorrect CAS numbers are listed in the regulations. The compound name was taken to be the correct reference, and the corresponding CAS number was taken from national chemical databases. Table D-1 (Appendix D) lists the substitutions, the NOS compounds, and indicates the origin of the compound versus the regulatory list. For instance, some compounds are both on the Appendix VIII and the UTS lists, while others originate from only one regulatory list.

During the Regulatory DQO, extensive work was performed to remove compounds from consideration that were from industries not related to Hanford (Wiemers, Lerchen, Miller, and Meier 1998). The same approach was used for the ETF delisting petition (DOE-RL 1993b). Table B.16 from the Regulatory DQO process report listed these compounds. Compounds excluded from the Regulatory DQO that were determined not to have been used at Hanford are removed from further consideration here. The Regulatory DQO Process Industry Use Excluded Compounds are shown in Appendix D (Table D-2) (124 compounds). The decision to remove the compounds not related to Hanford was made at D-4 in Figure 3-2.

During the Regulatory DQO, extensive work was performed to remove compounds that were unstable in the highly alkaline, oxidizing, and high-radiation environment of the tanks. The list to be excluded was agreed upon by regulators and DOE-ORP during the Regulatory DQO Process. The 45 compounds listed in the Regulatory DQO (Table B.21) as unstable in the single-shell and double-shell tank matrices were excluded from consideration, and are listed in Appendix D, Table D-3. The decision to remove the unstable compounds was made at D-5 in Figure 3-3.

The Regulatory DQO (Table B.1) reviewed historical data from the Tank Waste Information Network System (TWINS) database and identified the detected compounds in Hanford Tank Waste. While not all the underlying hazardous constituents (UHCs) and DST Part A compounds have been quantified, the goal is to ensure that regulated compounds that have been detected in either the vapor, sludge, or liquid of Hanford tank waste are not deleted from consideration. The detected list of regulated compounds was checked against the list of TWINS compounds for further evaluation, and it was verified that these detected compounds remain on the list. No compounds were deleted from consideration based on this evaluation. Table B.1 from the Regulatory DQO is not included here.

During the development of the testing approach after the Regulatory DQO meetings, three compounds were removed from further consideration; this agreement is documented in meeting minutes (Dahl 2001). Of the three compounds, only methyl isocyanate was on the COPCs list at that point in time. Based on the agreement, methyl isocyanate was removed from further consideration (Figure 3-3, Q7b). Since this is a single compound, no table lists the compound.

During the Regulatory DQO, regulators and DOE-Office of River Protection left the chlorinated pesticides and herbicides on the list for consideration. It was agreed that these compounds would be evaluated for stability in the tank waste matrix. Other pesticides were removed based on industry usage, as previously discussed. Only the chlorinated pesticides and herbicides that are stable in tank waste and are on the applicable starting list were retained in the final compound list.

The last decision in the selection logic, D-6, evaluated the list of compounds remaining for consideration using the same stability assessment as in the Regulatory DQO. The question considered in D-6 is whether the compound is stable in the highly alkaline, oxidizing, and high-radiation environment of the tanks. Of the original 315 compounds, 138 were removed for instability (Appendix D, Table D-4). Table D-4 outlines the logic for the removal of each compound, including a summary of the reactive functional group and how it reacts (for example, amines readily oxidize), and a basis for the instability assessment. The term "organic text" refers to any standard text normally used in college-level chemistry. When the basis for removal is found on a web site, the table lists the web site that provided the information used in the instability assessment.

Table 3-5 lists the 177 organic, metals, and organometallic compounds that remain on the delisting COPCs list. Of the 177 compounds and metals, there are 46 metals and inorganic compounds, 6 organometallics, and 125 organics on the list. The organometallic compounds in Table 3-5 were evaluated as to the cation (metal) that is in the compound. Current EPA methods analyze for the cation and/or anion that is part of the molecule, as opposed to the organic portion. The list of metals proposed for delisting is presented in Table 3-1.

Table 3-2 lists the metals and anions removed as COPCs from Delisting and LDR. Osmium is a very toxic, rarely used metal that was eliminated from consideration based on its removal during the Regulatory DQO process, based on the high toxicity of the metal and the fact that there is no reason to believe it is present in the tanks based on the Klem and Agnew publications cited in the Regulatory DQO.

In the glass, the anions will not be closely bonded to any single element, as they will associate with various alkali or alkaline earth metals. This means that the inorganic compound will not exist in the form listed in the regulations. In the glass, the cations will normally be in the oxide or silica form and will be in the tetrahedral bond system. Therefore, the cations will not be in the compound form listed in the regulations. This logic is similar to that used for organometallic compounds. The inorganic compound will not be stable and exist in the form listed in the regulations. Additional discussion pertaining to the remaining metals and anions that are the components of the inorganic and organometallic compounds are presented below.

Vanadium and zinc remain as delisting COPCs. Nitrogen is volatile and non-toxic and a major component of air, and is removed as a COPC. Sulfur will oxidize to sulfate, which is discussed subsequently. The following presents the logic used for the evaluation of whether analytical data are needed for ammonia, bromide, chloride, fluoride, nitrate and sulfate anions. Ammonia is extremely volatile and at the melter temperatures will not be present in the glass. A thorough search of 4 sources of

the information required by Delisting Risk Assessment Software (DRAS) discussed in Section 3.2 of this document was performed. The sources are listed below:

- Region 6 RCRA Delisting Technical Support Document (DTSD)
- Region 9 Preliminary Remediation Goals (PRGs)
- Appendix A of EPA Integrated Risk Information System (IRIS)
- LC50 toxicological data from the NIOSH Registry of Toxic Effects of Chemical Substances (RTECS) and Hazardous Substance Data Bank (HSDB) databases

The above sources did not provide sufficient human health risk information coupled with the added properties to allow calculations of the DRAS limits. In addition, the amount of risk presented by these anions is likely to be low as compared to the other metals and organics that remain as COPCs. A paper will be written to provide additional details regarding the risk evaluation. Based on this approach no additional analytical data will be gathered for the bromide, chloride, fluoride, nitrate and sulfate anions.

Cyanide is the only anion that has a delisting level applicable to this project in the DRAS model. Cyanide has been reported in the tanks, and is identified as a COPC in a variety of inorganic compounds. While the EPA *Vitrification Handbook* (EPA 1992) indicates that “compounds such as cyanide...decompose to their constituent molecules and atoms, and then follow the path typical of inorganics...,” meaning that cyanide decomposes to carbon and nitrogen, it was felt that data showing the decomposition will be needed for the cyanide. Evaluation of LDRs with respect to cyanide, and cyanide complex compounds, can be done by evaluating total and amenable cyanide levels. Total cyanide analysis will also be used to represent cyanide and complex cyanide compounds for evaluation against DRAS limits for total cyanide. It is envisioned that spiking the simulant with KCN or NaCN and evaluating the result per the DRAS limit will provide the data to support its destruction.

Decision D-7 in Figure 3-3 represents the logic that will be applied to evaluate additional R&T data once they have been generated. All text inside the dotted line describes activities that will be performed after the initial R&T data are obtained.

3.1.2 COPCs Selection for LDR

Figure 3-4 provides a summary of the LDR COPC selection logic. The COPCs selection for LDR has been conducted using the logic in Figure 3-5 and Figure 3-6. Tables of compounds that are the basis for the logic steps in these figures can be found in Appendix D, except for the final lists of COPCs that are shown in Table 3-1 and Table 3-3. All tables and queries are linked to a database and designated by a “Q” (listed in the table captions). The text, figures, and tables provide the number of compounds that remain after each step illustrated in the flow chart. Decisions designated by “D” are numbered for ease of discussion.

The input list included the universal treatment standard (UTS) constituents, minus fluoride, sulfides, vanadium, and zinc; the resulting compounds represent the underlying hazardous constituents (UHC) list, based on 40 CFR 268.2(i). The constituents from the DST Part A were also added. Compounds that solely relate to F039 have not been considered because F039 coded waste has not been placed in the tanks. Therefore, should F039 waste codes be placed in the tanks, the LDR/Delisting DQO would need to be revisited.

The same process described for delisting was used with respect to the substitutions for isomers. For many compounds, the regulatory lists present isomers or classes of compounds. An example is xylene; all isomers and total xylene are listed, and total xylene was substituted for each isomer. Where dioxins were listed, 2, 3, 7, 8 tetrachlorodibenzo(p)dioxin (TCDD) was used; 2, 3, 7, 8 TCDD is listed in risk databases as the most toxic of the dioxins. For polychlorinated biphenyls (PCBs), some Aroclors are listed in the UHC list, and some are not. In this case, total PCBs were substituted for all the Aroclors. Table D-1 (Appendix D), previously mentioned, lists the compounds and their substitutions. Table D-1 also shows the compounds that originate from the UTS list and DST Part A, along with their substitutions; these compounds form the LDR COPCs starting list of 240 constituents.

Following the above actions, all compound names and CAS numbers were consolidated. This consolidation was performed because each list may use differing names for the various organic compounds and, in a few cases, incorrect CAS numbers are listed in the regulations. The compound name was taken to be the correct reference, and the correct CAS number was taken from national chemical databases. Table D-1 (Appendix D) lists the compounds used, as verified by the check mark for the UTS and the DST, Part A.

During the Regulatory DQO process, extensive work was conducted to remove compounds that were from industries unrelated to Hanford (Wiemers, Lerchen, Miller, Meier 1998). The same approach was used for the ETF delisting petition (DOE 1993b). Table B.16 from the Regulatory DQO lists these compounds. The same compounds are excluded from further consideration here. The decision was made at D-1 in Figure 3-5. Table D-5 (Appendix D) identifies the 71 compounds that were removed on the basis of not being used at Hanford.

During the Regulatory DQO process, extensive work was done to remove compounds that were unstable in the highly alkaline, oxidizing, and high-radiation environment of the tanks. The list to be excluded was agreed upon by regulators and DOE-Office of River Protection during the Regulatory DQO Process. The compounds listed in the Regulatory DQO (Wiemers, Lerchen, Miller, and Meier 1998, Table B.21) as unstable in the Hanford tank waste matrix were excluded from consideration (Appendix D, Table D-6). The decision was made at D-2 in Figure 3-6.

During the Regulatory DQO process, regulators and DOE-ORP left the chlorinated pesticides and herbicides on the list for consideration. During this DQO process, it was agreed that these compounds would be evaluated for stability in the tank waste matrix. Other pesticides were removed based on industry usage as previously discussed. Only the chlorinated pesticides and herbicides that are stable in tank waste and are on the applicable starting list were retained in the final compound list.

The Regulatory DQO (Wiemers, Lerchen, Miller, and Meier 1998, Table B.1) reviewed historical data from the TWINS database, and identified the detected compounds in the Hanford tank waste systems. While not all the UHCs and DST Part A compounds had been quantified, the goal was to assure regulated compounds detected in the vapor, sludge, or liquid of Hanford tank wastes were not deleted from consideration. The detected list of regulated compounds was checked against the list of compounds for further evaluation, and it was verified that these compounds remain on the list. No compounds were deleted from consideration based on this evaluation.

A similar process to evaluate the organometallics was performed for LDR COPCs as was performed for delisting, and a list of metals remaining as COPCs are shown in Table 3-1. Table 3-2 lists the metals and anions removed from consideration for LDR. Fluoride, vanadium, and zinc are removed from consideration under the UTS per footnote #5 in the UTS tables in 40 CFR 248.48. Footnote 5 in the UTS

tables indicate that these are not UHCs. Ammonia, bromide, chloride, nitrate, nitrogen, osmium, sulfate and sulfur are not on the UTS list and therefore logic for exclusion is not applicable as noted in Table 3-2.

The last decision in the logic diagram for LDR, D-3 (Figure 3-6), used the same stability assessment as presented in the Regulatory DQO and in the previous delisting discussion. Table D-7 (Appendix D) presents the 26 compounds that were removed as being unstable in tank waste. Table 3-3 presents the 99 organics. Table 3-4 lists the UTS limits for all LDR COPCs including 99 organics, 13 metals, and total and amenable cyanide that were maintained.

3.1.3 Test Compound Selection

Organics destruction has been demonstrated with previous research data (refer to Appendix H), and is also discussed in the EPA *Vitrification Handbook* (EPA 1992). Since organic compounds do not survive the vitrification process, there is no need for a research program to ascertain the level of organic compounds in the glass for comparison to DRAS derived delisting limits or universal treatment standards. Accordingly, no organic test compounds are identified.

Table 3-1 consolidates the metals recommended for analysis. All of the metals listed in Table 3-1 are recommended for testing. The metals were screened as discussed in the previous subsections of this document.

3.2 Performance Criteria

RCRA establishes the criteria by which the treated waste will be evaluated for compliance with the LDR and delisting programs. Criteria for the relevant COPCs are discussed below. The regulatory criteria are critical inputs to establish the basis for adequate treatment.

3.2.1 Delisting Criteria

EPA's Region 6 delisting Program developed the Delisting Risk Assessment Software (DRAS) (www.epa.gov/earth1r6/6rd/rcra_c/pd-o/midlo.htm#risk, EPA 2000b) model in order to evaluate delisting petitions in a timely fashion. This Microsoft Windows-based program analyzes the risks and hazards posed by the constituents of a waste petitioned for delisting. It provides a tool for regulators, which facilitates consistency in decisions and, at the same time allows for consideration of exposure pathways other than groundwater in the delisting decision. A description of the DRAS is provided below. The delisting action levels (ALs) are presented in Table 3-6 at the conclusion of the model description in the column titled "Delisting Level Using Rule". The following discussion presents an overview of the DRAS model, inputs to the model, and outputs from the model, as well as the resulting delisting criteria. The DRAS computations were performed for both organic and inorganic COPCs, although testing for organics is unwarranted since they are destroyed during vitrification. The DRAS derived delisting action levels are presented for the organic COPCs in Table 3-6 for information, and for comparison against the UTS limits applicable to the underlying hazardous constituents of a LDR waste form.

3.2.1.1 DRAS Description

The DRAS performs 2 types of analyses: screening-level analyses, and cumulative risk and hazard analyses. The screening-level analyses compute chemical-specific exit values, or "delisting levels", for multiyear delistings. The cumulative risk and hazard analyses compute the cumulative carcinogenic risk and non-carcinogenic hazard index for a waste petitioned for a one-time delisting. The delisting levels

and cumulative risk and hazard estimates are calculated using modeled, medium-specific, chemical concentrations, and standard EPA exposure assessment and risk characterization algorithms.

In addition to calculating the most limiting and most sensitive combination of exposure pathway and receptor, the DRAS provides the calculated chemical-specific delisting level for that combination. A delisting level is the maximum allowable concentration for each constituent of a waste petitioned for a multiyear delisting. For each waste constituent, the DRAS computes a total delisting level (mg/kg), based on a surface exposure pathway, and a TCLP delisting level (mg/L), based on a groundwater exposure pathway. The TCLP delisting levels for the groundwater exposure pathways are calculated with standard risk assessment algorithms, and with groundwater chemical concentrations at the point of exposure derived from waste volume-specific dilution/attenuation factors (DAFs) using the EPA *Composite Model for Leachate Migration and Transformation Products* (EPACMTP) fate and transport model. The chemical-specific total delisting levels for the surface exposure pathways are not expected to be significant factors in any decision relating to delisting of vitrified Hanford tank waste. The DRAS derived chemical specific concentration outputs for surface routes are higher than the groundwater pathway for all of the inorganic constituents of concern, except mercury. Mercury is a metal that tends to volatilize in the melter and very little retention of mercury in the glass is expected. The expectation that organic constituents of concern will not be detectable in the glass further supports the position that surface exposure pathways will not be significant to decision-making.

The analysis identifies the pathway-receptor combination that is the limiting combination or, in the case of multiple pathway-receptor combinations that fail the screening analysis, the most sensitive combination of pathway and receptor. The program also provides the calculated delisting levels for all pathway-receptor combinations.

Computing the cumulative risk for a petitioned waste provides the user with detailed analysis of the petitioned waste. The DRAS indicates which chemicals and which pathways or receptors are driving the risk for a particular waste. The DRAS computes the cumulative carcinogenic risk by summing the carcinogenic risks for all waste constituents for a given exposure pathway, and then summing the carcinogenic risks for each pathway analyzed in the delisting risk assessment. The DRAS computes the cumulative non-carcinogenic risk by summing the non-carcinogenic hazard quotients (HQs) for all waste constituents for a given exposure pathway, and then summing the non-carcinogenic hazards associated with each exposure pathway analyzed.

3.2.1.2 DRAS Model Inputs

Chemicals for which delisting levels are to be calculated must be specified. The model allows the user to select from a list of chemicals for which the DRAS has data. The COPCs (organic compounds, anions, and metals) that resulted from the delisting COPCs selection logic were entered into DRAS. Table 3-6 provides the results from DRAS for each compound. Note that because certain compounds, anions, or elements are not listed in DRAS, no delisting levels are calculated for these constituents. For select compounds, 1 or more isomers were input instead of the total (for example, dinitrotoluene was input to DRAS as 1,3-dinitrotoluene). When the sum of all isomers was listed in the selected COPCs, the isomers that provided the most conservative delisting levels were input to the model.

Other inputs to the DRAS include the volume to be disposed of in the landfill, the target HQ, the target cancer risk level, and whether the disposal unit is a landfill or a surface impoundment. For this project, 1000 m³/yr was used for the volume, a HQ of 0.25, a cancer risk of 10E-05, and a landfill were input. The HQ and cancer risk levels were selected based on DOE and regulator discussions in DQO Meetings.

The volume is based on disposal of the estimated inventory of IHLW. Note that, if ILAW is delisted, the volume will change and the model must be rerun due to the different disposal pathways. If ILAW were delisted 2 sets of delisting limits would be required, 1 for ILAW and 1 for IHLW.

Volume is input in 2 parts: the annual volume, and the landfill lifetime, or duration of disposal in the landfill. Multiplied together, these give a total volume for disposal. The DRAS results are dependent on the total volume, and not the individual input factors. For example, the same delisting level is calculated for a specific chemical, regardless of whether 20,000 yd³ are generated in only 1 year, if the generation is 1,000 yd³/yr for 20 years, or 5,000 yd³/y for 4 years.

The model also requires that maximum TCLP and total concentrations for each constituent be entered. These numbers are not used in the calculation of delisting levels, but are used in the development of the output tables described below. Because the information is required to get the program to run, place-holders were used for TCLP and total concentrations in lieu of actual data (which is not available) so that DRAS subroutines would run properly.

3.2.1.3 DRAS Outputs

The DRAS results are displayed on 4 screens, which are described below:

Chemicals Exceeding Delisting Levels

The model output includes a screen showing each chemical that exceeds the DRAS calculated delisting level. The maximum TCLP and total concentrations, which are required input data, are the basis for the comparison. In the case of a waste that has not been generated, this output screen is not useful. After more R&T data are generated from IHLW testing, the results from the leach tests can be compared to the DRAS delisting level to assess whether the delisting levels are exceeded.

Chemical Specific Results

The model calculates delisting levels for each of the following exposure scenarios:

- Groundwater ingestion pathway
- Groundwater adult dermal pathway
- Groundwater child dermal pathway
- Groundwater inhalation pathway
- Surface water ingestion pathway
- Air particulate pathway
- Fish ingestion pathway
- Soil ingestion pathway
- Air volatile inhalation pathway

For each chemical, the DRAS provides a pathway-allowable TCLP concentration (for the groundwater pathways) or total concentration, and a HQ or cancer risk level. In a few cases, the model will provide both hazard quotients and cancer risk levels for the same chemical.

Cumulative Results and Summary of Results

The DRAS provides cumulative results on a screen that lists each chemical and the risk, and then sums the risks to provide a total risk for the waste. The DRAS also provides a summary screen showing the total cancer risk and hazard index. Because the cumulative results are related to one-time disposals, this output was not used.

Printed Results

Printed results include 6 separate reports. The user can select individual reports to print.

The first report, the program report, contains basic information on the petition, including the site, petition identification, person running the program, batch identification, and the date of waste sample analysis. Not all of this information needs to be entered in order to run the model.

The second report is a compilation of input information.

The third report gives limiting pathways and concentrations.

The fourth report contains a risk and hazard index for each chemical via the groundwater pathway and surface pathway, and cumulative risk. In most cases, one pathway dominates.

The fifth report shows chemicals that exceed toxicity characteristic (TC), soil saturation, and ecological benchmark values. The report contains information on all input chemicals, and contains columns for TC, soil saturation, and ecological toxicity reference value, and indicates yes or no in each column for each chemical. The comparisons to soil saturation and ecological benchmark values were not used. The soil saturation is for surface dispersal, which all parties to this DQO process have agreed is not important. The ecological toxicity reference value is an aquatic toxicity value, and related to surface pathways, which do not apply to this delisting. The TC limits are listed and used.

The sixth report shows the waste concentrations exceeding allowable concentrations. This report is based on the information from TCLP and total results based on analytical data. Because waste has not yet been generated, this report is not useful at this time. This report may be used to evaluate the results of R&T analyses to assure that the treated waste will meet delisting levels.

Table 3-6 lists the CAS number, chemical name, the TC level from RCRA regulations, and the MCL, as applicable, the volume adjusted DAF from the DRAS model, the back-calculated TCLP limit, and various other back-calculated TCLP limits, based on various risk scenarios. The table also lists which compounds are carcinogens. The column entitled "DRAS TCLP Path Limit" lists the exposure pathway that is the limiting factor (lowest limit); for this analysis, the groundwater pathway was determined to be the most limiting. The MCL is adjusted for the volume and DAF. The final two columns provide delisting levels based on which limit presents the lowest concentration (MCL, DRAS, old CML model), along with the basis for the selection of the appropriate delisting level. The DRAS software contains the various potential action levels such as MCL, old CML, TC levels. The model calculates risk pathway based concentrations, compares these calculated concentrations to the various other potential action levels and selects the most limiting level as the delisting level. The column titled "Delisting Level Using Rule: MCL or DRAS, but TC Limited" in Table 3-6 provides the proposed delisting levels. Unless alteration of a model input is needed, these levels will be the ALs for the delisting petition.

The last column in Table 3-6 simply provides the lowest of the MCL, DRAS or TC limit. This data is useful for establishing target analytical detection limits in case the proposed delisting levels are rejected in favor of the most restrictive of the MCL, DRAS or TC derived action level.

3.2.2 State-only Criteria

Before waste can be shipped to the proposed federal repository, it must also be shown that it is not a dangerous waste (DW) or extremely hazardous waste (EHW) under Washington state-only requirements contained in WAC 173-303-070 and WAC 173-303-080 through 173-303-100. The *Waste Treatment Plant Waste Analysis Plan (WAP)* (24590-WTP-RPT-ENV-01-003) identifies the listed and characteristic waste numbers that the WTP will be permitted to receive. The listed waste numbers and contaminant specific characteristic waste numbers will be addressed individually, by demonstrating that the IHLW meets the proposed delisting action levels shown in the last column of Table 3-6. Note that in cases where the DRAS derived limit is greater than the toxicity characteristic concentration, the TC concentration has been identified as the proposed delisting action level. The waste feed to the WTP will carry the numbers for ignitable (D001) and reactive (D003) waste. The WAP states that:

However, based on past process knowledge, which includes the age, temperature, history, and chemical composition of the waste feed stored in the DST system unit, it is not expected to exhibit the characteristics of ignitability or reactivity found in WAC 173-303-090. After the waste feed has been received into the WTP, this process knowledge will be used to remove the dangerous waste number for ignitability and reactivity.

Additional information and process knowledge pertaining to the removal of the ignitable and reactive waste numbers are discussed in Section 3.6 of the WAP (Sipkowski 2001). Since ignitable or reactive materials are not added in the WTP process, the IHLW will not exhibit either of the D001 or D003 characteristic. Likewise, glass waste forms produced by the vitrification process will no longer be corrosive. This is consistent with EPA's determination under the Land Disposal Restrictions that vitrification of high level mixed radioactive wastes (HLVIT) was the specified treatment standard for mixed waste carrying the corrosivity waste number. Based upon this information, the D002 waste number will not apply to the IHLW or ILAW.

The state-only waste numbers carried by the waste feed to the WTP include WT01 (toxic dangerous waste - EHW), WT02 (toxic dangerous waste - DW), WP01 (persistent dangerous waste - EHW) and WP02 (persistent dangerous waste DW). The WAC regulations allow a person to determine if a waste meets the toxicity criteria by following book designation instructions or bioassay designation instructions. If the designation acquired from book designation and bioassay data do not agree, then WAC 173-303-100 (5)(d) specifies that bioassay data will be used to designate a waste. In 1997, samples of tank waste were vitrified and subjected to the biological testing. A report on the testing was submitted to the State of Washington Department of Ecology on January 5, 1998 (Smith 1998). The results of this testing are summarized in Appendix B, Section 4 of this DQO. The tests, which were performed on active immobilized low activity wastes, show that the vitrified product does not qualify for even the lowest toxicity category (category D) and is, therefore, not a dangerous waste or EHW based upon the State of Washington's criteria for toxic dangerous wastes. Similar testing for IHLW has not been done to date. Differing results for IHLW would not be expected given the insolubility of the immobilized waste and the requirement to meet similar TCLP leachate standards. Based upon the existing bioassay test data, the WT01 and WT02 waste numbers do not apply to the ILAW or IHLW.

The WTP waste feeds were originally designated as persistent waste (WP01 and WP02) by virtue of their containing either halogenated organic compounds (HOC) or polycyclic aromatic hydrocarbons (PAH) as defined under WAC 173-303-040. The destruction/volatilization of organic constituents during vitrification, including HOCs and PAHs, means that the vitrified waste is not a dangerous waste or EHW based upon the State of Washington's criteria for persistent dangerous wastes, and that the WP01 and WP02 waste numbers do not apply to the ILAW or IHLW.

3.2.3 LDR Criteria

In order for EPA and Ecology to approve a petition for a treatability variance for vitrification, the petitioner must show that the treatment process will minimize threats to human health and the environment (40 CFR 268.44). There are no regulatory limits associated with a treatability variance that establish a threshold level for approving a variance. For the purposes of R&T data collection and planning, the UTS limits and the predicted health-based delisting levels for COPCs resulting from the selection logic represent benchmarks to evaluate the effectiveness of treatment. Those limits are presented in Table 3-4.

3.3 Analytical Methods and QC

The WAC 173-303-110 and 40 CFR Part 261 Appendix III require the use of the methods described in SW-846 (EPA 1997) to analyze many of these compounds and constituents to meet the regulatory data needs. SW-846 allows some flexibility for using other established methods that have been developed by the EPA or the American Society for Testing and Materials (ASTM). The test methods listed in Table 3-7 will be used for analysis of inactive samples, simulants, and non-radioactive glasses. The sample collection, sample preparation, and analytical quality assurance (QA) or quality control (QC) associated with each analytical method listed in Table 3-8 and Table 3-9 will be required and will be implemented through this DQO, as cited in R&T test specifications to be developed in support of this project. In addition, a case-by-case comparison of method detection limits (MDLs) to regulatory criteria will be made for the test compounds to ensure that analytical results will support decisions.

The SW-846 methods have been developed to analyze water and soils. Due to the radioactivity and complex sample matrix for the tank waste, it is likely that the SW-846 methods will need to be modified or alternative methods selected, as stipulated under WAC 173-303-110. For most of the alternative compounds and constituents, minor to major modifications to the analytical methods will be required, or methods will need to be developed. The Regulatory DQO (Wiemers, Lerchen, Miller, and Meier 1998) was prepared to address the regulatory data needs for waste currently stored in Hanford waste tanks; this DQO addresses issues and uncertainties associated with analysis of Hanford's tank waste and establishes a path forward for its characterization. More detailed information is available in the Regulatory DQO (Wiemers, Lerchen, Miller, and Meier 1998) and associated testing strategy, *Regulatory DQO Test Plan for Determining Method Detection Limits, Estimated Quantitation Limits, and Quality Assurance Criteria for Specified Analytes* (Patello 2000). Generally, performance requirements of the Regulatory DQO will be required for radioactive tank waste matrices. TCLP leachate from active glass, a buffered acetic acid solution, is reported to be low in radioactivity, and will likely be analyzed by a licensed commercial laboratory capable of complying with SW-846 requirements. If analyzed in a research laboratory, the method of analysis will be subject to qualification as described by the WTP QAPjP for environmental/regulatory data (PL-24590-QA-00001).

These method-specific criteria agree with the criteria published in the individual SW-846 methods, when criteria are provided. When criteria are not provided specifically in an SW-846 method, they are adapted

from other methods because many of the criteria are the same from method to method. Table 3-8 and Table 3-9 provide the details of the method-specific QC criteria.

3.4 Method Detection Limits

Method detection limits (MDLs) will be determined in accordance with the MDL definition in Chapter 1, SW-846. This approach is the basis for the Regulatory DQO MDL determination. For laboratories that handle radioactive waste, the MDLs will either be determined in water/sand, or determined per the approach that is negotiated as part of the Regulatory DQO. For laboratories that are not handling radioactive waste, MDLs will be determined using water or sand. For glass compositional analysis (active or inactive), establishing detection limits using a standard glass matrix such as the NIST standard for glass analysis is preferred alternative to sand/water derived MDLs. For all laboratories, the MDLs will be documented by the laboratory and supplied as part of the quality system documents before analysis begins on the LDR/Delisting matrices.

3.5 Estimated Quantitation Limits

Section 5.4 addresses the comparison of action limits versus estimated quantitation limits (EQL). The goal is to establish EQLs that are below the action limits. Section 5.4 lists the analytes for which the EQL may be above the action limits and describes how this situation will be managed.

Table 3-1 Metals and Anions Proposed as COPCs for Delisting and LDR

CAS#	Metal/Cation/Anion	Based on Delisting	Based on LDR
7429-90-5	Aluminum	X	
7440-36-0	Antimony	X	X
7440-38-2	Arsenic	X	X
7440-39-3	Barium	X	X
7440-41-7	Beryllium	X	X
7440-43-9	Cadmium	X	X
7440-70-2	Calcium	X	
7440-47-3	Chromium	X	X
7440-50-8	Copper	X	
57-12-5	Cyanide	X	X
7439-92-1	Lead	X	X
7439-97-6	Mercury	X	X
7440-02-0	Nickel	X	X
7723-14-0	Phosphorus	X	
7440-09-7	Potassium	X	
7782-49-2	Selenium	X	X
7440-22-4	Silver	X	X
7440-23-5	Sodium	X	
7440-28-0	Thallium	X	X
7440-62-2	Vanadium	X	
7440-66-6	Zinc	X	

Table 3-2 Metals and Anions Removed as COPCs for Delisting and LDR

Metal/Anion	Basis for Initial Consideration as a Delisting COPC	Basis for Exclusion from Delisting	Basis for Initial Consideration as a LDR COPC	Basis for Exclusion from LDR
Ammonia	261 Appendix VIII ^(b)	Removed as will be gas and volatilize in the melter	NA	NA
Bromide	261 Appendix VIII ^(b)	Data required for DRAS input is not available	NA	NA
Chloride	261 Appendix VIII ^(b)	Data required for DRAS input is not available	NA	NA
Fluoride ^(a)	261 Appendix VIII ^(b)	Data required for DRAS input is not available	268.48 UTS	Removed as COPC 268.48 UTS footnote 5
Nitrate	261 Appendix VIII ^(b)	Data required for DRAS input is not available	NA	NA
Nitrogen	261 Appendix VIII ^(b)	Gas, non hazardous, removed.	NA	NA
Osmium	261 Appendix VIII ^(b)	Based on Regulatory DQO, not in feed. Not used at Hanford based on Klem and Agnew.	NA	NA
Sulfate	261 Appendix VIII ^(b)	Data required for DRAS input is not available.	NA	NA
Sulfide ^(a)		Not on the list	268.48 UTS	Removed as COPC 268.48 UTS footnote 5
Sulfur	261 Appendix VIII ^(b) EPA/R-93/007	Not included in DRAS modeling	NA	NA

Table 3-2 Metals and Anions Removed as COPCs for Delisting and LDR

Metal/Anion	Basis for Initial Consideration as a Delisting COPC	Basis for Exclusion from Delisting	Basis for Initial Consideration as a LDR COPC	Basis for Exclusion from LDR
Vanadium ^(a)	261 Appendix VIII ^(b)	Remain for delisting	268.48 UTS	Removed as COPC 268.48 UTS footnote 5
Zinc ^(a)	261 Appendix VIII ^(b)	Remain for delisting	268.48 UTS	Removed as COPC 268.48 UTS footnote 5

^a Fluoride, vanadium, sulfide, and zinc removed from LDR per 40 CFR 268.48, footnote #5, to UTS tables in regulations.

^b 261 Appendix VIII cites these as inorganic or organo-metallic compounds, however, analytical methods only analyze the separate cations and anions, and not the inorganic and organo-metallic compounds. Therefore, these metals, cations, and anions were evaluated. This is consistent with the approach used in the Regulatory DQO (Wiemers, Lerchen, Miller, and Meier 1998) for inorganic and organo-metallic compounds.

NA - not applicable

Table 3-3 Organic Compounds Remaining for LDR

CAS#	Constituent
100-21-0	p-Phthalic acid
100-41-4	Ethyl benzene
10061-01-5	cis-1, 3-Dichloropropene
10061-02-6	trans-1, 3-Dichloropropene
101-55-3	4-Bromophenylphenyl ether
106-46-7	1, 4-Dichlorobenzene
106-93-4	Ethylene dibromide
107-02-8	Acrolein
107-05-1	3-Chloropropene
107-06-2	1, 2-Dichloroethane
107-12-0	Propionitrile
107-13-1	Acrylonitrile
108-10-1	4-Methyl-2-pentanone (MIBK)
108-88-3	Toluene
108-90-7	Chlorobenzene
108-95-2	Phenol
110-86-1	Pyridine
117-81-7	Bis(2-ethylhexyl) phthalate
117-84-0	Di-n-octylphthalate
120-12-7	Anthracene
120-82-1	1, 2, 4-Trichlorobenzene
120-83-2	2, 4-Dichlorophenol
122-39-4	N, N-Diphenylamine
123-91-1	1, 4-Dioxane
126-98-7	2-Methyl-2-propenenitrile
127-18-4	1, 1, 2, 2-Tetrachloroethene
129-00-0	Pyrene
1319-77-3	Cresols (total)
1330-20-7	Xylene (total)
1336-36-3	Polychlorinated biphenyls (PCBs)
156-60-5	1, 2-trans-Dichloroethene
191-24-2	Benzo(ghi)perylene

Table 3-3 Organic Compounds Remaining for LDR

CAS#	Constituent
192-65-4	Dibenzo[a,e]pyrene
193-39-5	Indeno(1,2,3-cd)pyrene
205-99-2	Benzo(b)fluoranthene
206-44-0	Fluoranthene
207-08-9	Benzo(k)fluoranthene
208-96-8	Acenaphthylene
218-01-9	Chrysene
319-84-6	alpha-BHC
319-85-7	beta-BHC
319-86-8	delta-BHC
41903-57-5	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8)
465-73-6	Isodrin
50-32-8	Benzo(a)pyrene
53-70-3	Dibenz[a,h]anthracene
541-73-1	1, 3-Dichlorobenzene
56-23-5	Carbon tetrachloride
56-49-5	3-Methylcholanthrene
56-55-3	Benzo(a)anthracene
58-89-9	gamma-BHC (Lindane)
58-90-2	2, 3, 4, 6-Tetrachlorophenol
59-50-7	4-Chloro-3-methylphenol
59-89-2	N-Nitrosomorpholine
621-64-7	N-Nitroso-di-n-propylamine
62-75-9	N-Nitroso-N,N-dimethylamine
630-20-6	1, 1, 1, 2-Tetrachloroethane
67-64-1	2-Propanone (Acetone)
67-66-3	Chloroform
67-72-1	Hexachloroethane
71-43-2	Benzene
71-55-6	1, 1, 1-Trichloroethane
74-83-9	Bromomethane
74-87-3	Chloromethane

Table 3-3 Organic Compounds Remaining for LDR

CAS#	Constituent
75-00-3	Chloroethane
75-01-4	1-Chloroethene
75-05-8	Acetonitrile
75-09-2	Dichloromethane (Methylene Chloride)
75-15-0	Carbon disulfide
75-27-4	Bromodichloromethane
75-34-3	1, 1-Dichloroethane
75-35-4	1, 1-Dichloroethene
75-69-4	Trichlorofluoromethane
75-71-8	Dichlorodifluoromethane
78-83-1	2-Methylpropyl alcohol
78-87-5	1, 2-Dichloropropane
78-93-3	2-Butanone (Methyl ethyl ketone)
79-00-5	1, 1, 2-Trichloroethane
79-01-6	1, 1, 2-Trichloroethylene
79-34-5	1, 1, 2, 2-Tetrachloroethane
82-68-8	Pentachloronitrobenzene (PCNB)
83-32-9	Acenaphthene
84-66-2	Diethyl phthalate
84-74-2	Di-n-butylphthalate
85-01-8	Phenanthrene
85-68-7	Butylbenzylphthalate
86-73-7	Fluorene
87-68-3	Hexachlorobutadiene
88-06-2	2, 4, 6-Trichlorophenol
88-75-5	2-Nitrophenol
88-85-7	2-sec-Butyl-4, 6-dinitrophenol; syn Dinoseb
91-20-3	Naphthalene
91-58-7	2-Chloronaphthalene
93-72-1	Silvex (2, 4, 5-TP)
95-50-1	1, 2-Dichlorobenzene
95-57-8	2-Chlorophenol

Table 3-3 Organic Compounds Remaining for LDR

CAS#	Constituent
95-95-4	2, 4, 5-Trichlorophenol
98-86-2	Acetophenone
98-95-3	Nitrobenzene

Table 3-4 UTS Limits for COPCs

Chemical Name	CAS Number	LDR Treatment Standard (mg/kg) unless noted
alpha-BHC	319-84-6	0.066
beta-BHC	319-85-7	0.066
delta-BHC	319-86-8	0.066
Isodrin	465-73-6	0.066
gamma-BHC (Lindane)	58-89-9	0.066
2, 3, 4, 6-Tetrachlorophenol	58-90-2	7.4
2-sec-Butyl-4, 6-dinitrophenol; syn Dinoseb	88-85-7	2.5
Silvex (2, 4, 5-TP)	93-72-1	7.9
Antimony	7440-36-0	1.15 mg/L TCLP
Arsenic	7440-38-2	HLVIT
Barium	7440-39-3	HLVIT
Beryllium	7440-41-7	1.22 mg/L TCLP
Cadmium	7440-43-9	HLVIT
Chromium	7440-47-3	HLVIT
Lead	7439-92-1	HLVIT
Mercury	7439-97-6	HLVIT
Nickel	7440-02-0	11 mg/L TCLP
Selenium	7782-49-2	HLVIT
Silver	7440-22-4	HLVIT
Thallium	7440-28-0	0.20 mg/L TCLP
Dibenzo[a,e]pyrene	192-65-4	N/A
p-Phthalic acid	100-21-0	28
Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5	0.001
Ethyl benzene	100-41-4	10
cis-1, 3-Dichloropropene	10061-01-5	18
trans-1, 3-Dichloropropene	10061-02-6	18
4-Bromophenylphenyl ether	101-55-3	15
1, 4-Dichlorobenzene	106-46-7	6.0
Ethylene dibromide	106-93-4	15
Acrolein	107-02-8	NA

Table 3-4 UTS Limits for COPCs

Chemical Name	CAS Number	LDR Treatment Standard (mg/kg) unless noted
3-Chloropropene	107-05-1	30
1,2-Dichloroethane	107-06-2	6.0
Propionitrile	107-12-0	360
Acrylonitrile	107-13-1	84
4-Methyl-2-pentanone (MIBK)	108-10-1	33
Toluene	108-88-3	10
Chlorobenzene	108-90-7	6.0
Phenol	108-95-2	6.2
Pyridine	110-86-1	16
Bis(2-ethylhexyl) phthalate	117-81-7	28
Di-n-octylphthalate	117-84-0	28
Anthracene	120-12-7	3.4
1, 2, 4-Trichlorobenzene	120-82-1	19
2, 4-Dichlorophenol	120-83-2	14
N, N-Diphenylamine	122-39-4	13
1, 4-Dioxane	123-91-1	170
2-Methyl-2-propenenitrile	126-98-7	84
1, 1, 2, 2-Tetrachloroethene	127-18-4	6.0
Pyrene	129-00-0	8.2
Cresols (total)	1319-77-3	N/A
Xylene (total)	1330-20-7	30
Polychlorinated biphenyls (PCBs)	1336-36-3	10
1, 2-trans-Dichloroethene	156-60-5	30
Benzo(ghi)perylene	191-24-2	1.8
Indeno(1, 2, 3-cd)pyrene	193-39-5	3.4
Benzo(b)fluoranthene	205-99-2	6.8
Fluoranthene	206-44-0	3.4
Benzo(k)fluoranthene	207-08-9	6.8
Acenaphthylene	208-96-8	3.4
Chrysene	218-01-9	3.4
Benzo(a)pyrene	50-32-8	3.4

Table 3-4 UTS Limits for COPCs

Chemical Name	CAS Number	LDR Treatment Standard (mg/kg) unless noted
Dibenz[a,h]anthracene	53-70-3	8.2
1, 3-Dichlorobenzene	541-73-1	6.0
Carbon tetrachloride	56-23-5	6.0
3-Methylcholanthrene	56-49-5	15
Benzo(a)anthracene	56-55-3	3.4
Cyanide (total)	57-12-5	590
Cyanide (amenable)	57-12-5	30
4-Chloro-3-methylphenol	59-50-7	14
N-Nitrosomorpholine	59-89-2	2.3
N-Nitroso-di-n-propylamine	621-64-7	14
N-Nitroso-N,N-dimethylamine	62-75-9	2.3
1, 1, 1, 2-Tetrachloroethane	630-20-6	6.0
2-Propanone (Acetone)	67-64-1	160
Chloroform	67-66-3	6.0
Hexachloroethane	67-72-1	30
Benzene	71-43-2	10
1, 1, 1-Trichloroethane	71-55-6	6.0
Bromomethane	74-83-9	15
Chloromethane	74-87-3	30
Chloroethane	75-00-3	6.0
1-Chloroethene	75-01-4	6.0
Acetonitrile	75-05-8	38
Dichloromethane (Methylene Chloride)	75-09-2	30
Carbon disulfide	75-15-0	4.8 mg/L TCLP
Bromodichloromethane	75-27-4	15
1, 1-Dichloroethane	75-34-3	6.0
1, 1-Dichloroethene	75-35-4	6.0
Trichlorofluoromethane	75-69-4	30
Dichlorodifluoromethane	75-71-8	7.2
2-Methylpropyl alcohol	78-83-1	170
1, 2-Dichloropropane	78-87-5	18

Table 3-4 UTS Limits for COPCs

Chemical Name	CAS Number	LDR Treatment Standard (mg/kg) unless noted
2-Butanone (Methyl ethyl ketone)	78-93-3	36
1, 1, 2-Trichloroethane	79-00-5	6.0
1, 1, 2-Trichloroethylene	79-01-6	6.0
1, 1, 2, 2,-Tetrachloroethane	79-34-5	6.0
Pentachloronitrobenzene (PCNB)	82-68-8	4.8
Acenaphthene	83-32-9	3.4
Diethyl phthalate	84-66-2	28
Di-n-butylphthalate	84-74-2	28
Phenanthrene	85-01-8	5.6
Butylbenzylphthalate	85-68-7	28
Fluorene	86-73-7	3.4
Hexachlorobutadiene	87-68-3	5.6
2, 4, 6-Trichlorophenol	88-06-2	7.4
2-Nitrophenol	88-75-5	13
Naphthalene	91-20-3	5.6
2-Chloronaphthalene	91-58-7	5.6
1, 2-Dichlorobenzene	95-50-1	6.0
2-Chlorophenol	95-57-8	5.7
2, 4, 5-Trichlorophenol	95-95-4	7.4
Acetophenone	98-86-2	9.7
Nitrobenzene	98-95-3	14

N/A = Not applicable. Not a UHC and no UTS established in 409 CFR 268.

HLVIT: High-level vitrification is the current LDR technology-based standard (40 CFR 268.40) for mixed high-level radioactive waste with toxicity characteristic concentrations of the indicated constituent.

Table 3-5 Organic and Inorganic Compounds Remaining for Delisting

CAS #	Constituent	Compound Type:
100-21-0	p-Phthalic acid	Organic
100-41-4	Ethyl benzene	Organic
100-42-5	Styrene	Organic
10061-01-5	cis-1, 3-Dichloropropene	Organic
10061-02-6	trans-1, 3-Dichloropropene	Organic
10102-43-9	Nitric oxide	Inorganic
10102-44-0	Nitrogen dioxide	Inorganic
10102-45-1	Thallium(I) nitrate	Inorganic
101-55-3	4-Bromophenylphenyl ether	Organic
106-46-7	1, 4-Dichlorobenzene	Organic
106-93-4	Ethylene dibromide	Organic
107-02-8	Acrolein	Organic
107-05-1	3-Chloropropene	Organic
107-06-2	1, 2-Dichloroethane	Organic
107-12-0	Propionitrile	Organic
107-13-1	Acrylonitrile	Organic
108-10-1	4-Methyl-2-pentanone (MIBK)	Organic
1319-77-3	Cresols (total)	Organic
108-88-3	Toluene	Organic
108-90-7	Chlorobenzene	Organic
108-95-2	Phenol	Organic
109-06-8	2-Methylpyridine	Organic
110-86-1	Pyridine	Organic
117-81-7	Bis(2-ethylhexyl) phthalate	Organic
117-84-0	Di-n-octylphthalate	Organic
120-12-7	Anthracene	Organic
12039-52-0	Thallium selenite	Inorganic
120-82-1	1, 2, 4-Trichlorobenzene	Organic
120-83-2	2, 4-Dichlorophenol	Organic
122-09-8	alpha, alpha- Dimethylphenethylamine	Organic
122-39-4	N, N-Diphenylamine	Organic

Table 3-5 Organic and Inorganic Compounds Remaining for Delisting

CAS #	Constituent	Compound Type:
123-91-1	1, 4-Dioxane	Organic
126-68-1	O, O, O-Triethyl phosphorothioate	Organic
126-98-7	2-Methyl-2-propenenitrile	Organic
127-18-4	1, 1, 2, 2-Tetrachloroethene	Organic
129-00-0	Pyrene	Organic
130-15-4	1, 4-Naphthoquinone	Organic
1303-28-2	Arsenic pentoxide	Inorganic
1314-32-5	Thallic oxide	Inorganic
1314-62-1	Vanadium pentoxide	Inorganic
1314-84-7	Zinc phosphide	Inorganic
13256-22-9	N-Nitrososarcosine	Organic
1327-53-3	Arsenic trioxide	Inorganic
1330-20-7	Xylene (total)	Organic
1335-32-6	Lead subacetate	Organometallic
1336-36-3	Polychlorinated biphenyls (PCBs)	Organic
13463-39-3	Nickel carbonyl	Inorganic
13765-19-0	Calcium chromate	Inorganic
143-33-9	Sodium cyanide	Inorganic
151-50-8	Potassium cyanide	Inorganic
152-16-9	Octamethylpyrophosphoramidate	Organic
156-60-5	1, 2-trans-Dichloroethene	Organic
189-55-9	Dibenzo[a,i]pyrene	Organic
189-64-0	Dibenzo[a,h]pyrene	Organic
191-24-2	Benzo(ghi)perylene	Organic
192-65-4	Dibenzo[a,e]pyrene	Organic
193-39-5	Indeno(1, 2, 3-cd)pyrene	Organic
205-82-3	Benzo[j]fluoranthene	Organic
205-99-2	Benzo(b)fluoranthene	Organic
206-44-0	Fluoranthene	Organic
207-08-9	Benzo(k)fluoranthene	Organic
20859-73-8	Aluminum phosphide	Inorganic
208-96-8	Acenaphthylene	Organic

Table 3-5 Organic and Inorganic Compounds Remaining for Delisting

CAS #	Constituent	Compound Type:
218-01-9	Chrysene	Organic
224-42-0	Dibenz[a,j]acridine	Organic
225-51-4	Benz[c]acridine	Organic
226-36-8	Dibenz[a,h]acridine	Organic
2303-16-4	Diallate	Organic
25567-55-9	2, 3, 4, 6-Tetrachlorophenol, sodium salt	Organometallic
26952-23-8	Dichloropropene	Organic
297-97-2	O, O-Diethyl O-pyrazinyl phosphoro- thioate	Organic
301-04-2	Lead acetate	Organometallic
30402-15-4	Pentachlorodibenzofurans	Organic
319-84-6	alpha-BHC	Organic
319-85-7	beta-BHC	Organic
319-86-8	delta-BHC	Organic
34465-46-8	Hexachlorodibenzo-p-dioxins	Organic
41903-57-5	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	Organic
465-73-6	Isodrin	Organic
492-80-8	Auramine	Organic
50-32-8	Benzo(a)pyrene	Organic
50-55-5	Reserpine	Organic
506-61-6	Potassium silver cyanide	Inorganic
506-64-9	Silver cyanide	Inorganic
53535-27-6	2, 3, 4, 6-Tetrachlorophenol, potassium salt	Organometallic
53-70-3	Dibenz[a,h]anthracene	Organic
541-73-1	1, 3-Dichlorobenzene	Organic
542-62-1	Barium cyanide	Inorganic
544-92-3	Copper cyanide	Inorganic
557-19-7	Nickel cyanide	Inorganic
557-21-1	Zinc cyanide	Inorganic
56-23-5	Carbon tetrachloride	Organic
563-68-8	Thallium(I) acetate	Organometallic
56-49-5	3-Methylcholanthrene	Organic
56-55-3	Benzo(a)anthracene	Organic

Table 3-5 Organic and Inorganic Compounds Remaining for Delisting

CAS #	Constituent	Compound Type:
57-12-5	Cyanide	Inorganic
57-97-6	7, 12-Dimethylbenz[a]anthracene	Organic
58-89-9	gamma-BHC (Lindane)	Organic
58-90-2	2, 3, 4, 6-Tetrachlorophenol	Organic
592-01-8	Calcium cyanide	Inorganic
59-50-7	4-Chloro-3-methylphenol	Organic
59-89-2	N-Nitrosomorpholine	Organic
60-51-5	Dimethoate	Organic
621-64-7	N-Nitroso-di-n-propylamine	Organic
62-75-9	N-Nitroso-N,N-dimethylamine	Organic
628-86-4	Mercury fulminate	Inorganic
630-20-6	1, 1, 1, 2-Tetrachloroethane	Organic
6358-53-8	Citrus red No. 2	Organic
64-18-6	Formic acid	Organic
6533-73-9	Thallium(I) carbonate	Inorganic
67-64-1	2-Propanone (Acetone)	Organic
67-66-3	Chloroform	Organic
67-72-1	Hexachloroethane	Organic
70-30-4	Hexachlorophene	Organic
71-43-2	Benzene	Organic
71-55-6	1, 1, 1-Trichloroethane	Organic
7439-92-1	Lead	Inorganic
7439-97-6	Mercury	Inorganic
7440-02-0	Nickel	Inorganic
7440-22-4	Silver	Inorganic
7440-28-0	Thallium	Inorganic
7440-36-0	Antimony	Inorganic
7440-38-2	Arsenic	Inorganic
7440-39-3	Barium	Inorganic
7440-41-7	Beryllium	Inorganic
7440-43-9	Cadmium	Inorganic
7440-47-3	Chromium	Inorganic

Table 3-5 Organic and Inorganic Compounds Remaining for Delisting

CAS #	Constituent	Compound Type:
7440-62-2	Vanadium	Inorganic
7440-66-6	Zinc	Inorganic
7446-18-6	Thallium(I) sulfate	Inorganic
7446-27-7	Lead phosphate	Inorganic
74-83-9	Bromomethane	Organic
74-87-3	Chloromethane	Organic
7488-56-4	Selenium sulfide	Inorganic
74-90-8	Hydrogen cyanide	Inorganic
75-00-3	Chloroethane	Organic
75-01-4	1-Chloroethene	Organic
75-05-8	Acetonitrile	Organic
75-09-2	Dichloromethane (Methylene Chloride)	Organic
75-15-0	Carbon disulfide	Organic
75-27-4	Bromodichloromethane	Organic
75-34-3	1, 1-Dichloroethane	Organic
75-35-4	1, 1-Dichloroethene	Organic
75-69-4	Trichlorofluoromethane	Organic
75-71-8	Dichlorodifluoromethane	Organic
7778-39-4	Arsenic acid	Inorganic
7782-49-2	Selenium	Inorganic
7783-00-8	Selenium dioxide	Inorganic
7791-12-0	Thallium(I) chloride	Inorganic
7803-55-6	Ammonium vanadate	Inorganic
78-83-1	2-Methylpropyl alcohol	Organic
78-87-5	1, 2-Dichloropropane	Organic
78-93-3	2-Butanone (Methyl ethyl ketone)	Organic
79-00-5	1, 1, 2-Trichloroethane	Organic
79-01-6	1, 1, 2-Trichloroethylene	Organic
79-34-5	1, 1, 2, 2-Tetrachloroethane	Organic
82-68-8	Pentachloronitrobenzene (PCNB)	Organic
83-32-9	Acenaphthene	Organic
84-66-2	Diethyl phthalate	Organic

Table 3-5 Organic and Inorganic Compounds Remaining for Delisting

CAS #	Constituent	Compound Type:
84-74-2	Di-n-butylphthalate	Organic
85-01-8	Phenanthrene	Organic
85-68-7	Butylbenzylphthalate	Organic
86-73-7	Fluorene	Organic
87-68-3	Hexachlorobutadiene	Organic
88-06-2	2, 4, 6-Trichlorophenol	Organic
88-75-5	2-Nitrophenol	Organic
88-85-7	2-sec-Butyl-4,6-dinitrophenol; syn Dinoseb	Organic
91-20-3	Naphthalene	Organic
91-58-7	2-Chloronaphthalene	Organic
93-72-1	Silvex (2, 4, 5-TP)	Organic
95-50-1	1, 2-Dichlorobenzene	Organic
95-57-8	2-Chlorophenol	Organic
95-95-4	2, 4, 5-Trichlorophenol	Organic
98-05-5	Benzeneearsonic acid	Organometallic
98-86-2	Acetophenone	Organic
98-95-3	Nitrobenzene	Organic
99-35-4	1, 3, 5-Trinitrobenzene	Organic

Table 3-6 DRAS Output, Delisting Action Levels

CAS Number	Chemical Name	Dilution Attenuation Factor (DAF)	Waste Volume Adjusted DAF	Max. Allowable TCLP Conc. Based on GW Ingestion (mg/L)	Max. Allowable TCLP Conc. Based on GW Inhalation (mg/L)	Max. Allowable TCLP Conc. Based on Adult GW Dermal Absorption (mg/L)	Max. Allowable TCLP Conc. Based on Child GW Dermal Absorption (mg/L)	DRAS V2.0 Maximum Allowable TCLP Conc. (mg/L)	Max. Allowable Conc. Based on MCL (mg/L)	Toxicity Characteristic Levels (mg/L)	Delisting Level Using Rule: MCL or DRAS, but TC Limited ^(a) (as measured by TCLP) (mg/L)	Delisting Level Using Rule: Lower of MCL or DRAS, but TC Limited ^(b) (as measured by TCLP) (mg/L)
Organic Compounds												
100-21-0	p-Phthalic acid			Not in DRAS								
100-41-4	Ethylbenzene	1.90E+01	6.08E+01	5.71E+01	8.06E+01	9.07E+01	4.16E+01	4.16E+01	4.26E+01		4.26E+01	4.16E+01
100-42-5	Styrene	1.90E+01	6.08E+01	1.14E+02	2.76E+02	2.48E+02	1.14E+02	6.08E+00	6.08E+00		6.08E+00	6.08E+00
10061-01-5	Dichloropropene, cis-1, 3-	3.30E+08	1.06E+09	4.41E+06	6.87E+06	5.75E+07	1.32E+08	4.41E+06	---		4.41E+06	4.41E+06
10061-02-6	Dichloropropene, trans-1, 3-	3.30E+08	1.06E+09	4.41E+06	7.11E+06	5.75E+07	1.32E+08	4.41E+06	---		4.41E+06	4.41E+06
101-55-3	Bromophenyl-phenyl ether 4-	1.80E+01	5.76E+01	3.14E+01	---	2.12E+01	9.73E+00	9.73E+00	---		9.73E+00	9.73E+00
106-44-5	Cresol, p- (represents total Cresols,	1.90E+01	6.08E+01	2.86E+00	---	3.27E+01	1.50E+01	2.86E+00	---	2.00E+02	2.00E+02	2.86E+00
106-46-7	Dichlorobenzene, 1, 4-	1.80E+01	5.76E+01	1.76E+00	2.86E+00	3.02E+00	6.94E+00	1.76E+00	4.32E+01	7.50E+00	7.50E+00	1.76E+00
106-93-4	Ethylene Dibromide	1.50E+03	4.80E+03	4.13E-02	8.98E+00	1.46E+00	3.35E+00	4.13E-02	2.40E-01		2.40E-01	4.13E-02
107-02-8	Acrolein	1.43E+06	4.58E+06	8.59E+05	1.06E+03	1.68E+08	7.70E+07	1.06E+03	---		1.06E+03	1.06E+03
107-05-1	Allyl chloride	---	---	---	---	---	---	---	---			
107-06-2	Dichloroethane, 1, 2-	1.00E+00	3.20E+00	---	---	---	---	1.60E-02	1.60E-02	5.00E-01	1.60E-02	1.60E-02
107-12-0	Propionitrile (Ethyl cyanide)			Not in DRAS								
107-13-1	Acrylonitrile	1.80E+01	5.76E+01	7.80E-02	7.03E-01	1.20E+01	2.74E+01	7.80E-02	---		7.80E-02	7.80E-02
108-10-1	Methyl isobutyl ketone	1.90E+01	6.08E+01	4.57E+01	---	1.67E+03	7.67E+02	4.57E+01	---		4.57E+01	4.57E+01
108-39-4	Cresol, m-	1.90E+01	6.08E+01	2.86E+01	---	3.27E+02	1.50E+02	2.86E+01	---	2.00E+02	2.00E+02	2.00E+02
108-88-3	Toluene	1.90E+01	6.08E+01	1.14E+02	---	3.11E+02	1.43E+02	6.08E+01	6.08E+01		6.08E+01	6.08E+01
108-90-7	Chlorobenzene	1.90E+01	6.08E+01	1.14E+01	1.59E+01	3.00E+01	1.38E+01	6.08E+00	6.08E+00	1.00E+02	6.08E+00	6.08E+00
108-95-2	Phenol	1.90E+01	6.08E+01	3.43E+02	---	7.57E+03	3.48E+03	3.43E+02	---		3.43E+02	3.43E+02
109-06-8	Picoline a-	1.80E+01	5.76E+01	---	---	---	---	---	---			
110-86-1	Pyridine	1.90E+01	6.08E+01	5.71E-01	---	4.19E+01	1.92E+01	5.71E-01	---	5.00E+00	5.71E-01	5.71E-01
117-81-7	Bis(2-ethylhexyl)phthalate	1.90E+01	6.08E+01	1.14E+01	---	5.47E+00	2.51E+00	3.65E-01	3.65E-01		3.65E-01	3.65E-01
117-84-0	Di-n-octyl phthalate	2.70E+01	8.65E+01	1.62E+01	---	6.10E-02	2.80E-02	2.80E-02	---		2.80E-02	2.80E-02
120-12-7	Anthracene	1.80E+01	5.76E+01	1.62E+02	---	4.36E+01	2.00E+01	2.00E+01	---		2.00E+01	2.00E+01
120-82-1	Trichlorobenzene, 1, 2, 4-	1.90E+01	6.08E+01	5.71E+00	2.65E+01	3.94E+00	1.81E+00	1.81E+00	4.26E+00		4.26E+00	1.81E+00
120-83-2	Dichlorophenol, 2, 4-	1.90E+01	6.08E+01	1.71E+00	---	4.46E+00	2.05E+00	1.71E+00	---		1.71E+00	1.71E+00
122-09-8	alpha, alpha-			Not in DRAS								
122-39-4	Diphenylamine	1.90E+01	6.08E+01	1.43E+01	---	2.05E+01	9.41E+00	9.41E+00	---		9.41E+00	9.41E+00
123-91-1	Dioxane, 1, 4-	1.80E+01	5.76E+01	3.83E+00	2.35E+02	2.24E+03	5.14E+03	3.83E+00	---		3.83E+00	3.83E+00
126-68-1	Triethylphosphorothiate o, o, o-	1.80E+01	5.76E+01	---	---	---	---	---	---			
126-98-7	Methacrylonitrile	1.90E+01	6.08E+01	5.71E-02	3.12E-01	4.90E+00	2.25E+00	5.71E-02	---		5.71E-02	5.71E-02
127-18-4	Tetrachloroethylene	1.90E+01	6.08E+01	5.71E+00	---	2.90E+01	1.33E+01	3.04E-01	3.04E-01	7.00E-01	3.04E-01	3.04E-01
129-00-0	Pyrene	1.90E+01	6.08E+01	1.71E+01	---	2.15E+00	9.89E-01	9.89E-01	---		9.89E-01	9.89E-01
130-15-4	Naphthaquinone 1, 4-	1.80E+01	5.76E+01	---	---	---	---	---	---			
13256-22-9	N-Nitrososarcosine			Not in DRAS								
1330-20-7	Xylenes (total)	1.90E+01	6.08E+01	1.14E+03	---	1.74E+03	7.99E+02	6.08E+02	6.08E+02		6.08E+02	6.08E+02
1336-36-3	Polychlorinated biphenyls	1.80E+01	5.76E+01	2.11E-02	4.31E-02	6.54E-04	1.50E-03	6.54E-04	2.88E-02		2.88E-02	6.54E-04
152-16-9	Octamethylpyrophosphoramide	1.90E+01	6.08E+01	1.14E+00	---	2.49E+03	1.14E+03	1.14E+00	---		1.14E+00	1.14E+00
156-60-5	Dichloroethylene, trans-1, 2-	1.90E+01	6.08E+01	1.14E+01	---	1.01E+02	4.65E+01	6.08E+00	6.08E+00		6.08E+00	6.08E+00
1746-01-6	Tetrachlorodibenzo-p-dioxin, 2, 3,	1.80E+01	5.76E+01	2.81E-07	6.20E-06	6.55E-09	1.50E-08	6.55E-09	---		6.55E-09	6.55E-09

Table 3-6 DRAS Output, Delisting Action Levels

CAS Number	Chemical Name	Dilution Attenuation Factor (DAF)	Waste Volume Adjusted DAF	Max. Allowable TCLP Conc. Based on GW Ingestion (mg/L)	Max. Allowable TCLP Conc. Based on GW Inhalation (mg/L)	Max. Allowable TCLP Conc. Based on Adult GW Dermal Absorption (mg/L)	Max. Allowable TCLP Conc. Based on Child GW Dermal Absorption (mg/L)	DRAS V2.0 Maximum Allowable TCLP Conc. (mg/L)	Max. Allowable Conc. Based on MCL (mg/L)	Toxicity Characteristic Levels (mg/L)	Delisting Level Using Rule: MCL or DRAS, but TC Limited ^(a) (as measured by TCLP) (mg/L)	Delisting Level Using Rule: Lower of MCL or DRAS, but TC Limited ^(b) (as measured by TCLP) (mg/L)
189-55-9	Dibenzo[a, i]pyrene			Not in DRAS								
189-64-0	Dibenzo[a, h]pyrene			Not in DRAS								
191-24-2	Benzo (ghi) perylene	1.80E+01	5.76E+01	---	---	---	---	---	---			
192-65-4	Dibenzo[a, e]pyrene			Not in DRAS								
193-39-5	Indeno(1, 2, 3-cd) pyrene	1.90E+01	6.08E+01	6.09E-02	9.46E+03	1.32E-03	3.02E-03	1.32E-03	---		1.32E-03	1.32E-03
205-82-3	Benzo[j]fluoranthene			Not in DRAS								
205-99-2	Benzo(b)fluoranthene	1.90E+01	6.08E+01	6.09E-02	7.52E+00	2.33E-03	5.36E-03	2.33E-03	---		2.33E-03	2.33E-03
206-44-0	Fluoranthene	1.90E+01	6.08E+01	2.28E+01	---	2.81E+00	1.29E+00	1.29E+00	---		1.29E+00	1.29E+00
207-08-9	Benzo(k)fluoranthene	1.90E+01	6.08E+01	6.09E-01	1.09E+03	3.25E-02	7.45E-02	3.25E-02	---		3.25E-02	3.25E-02
208-96-8	Acenaphthylene	1.80E+01	5.76E+01	---	---	---	---	---	---			
218-01-9	Chrysene	1.90E+01	6.08E+01	6.09E+00	3.74E+03	4.44E-01	1.02E+00	4.44E-01	---		4.44E-01	4.44E-01
224-42-0	Dibenz[a, i]acridine			Not in DRAS								
225-51-4	Benz[c]acridine			Not in DRAS								
226-36-8	Dibenz[a, h]acridine			Not in DRAS								
2303-16-4	Diallate	2.20E+05	7.05E+05	8.44E+03	6.12E+04	6.02E+03	1.38E+04	6.02E+03	---		6.02E+03	6.02E+03
26952-23-8	Dichloropropene			Not in DRAS								
297-97-2	Thionazin	2.00E+06	6.41E+06	---	---	---	---	---	---			
30402-15-4D	Pentachlorodibenzofurans			Not in DRAS								
319-84-6	Hexachlorocyclohexane, alpha-	1.90E+06	6.08E+06	7.06E+02	3.43E+04	1.80E+03	4.13E+03	7.06E+02	---		7.06E+02	7.06E+02
319-85-7	Hexachlorocyclohexane, beta-	1.80E+01	5.76E+01	2.34E-02	2.17E+01	5.96E-03	1.37E-01	2.34E-02	---		2.34E-02	2.34E-02
319-86-8	delta-BHC			Not in DRAS								
34465-46-8D	Hexachlorodibenzo-p-dioxins			Not in DRAS								
465-73-6	Isodrin			Not in DRAS								
492-80-8	Auramine			Not in DRAS								
50-32-8	Benzo(a)pyrene	1.80E+01	5.76E+01	5.77E-03	5.17E+00	2.58E-04	5.92E-04	2.58E-04	1.15E-02		1.15E-02	2.58E-04
50-55-5	Reserpine			Not in DRAS								
53-70-3	Dibenz(a,h)anthracene	1.80E+01	5.76E+01	5.77E-03	3.91E+02	1.22E-04	2.79E-04	1.22E-04	---		1.22E-04	1.22E-04
541-73-1	Dichlorobenzene 1, 3-	1.90E+01	6.08E+01	---	5.59E-02	---	---	5.59E-02	---		5.59E-02	5.59E-02
56-23-5	Carbon tetrachloride	2.50E+01	8.01E+01	5.26E-01	---	2.30E+00	1.05E+00	4.00E-01	4.00E-01	5.00E-01	4.00E-01	4.00E-01
56-49-5	Methylcholanthrene, 3-	1.80E+01	5.76E+01	1.62E-03	5.50E-01	4.83E-05	1.11E-04	4.83E-05	---		4.83E-05	4.83E-05
56-55-3	Benz(a)anthracene	1.80E+01	5.76E+01	5.76E-02	1.20E+01	4.20E-03	9.64E-03	4.20E-03	---		4.20E-03	4.20E-03
57-97-6	Dimethylbenz(a)anthracene, 7, 12	1.80E+01	5.76E+01	1.69E-03	2.63E+01	3.37E-05	7.73E-05	3.37E-05	---		3.37E-05	3.37E-05
58-89-9	Hexachlorocyclohexane, gamma	1.70E+06	5.44E+06	1.53E+04	---	3.47E+04	1.60E+04	1.09E+03	1.09E+03	4.00E-01	4.00E-01	4.00E-01
58-90-2	Tetrachlorophenol, 2, 3, 4, 6-	1.90E+01	6.08E+01	1.71E+01	---	9.85E+00	4.52E+00	4.52E+00	---		4.52E+00	4.52E+00
59-50-7	Chloro-3-methylphenol 4-	1.80E+01	5.76E+01	---	---	---	---	---	---			
59-89-2	Nitrosomorpholine N-	1.80E+01	5.76E+01	---	---	---	---	---	---			
60-51-5	Dimethoate	2.50E+04	8.01E+04	1.50E+02	---	3.06E+04	1.40E+04	1.50E+02	---		1.50E+02	1.50E+02
621-64-7	N-Nitrosodi-n-propylamine	1.80E+01	5.76E+01	6.02E-03	5.06E-02	2.54E-01	5.82E-01	6.02E-03	---		6.02E-03	6.02E-03
62-75-9	Nitrosodimethylamine	1.80E+01	5.76E+01	8.26E-04	2.13E-01	5.69E-01	1.31E+00	8.26E-04	---		8.26E-04	8.26E-04
630-20-6	Tetrachloroethane, 1, 1, 1, 2-	2.70E+01	8.65E+01	2.43E+00	3.93E+00	1.81E+01	4.16E+01	2.43E+00	---		2.43E+00	2.43E+00
6358-53-8	Citrus red No. 2			Not in DRAS								
64-18-6	Formic Acid	1.90E+01	6.08E+01	1.14E+03	---	4.89E+05	2.24E+05	1.14E+03	---		1.14E+03	1.14E+03

Table 3-6 DRAS Output, Delisting Action Levels

CAS Number	Chemical Name	Dilution Attenuation Factor (DAF)	Waste Volume Adjusted DAF	Max. Allowable TCLP Conc. Based on GW Ingestion (mg/L)	Max. Allowable TCLP Conc. Based on GW Inhalation (mg/L)	Max. Allowable TCLP Conc. Based on Adult GW Dermal Absorption (mg/L)	Max. Allowable TCLP Conc. Based on Child GW Dermal Absorption (mg/L)	DRAS V2.0 Maximum Allowable TCLP Conc. (mg/L)	Max. Allowable Conc. Based on MCL (mg/L)	Toxicity Characteristic Levels (mg/L)	Delisting Level Using Rule: MCL or DRAS, but TC Limited ^(a) (as measured by TCLP) (mg/L)	Delisting Level Using Rule: Lower of MCL or DRAS, but TC Limited ^(b) (as measured by TCLP) (mg/L)
67-64-1	Acetone	1.90E+01	6.08E+01	5.71E+01	---	1.62E+04	7.44E+03	5.71E+01	---		5.71E+01	5.71E+01
67-66-3	Chloroform	1.80E+01	5.76E+01	6.91E+00	7.79E-01	1.13E+02	2.59E+02	7.79E-01	5.76E+00	6.00E+00	5.76E+00	7.79E-01
67-72-1	Hexachloroethane	1.80E+01	5.76E+01	5.41E-01	---	5.38E-01	2.47E-01	2.47E-01	---	3.00E+00	2.47E-01	2.47E-01
70-30-4	Hexachlorophene	1.90E+01	6.08E+01	1.71E-01	---	1.70E-03	7.82E-04	7.82E-04	---		7.82E-04	7.82E-04
71-43-2	Benzene	1.80E+01	5.76E+01	5.41E-01	2.19E+00	3.66E+00	1.68E+00	5.41E-01	5.76E-01	5.00E-01	5.00E-01	5.00E-01
71-55-6	Trichloroethane, 1, 1, 1-	1.90E+01	6.08E+01	2.00E+01	7.38E+01	4.26E+01	1.90E+01	1.22E+01	1.22E+01		1.22E+01	1.22E+01
74-83-9	Methyl bromide (Bromomethane)	7.60E+03	2.43E+04	3.20E+02	4.83E+02	1.15E+04	5.28E+03	3.20E+02	---		3.20E+02	3.20E+02
74-87-3	Methyl chloride (Chloromethane)	---	---	---	---	---	---	---	---			
75-00-3	Chloroethane	1.80E+01	5.76E+01	1.45E+01	5.29E+01	---	---	1.45E+01	---		1.45E+01	1.45E+01
75-01-4	Vinyl chloride	1.90E+01	6.08E+01	2.97E-02	2.00E+00	6.54E-01	1.50E+00	2.97E-02	1.22E-01	2.00E-01	1.22E-01	2.97E-02
75-05-8	Acetonitrile	1.90E+01	6.08E+01	---	1.33E+02	---	---	1.33E+02	---		1.33E+02	1.33E+02
75-09-2	Methylene chloride	1.80E+01	5.76E+01	3.25E+01	2.02E+02	9.69E+02	4.45E+02	2.88E-01	2.88E-01		2.88E-01	2.88E-01
75-15-0	Carbon disulfide	1.90E+01	6.08E+01	5.71E+01	1.62E+02	4.86E+02	2.23E+02	5.71E+01	---		5.71E+01	5.71E+01
75-27-4	Bromodichloromethane	1.80E+01	5.76E+01	6.80E-01	1.03E+00	1.15E+01	2.63E+01	6.80E-01	---		6.80E-01	6.80E-01
75-34-3	Dichloroethane, 1, 1-	1.00E+00	3.20E+00	3.01E+00	6.68E+00	4.13E+01	1.90E+01	3.01E+00	---		3.01E+00	3.01E+00
75-34-4	Dichloroethylene, 1, 1-	1.80E+01	5.76E+01	7.02E-02	3.47E-01	6.99E-01	1.61E+00	7.02E-02	4.04E-01	7.00E-01	4.04E-01	7.02E-02
75-69-4	Trichlorofluoromethane	1.90E+01	6.08E+01	1.71E+02	5.10E+01	9.42E+02	4.32E+02	5.10E+01	---		5.10E+01	5.10E+01
75-71-8	Dichlorodifluoromethane	1.90E+01	6.08E+01	1.14E+02	5.24E+01	9.94E+02	4.56E+02	5.24E+01	---		5.24E+01	5.24E+01
78-83-1	Isobutyl alcohol	1.90E+01	6.08E+01	1.71E+02	---	1.08E+04	4.95E+03	1.71E+02	---		1.71E+02	1.71E+02
78-87-5	Dichloropropane, 1, 2-	3.30E+01	1.06E+02	---	1.86E+00	---	---	5.28E-01	5.28E-01		5.28E-01	5.28E-01
78-93-3	Methyl ethyl ketone	1.90E+01	6.08E+01	3.43E+02	1.57E+03	4.60E+04	2.11E+04	3.43E+02	---	2.00E+02	2.00E+02	2.00E+02
79-00-5	Trichloroethane, 1, 1, 2-	1.90E+01	6.08E+01	2.28E+00	---	2.64E+01	1.21E+01	3.04E-01	3.04E-01		3.04E-01	3.04E-01
79-01-6	Trichloroethylene	1.90E+01	6.08E+01	3.43E+00	---	5.00E+00	2.24E+00	3.04E-01	3.04E-01	5.00E-01	3.04E-01	3.04E-01
79-34-5	Tetrachloroethane, 1, 1, 2, 2-	3.75E+02	1.20E+03	4.39E+00	9.63E+00	4.72E+01	1.08E+02	4.39E+00	---		4.39E+00	4.39E+00
82-68-8	Pentachloronitrobenzene (PCNB)	1.80E+01	5.76E+01	1.62E-01	3.21E-01	1.09E-01	2.50E-01	1.09E-01	---		1.09E-01	1.09E-01
83-32-9	Acenaphthene	1.90E+01	6.08E+01	3.43E+01	---	2.19E+01	1.00E+01	1.00E+01	---		1.00E+01	1.00E+01
84-66-2	Diethyl phthalate	2.30E+01	7.37E+01	5.53E+02	---	5.66E+03	2.60E+03	5.53E+02	---		5.53E+02	5.53E+02
84-74-2	Di-n-butyl phthalate	2.00E+01	6.41E+01	6.01E+01	---	2.88E+01	1.32E+01	1.32E+01	---		1.32E+01	1.32E+01
85-01-8	Phenanthrene	1.80E+01	5.76E+01	---	---	---	---	---	---			
85-68-7	Butylbenzylphthalate	2.00E+01	6.41E+01	1.20E+02	---	5.06E+01	2.32E+01	2.32E+01	---		2.32E+01	2.32E+01
86-73-7	Fluorene	1.90E+01	6.08E+01	2.28E+01	---	9.68E+00	4.44E+00	4.44E+00	---		4.44E+00	4.44E+00
87-68-3	Hexachloro-1, 3-butadiene	1.80E+01	5.76E+01	1.08E-01	---	3.27E-02	1.50E-02	1.50E-02	---	5.00E-01	1.50E-02	1.50E-02
88-06-2	Trichlorophenol 2, 4, 6-	1.80E+01	5.76E+01	3.83E+00	3.02E+02	6.02E+00	1.38E+01	3.83E+00	---	2.00E+00	2.00E+00	2.00E+00
88-75-5	Nitrophenol 2-	1.80E+01	5.76E+01	---	---	---	---	---	---			
88-85-7	Butyl-4,6-dinitrophenol, 2-sec-	1.90E+01	6.08E+01	5.71E-01	---	2.33E+00	1.07E+00	4.26E-01	4.26E-01		4.26E-01	4.26E-01
91-20-3	Naphthalene	1.90E+01	6.08E+01	1.14E+01	1.04E+00	1.47E+01	6.77E+00	1.04E+00	---		1.04E+00	1.04E+00
91-58-7	chloronaphthalene 2-	1.80E+01	5.76E+01	4.33E+01	---	2.07E+01	9.50E+00	9.50E+00	---		9.50E+00	9.50E+00
93-72-1	Trichlorophenoxypropionic acid, 2,	1.90E+01	6.08E+01	4.57E+00	---	1.52E+01	6.99E+00	3.04E+00	3.04E+00	1.00E+00	1.00E+00	1.00E+00
95-48-7	Cresol, o-	1.90E+01	6.08E+01	2.86E+01	---	2.97E+02	1.36E+02	2.86E+01	---	2.00E+02	2.86E+01	2.86E+01
95-50-1	Dichlorobenzene, 1, 2-	1.90E+01	6.08E+01	5.14E+01	5.63E+01	6.78E+01	3.11E+01	3.11E+01	3.65E+01		3.65E+01	3.11E+01
95-57-8	Chlorophenol, 2-	1.90E+01	6.08E+01	2.86E+00	---	2.58E+01	1.18E+01	2.86E+00	---		2.86E+00	2.86E+00
95-95-4	Trichlorophenol, 2, 4, 5-	1.90E+01	6.08E+01	5.71E+01	---	4.99E+01	2.29E+01	2.29E+01	---	4.00E+02	2.29E+01	2.29E+01

Table 3-6 DRAS Output, Delisting Action Levels

CAS Number	Chemical Name	Dilution Attenuation Factor (DAF)	Waste Volume Adjusted DAF	Max. Allowable TCLP Conc. Based on GW Ingestion (mg/L)	Max. Allowable TCLP Conc. Based on GW Inhalation (mg/L)	Max. Allowable TCLP Conc. Based on Adult GW Dermal Absorption (mg/L)	Max. Allowable TCLP Conc. Based on Child GW Dermal Absorption (mg/L)	DRAS V2.0 Maximum Allowable TCLP Conc. (mg/L)	Max. Allowable Conc. Based on MCL (mg/L)	Toxicity Characteristic Levels (mg/L)	Delisting Level Using Rule: MCL or DRAS, but TC Limited ^(a) (as measured by TCLP) (mg/L)	Delisting Level Using Rule: Lower of MCL or DRAS, but TC Limited ^(b) (as measured by TCLP) (mg/L)
98-86-2	Acetophenone	1.90E+01	6.08E+01	5.71E+01	---	1.18E+03	5.43E+02	5.71E+01	---		5.71E+01	5.71E+01
98-95-3	Nitrobenzene	1.90E+01	6.08E+01	2.86E-01	---	4.34E+00	1.99E+00	2.86E-01	---	2.00E+00	2.86E-01	2.86E-01
99-35-4	Trinitrobenzene, sym-	1.80E+01	5.76E+01	1.62E+01	---	1.35E+03	6.21E+02	1.62E+01	---		1.62E+01	1.62E+01
Inorganic Compounds												
57-12-5	Cyanide	1.80E+01	5.76E+01	1.08E+01	---	---	---	1.08E+01	1.15E+01		1.15E+01	1.08E+01
7429-90-5	Aluminum			Not in DRAS								
7439-92-1	Lead	5.00E+03	1.60E+04	---	---	---	---	2.40E+02	2.40E+02	5.00E+00	5.00E+00	5.00E+00
7439-97-6	Mercury	7.45E+01	2.39E+02	2.24E-01	6.51E-02	---	---	6.51E-02	4.77E-01	2.00E-01	2.00E-01	6.51E-02
7440-02-0	Nickel	3.76E+01	1.21E+02	2.26E+01	---	---	---	2.26E+01	---		2.26E+01	2.26E+01
7440-09-7	Potassium			Not in DRAS								
7440-22-4	Silver	2.05E+01	6.55E+01	3.07E+00	---	---	---	3.07E+00	---	5.00E+00	3.07E+00	3.07E+00
7440-23-5	Sodium			Not in DRAS								
7440-28-0	Thallium	4.40E+01	1.41E+02	1.06E-01	---	---	---	1.06E-01	2.82E-01		2.82E-01	1.06E-01
7440-36-0	Antimony	3.43E+01	1.10E+02	4.12E-01	---	---	---	4.12E-01	6.59E-01		6.59E-01	4.12E-01
7440-38-2	Arsenic	1.92E+01	6.15E+01	3.00E-02	---	---	---	3.00E-02	3.08E+00	5.00E+00	3.08E+00	3.00E-02
7440-39-3	Barium	2.78E+01	8.91E+01	5.86E+01	---	---	---	5.86E+01	1.78E+02	1.00E+02	1.00E+02	5.86E+01
7440-41-7	Beryllium	1.04E+02	3.33E+02	6.25E+00	---	---	---	1.33E+00	1.33E+00		1.33E+00	1.33E+00
7440-43-9	Cadmium	3.00E+01	9.61E+01	4.51E-01	---	---	---	4.51E-01	4.80E-01	1.00E+00	4.80E-01	4.51E-01
7440-47-4	Chromium	3.85E+03	1.23E+04	1.74E+05	---	---	---	1.23E+03	1.23E+03	5.00E+00	5.00E+00	5.00E+00
7440-50-8	Copper	7.01E+03	2.24E+04	8.42E+03	---	---	---	8.42E+03	2.92E+04		2.92E+04	8.42E+03
7440-62-2	Vanadium	8.03E+01	2.57E+02	1.69E+01	---	---	---	1.69E+01	---		1.69E+01	1.69E+01
7440-66-6	Zinc	2.49E+01	7.97E+01	2.25E+02	---	---	---	2.25E+02	---		2.25E+02	2.25E+02
7440-70-2	Calcium			Not in DRAS								
7664-41-7	Ammonia/ammonium			Not in DRAS								
7697-37-2	Nitrate			Not in DRAS								
7723-14-0	Phosphorus			Not in DRAS								
7782-49-2	Selenium	1.16E+01	3.71E+01	1.74E+00	---	---	---	1.74E+00	1.86E+00	1.00E+00	1.00E+00	1.00E+00

DRAS = Delisting Risk Assessment Software, Version 2.0 (EPA 2000b).

- (a) **Delisting Level Using Rule: MCL or DRAS, but TC Limited:** Selection rule in which an MCL times a DAF is used for a delisting level (even if it is higher than the DRAS model result), or if there is no MCL, the DRAS computed delisting level is used. However, in either case, if a toxicity characteristic limit is available, it is used in lieu of both the MDL derived limit, or the DRAS derived limit (if the delisting level is higher than the TC level, the TC level takes precedence). This column indicates proposed delisting levels.
- (b) **Delisting Level Using Rule: Lower of MCL or DRAS, but TC Limited:** Selection rule in which the selected delisting level is the lower of the MDL or DRAS-derived levels. However, in either case, if a toxicity characteristic limit is available, it is used as the in lieu of both the MDL derived limit, or the DRAS derived limit (if the delisting level is higher than the TC level, the TC level takes precedence).

Table 3-7 Summary of Sample Preparation and Analytical Methods

Analytes of Interest	Prep Method	Analytical Method	Precision/Accuracy Requirements ⁽¹⁾
Metals	Liquids: 3005A, 3010A or equivalent Solids: 3052, 3050B, 3051A, or other ^(c)	6020 (ICP/MS) ^(a) 6010B (ICP/AES) ^(b) Lab Specific - DCP/AES ^(d)	RPD ≤ ±20 % 75 %-125 % recovery
Cyanide (Total and Amenable)	9010B Distillation or 9012A Automated analysis with Distillation 9013 Solids preparation	9012A Automated Spectroscopic	
Mercury	7470A/7471A	7470A/7471A	

⁽¹⁾ Applies to matrix spike and matrix spike duplicates (applies to like matrices, note that different simulants may be defined as different matrices, as do matrices with differing alkalinity). Additional method-specific calibration verification (not shown) applies. Failures will be assessed for data impact on a case-by-case basis.

^(a) ICP/MS = inductively coupled plasma/mass spectroscopy

^(b) ICP/AES = inductively coupled plasma/atomic emission spectroscopy

^(c) ASTM C 1317-95, ASTM C 1342-96, ASTM C 1412-99 may be required for certain refractory metals that are not amenable to full dissolution from glass using SW-846 methodologies. In such cases, equivalent SW-846 QC protocols shall apply, as appropriate to the dissolution method.

^(d) DCP/AES = direct coupled plasma/atomic emission spectroscopy, subject to the same QA/QC as SW-846 method 6010B
 Deviations to this table will be negotiated on a case-by-case basis

Table 3-8 Inorganic Preparative QC - All Inorganic Analytical Techniques (except pH)

QC Samples	Frequency	Acceptance Criteria	Failure Action
Preparation Blank (PB)	1 per batch	< EQL	Investigate. Determine usability by evaluating against analyte concentration in sample. Re-prepare, as appropriate.
Blank Spike (BS) ^(a)	1 per batch	80 % to 120 %	Investigate. Re-prepare for failed analytes.
Laboratory Control Sample (LCS)	1 per batch	Vendor specs/regulatory requirements/statistical	Investigate. Re-prepare for failed analytes.
Matrix Spike Duplicate (including Matrix Spike Duplicate (MSD))	1 per batch	± 20 % RPD, when result 10 times IDL	Investigate. Discuss in narrative.
Matrix Spike	1 per batch	75 % to 125 % recovery	Investigate. Post spike for ICP and Flame Atomic Absorption Spectroscopy (FLAA) for failed analyte. Discuss in narrative.

^(a) Techniques where the ICV analytical standard (ICV) is prepared with the samples; the ICV can serve as the blank spike.

Table 3-9 Inorganic Analytical QC - All Inorganic Analytical Techniques (except pH)

QC Samples	Frequency	Acceptance Criteria	Failure Action
Inductively Coupled Plasma Spectrometer and Flame Atomic Absorption (FLAA) and DCP			
ICV	Immediately after calibration (typically mid-range).	90 % to 110%	Investigate failure for analytes of interest. Recalibrate for analytes of interest.
Initial Calibration Blank (ICB)	After ICV	<EQL	Investigate failure for analytes of interest. Recalibrate for analytes of interest.
Continuing Calibration Verification (CCV) Standard	After every 10 samples and at the end of analytical run.	90 % to 110 %	Investigate failure for analytes of interest. Recalibrate for analytes of interest. Reanalyze samples, as appropriate.
Continuing Calibration Blank (CCB)	After every CCV.	< EQL	Investigate failure for analytes of interest. Recalibrate for analytes of interest. Reanalyze samples, as appropriate.
Low-Level Standard (LLS) ^b	Immediately after ICB.	75 % to 125 %	Investigate. Discuss in narrative.
Interference check standard (ICP only)	After ICB and just before last CCV.	80 % to 120 %	Investigate. Reanalyze all samples.
Serial dilution	One per batch as required or needed.	=10 % difference, when analyte 10 times EQL after 5-fold dilution	Investigate. Discuss in narrative.
Post spike	MS fails or new and/or unusual matrix is being analyzed.	75 % to 125 %	Investigate. Discuss in narrative.
ICP/MS			
ICV	Immediately after calibration (typically mid-point region).	90 % to 110 %	Investigate failure for analytes of interest. Correct. Recalibrate for analytes of interest.
CCV	Every 10 samples and at the end of the run.	90% to 110%	Investigate failure for analytes of interest. Correct. Recalibrate for analytes of interest.
ICB	After ICV.	< EQL	Investigate failure for analytes of interest. Correct. Recalibrate for analytes of interest.
CCB	After each CCV.	< EQL	Investigate failure for analytes of interest. Correct. Recalibrate for analytes of interest.

Table 3-9 Inorganic Analytical QC - All Inorganic Analytical Techniques (except pH)

QC Samples	Frequency	Acceptance Criteria	Failure Action
Interference check standard	After ICV and ICB and every 12 h.	Monitor for interference that will impact samples.	Investigate. Correct/Reanalyze/Flag.
Serial dilution	One per batch of samples prepared or when internal standard criteria failure occurs.	± 10% difference when analyte 100 times IDL	Investigate for analyst error. Discuss performance in narrative.
Post spike	When MS fails or when new or unusual matrix is encountered.	75 % to 125 %	Investigate for analyst error. Discuss performance in narrative.
Internal standard	Every sample, QC sample, blank, and standard.	30 % to 120 %	Perform serial dilution. Evaluate. Correct/Report.
Mercury, Cold Vapor Atomic Absorption (CVAA)			
ICV ^(a)	Immediately after calibration (typically mid-range).	90 % to 110 %	Investigate. Recalibrate.
ICB	After ICV.	< EQL	Investigate. Recalibrate.
CCV	After every 10 samples and at the end of analytical run.	90% to 110%	Investigate. Recalibrate. Re-prepare and reanalyze samples, as appropriate.
CCB	After every CCV.	< EQL	Investigate. Recalibrate. Re-prepare and reanalyze samples, as appropriate.
LLS ^b	After ICV and ICB.	75 % to 125 %	Investigate. Discuss in narrative.

Table 3-9 Inorganic Analytical QC - All Inorganic Analytical Techniques (except pH)

QC Samples	Frequency	Acceptance Criteria	Failure Action
Spectrophotometric			
ICV	Immediately after calibration.	90 % to 110 %	Investigate. Recalibrate.
ICB	After ICV.	< EQL	Investigate. Recalibrate.
CCV	After every 10 Samples for working-curve technique; at the end of the run for all other techniques.	Based on long-term statistical performance.	Rerun all samples since last valid.
CCB	After each CCV.	< EQL	Rerun all samples since last valid.

^(a) If the ICV is representative of the sample matrix and prepared with the samples, then the ICV may be used as both the BS and ICV.

^(b) The LLS is used to monitor instrument performance in the region at or near the EQL and is routinely applied to inorganic systems to monitor sensitivity in the EQL region. For ICP spectrometry systems, the LLS should be prepared at approximately 2 times the EQL. The majority of other inorganic techniques employ an LLS that is at or near the EQL. In those cases where it is used as part of instrument calibration, a separate LLS is not required.

Figure 3-1 Summary of Approach for Establishing the Regulated COPCs for Delisting IHLW

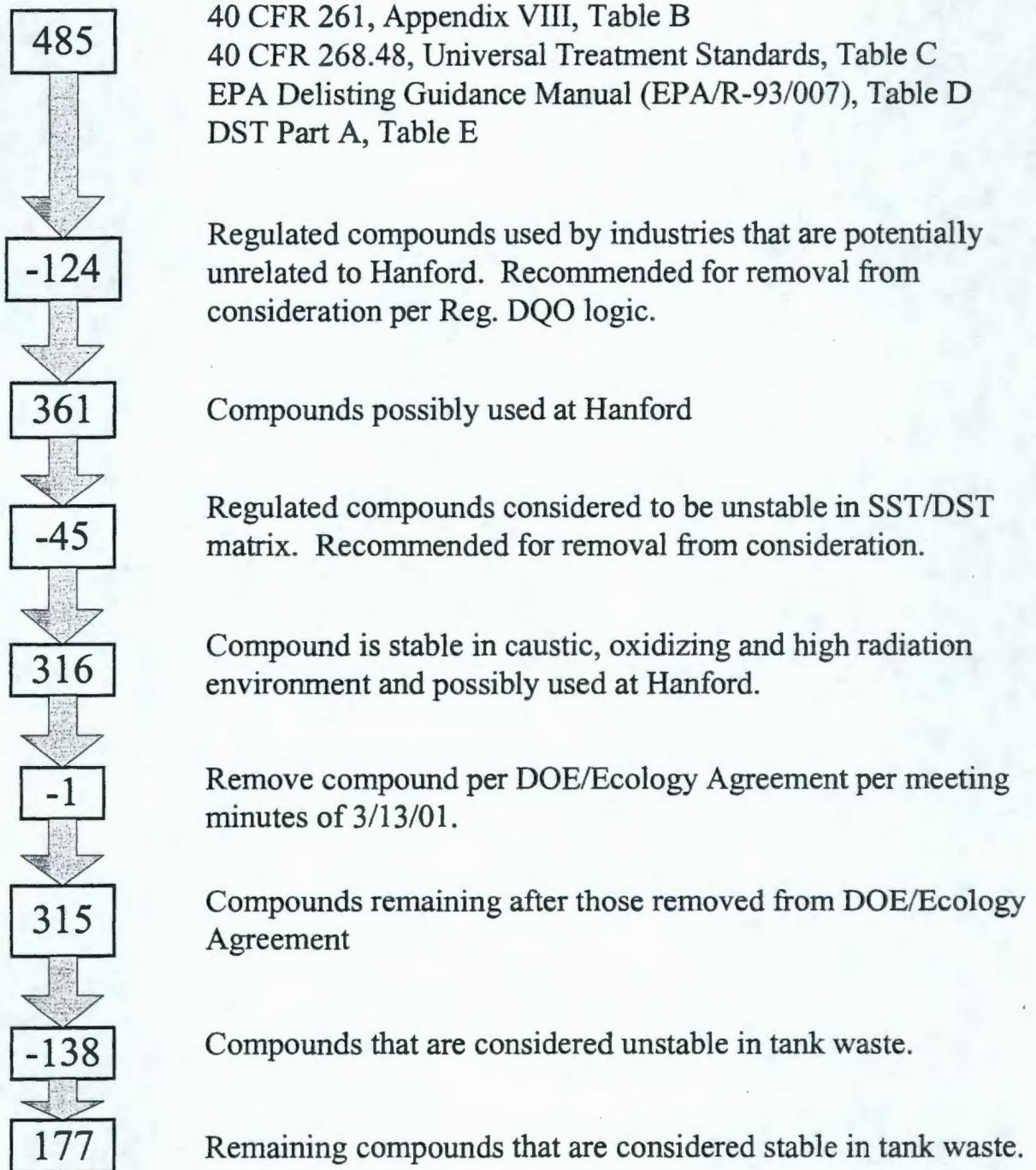


Figure 3-2 Establishing Regulated List for COPC Selection for Delisting IHLW (p. 1 of 2)

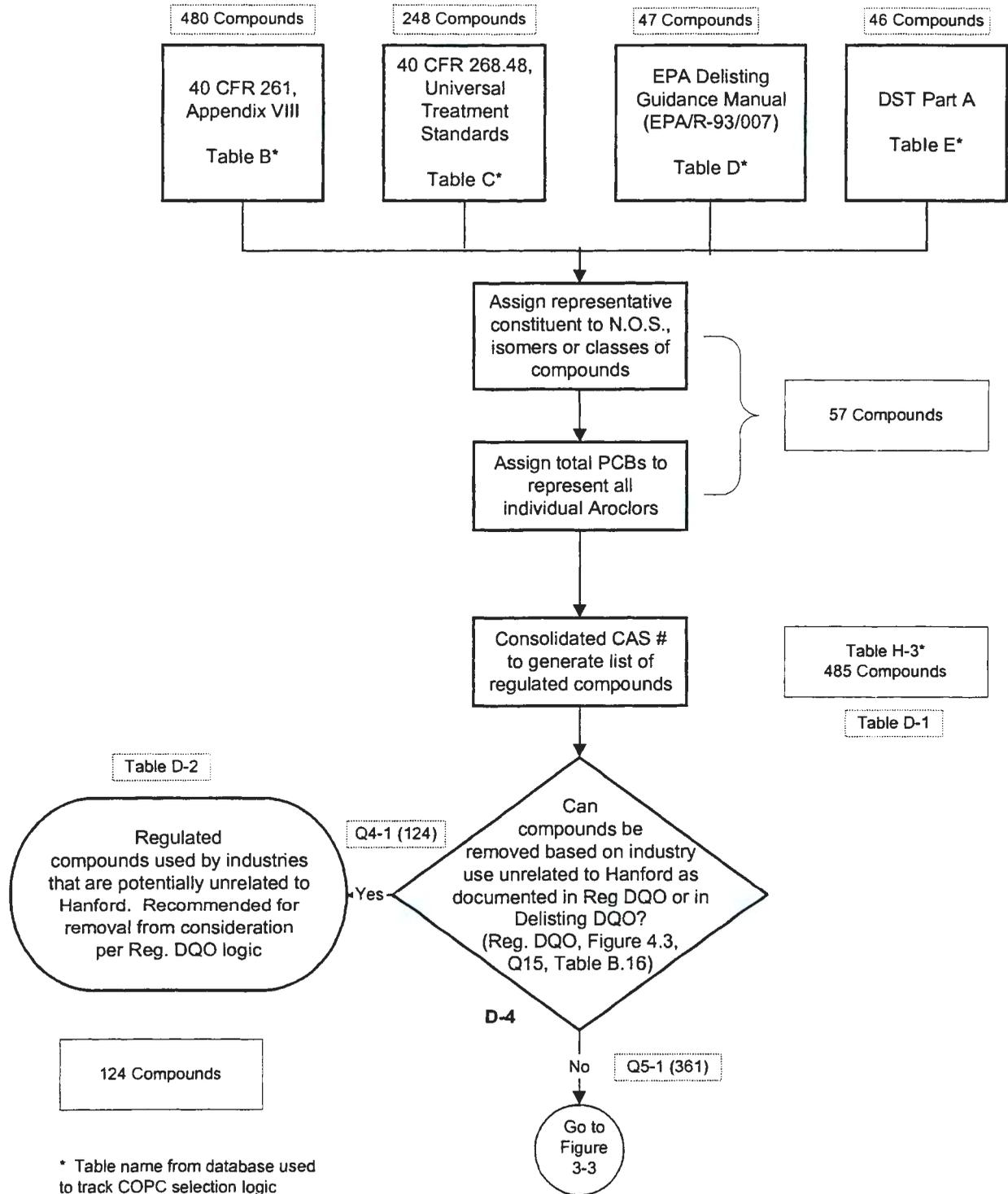


Figure 3-3 Establishing Regulated List for COPC Selection for Delisting IHLW (p. 2 of 2)

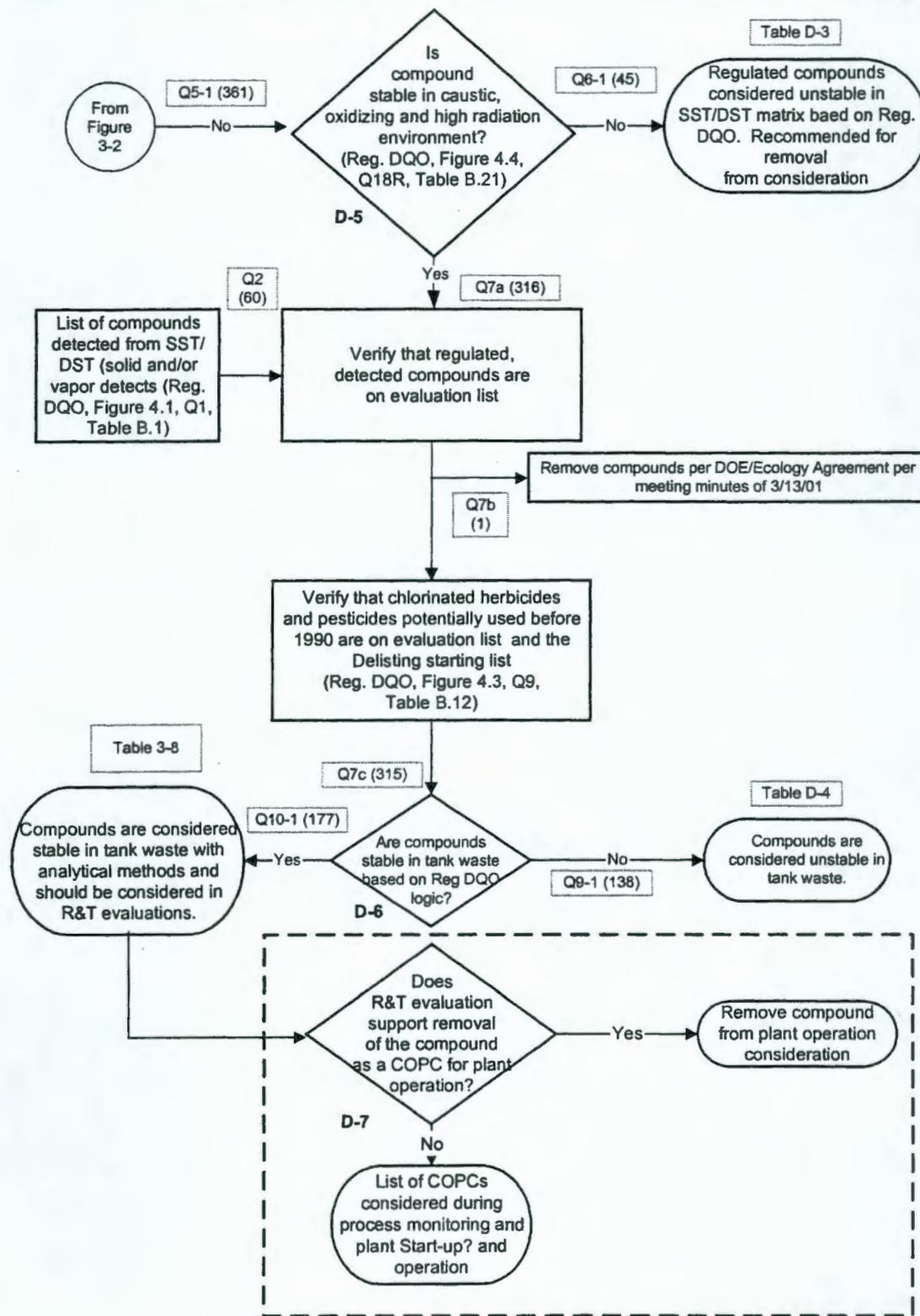


Figure 3-4 Summary of Approach to Establish Regulated List for COPC Selection for LDR

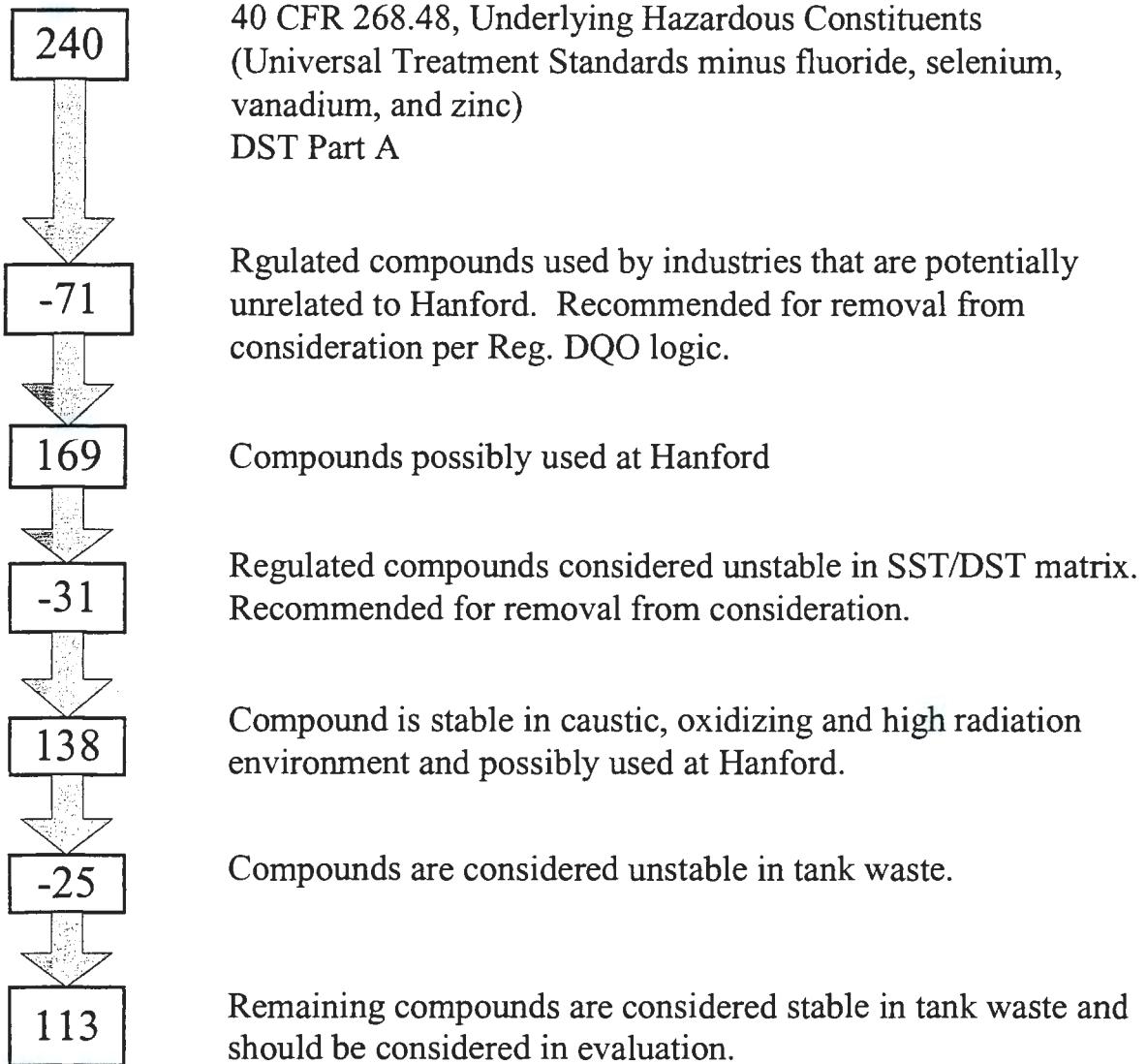


Figure 3-5 Establishing Regulated List for COPC Selection for LDR Evaluation of IHLW and ILAW (p. 1 of 2)

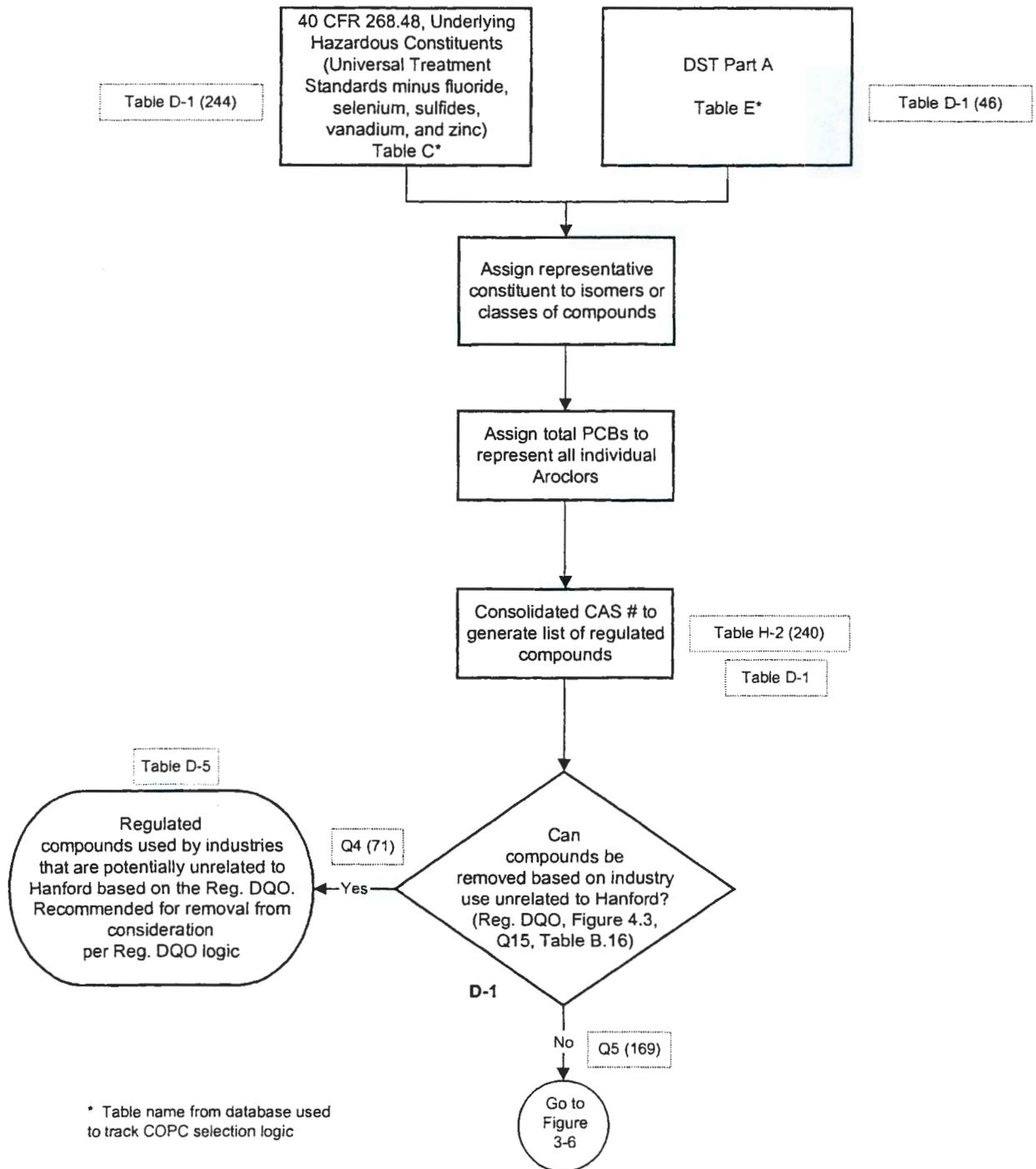
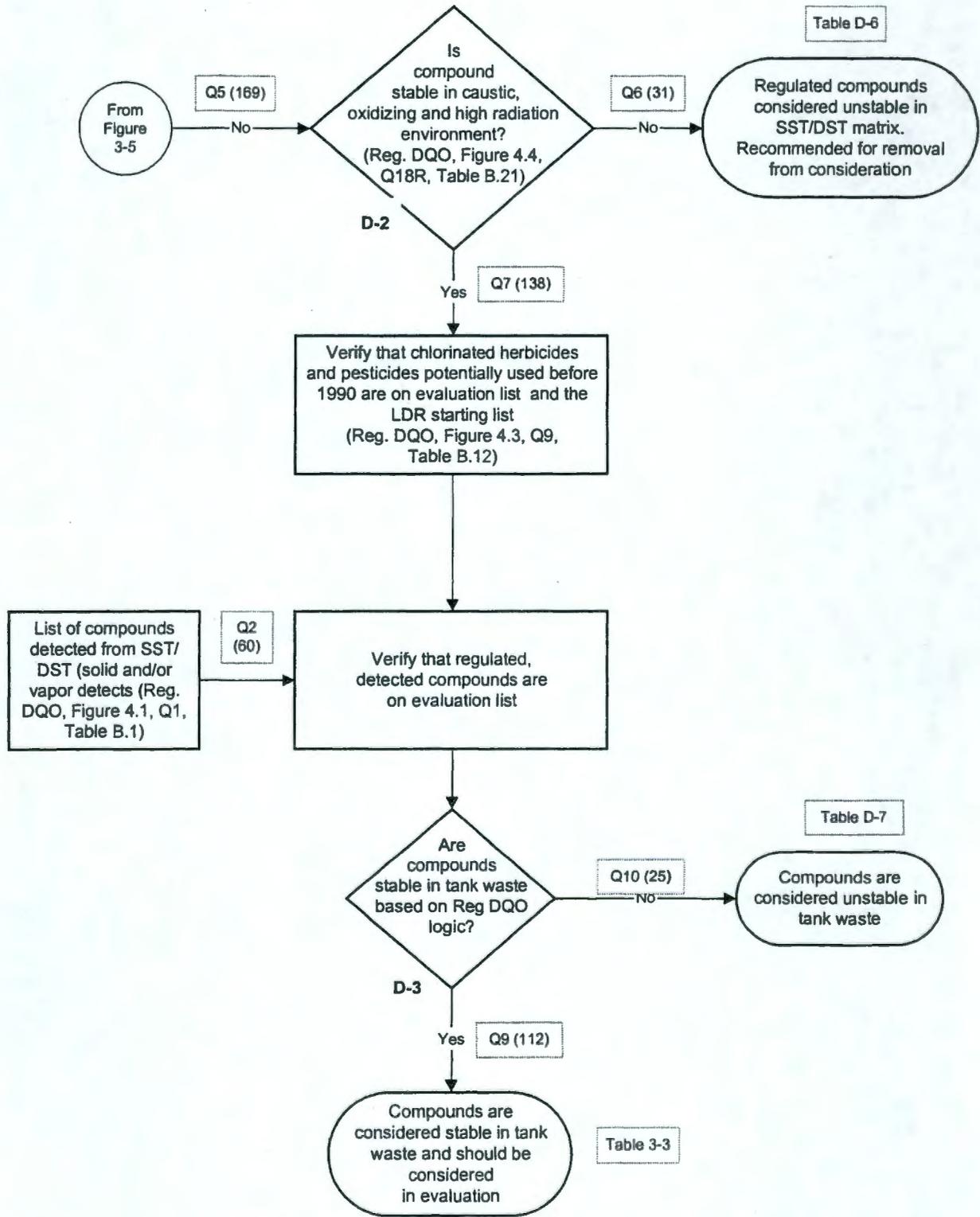


Figure 3-6 Establishing Regulated List for COPC Selection for LDR Evaluation of IHLW and ILAW (p. 2 of 2)



4 Step 4 - Define Boundaries

In step 4 of the data quality objectives (DQO) process, the study boundaries are defined. The “study boundaries” include the constraints of data collection and the applicability of the decisions to be made based on the data to be collected. Additionally, step 4 helps to establish well-defined targets for the study so that data interpretation will be focused and facilitate a clear decision. In step 4, the study population (source of the samples to be collected), physical, temporal (time-related), and practical constraints to data collection are summarized along with the scale (or applicability) of the decision so that an optimal data collection approach can be formulated in later DQO steps.

4.1 Population of Interest

The population of interest for this DQO process is the contents of the vitrified glass, which must comply with delisting requirements for IHLW, and comply with the land disposal restrictions for both ILAW and IHLW. Because DOE and the WTP intend to seek approval of a treatability variance that will establish vitrification as the specified treatment for Hanford tank waste for all waste codes and hazardous constituents, and to develop an upfront petition to support delisting the glass product, the ability to achieve compliance will be shown through the data generated by a research and technology (R&T) program. The R&T program is intended to show that waste that undergoes the proposed treatment process will meet the applicable delisting criteria and LDR treatment standards established through a treatability variance. Therefore, the population of interest for the purposes of this DQO process include the data that describe the characteristics of feed materials from tank waste, and simulants spiked with COPCs developed to determine the behavior of feed materials in the glass-forming process. In addition, the data developed from an evaluation of the glass-making process and the glass are critical to an understanding of the suitability of vitrification as a waste treatment process for the tank wastes.

The pretreatment products, up until CRV contents, are not included in the population of interest. Pretreatment is intended primarily to remove the specific radioactive elements from LAW and reduce the moisture content of LAW and HLW feed materials. As discussed in Section 1, the final control point for processing is CRV. Variability in the CRV content is accommodated by the addition of GFCs. The WTP does not claim credit for any destruction of organics through pretreatment activities. Accordingly, the pretreatment processes are not considered within the population of study parameters.

4.2 Physical Boundaries

Although the initial stages of operation for the WTP will be concerned with a limited subset of the Hanford double-shell tanks (DSTs) defined by the tank waste feed envelopes, the data that will be developed during the R&T program may be used to support regulatory determinations for all of the tank waste currently stored at the Hanford Site. Data must be generated to support petitions to delist IHLW and support an LDR treatability variance for IHLW and ILAW. Data are required to show the constituent makeup of the tank waste and any simulants of that waste, as well as any glass product that is produced from the bench-scale and pilot-scale treatment of these waste forms during R&T. These data should include qualified analytical results that describe the following materials:

- Constituent makeup of feed to the melters
- Glass to be disposed of in a non-RCRA facility (federal high-level waste repository, delisting). Objectives include demonstrating that the final waste form is delistable.

- Glass to be disposed of in an RCRA land disposal facility (LDR treatability variance). Data are required that demonstrate a substantial reduction in toxicity and mobility for all immobilized waste so that short-term and long-term threats to human health and the environment are minimized.

The decisions to apply for an LDR treatability variance and to delist IHLW, will apply to the Hanford tank waste as processed by vitrification. The WTP contract for design and initial startup of the WTP requires the facility to treat the waste represented by a specific subset of tanks. These tanks were selected to represent a significant portion of the total tank inventory. These tanks and their characterization will be used to demonstrate the efficiency (acceptability) of the treatment process (vitrification). Statistically designed simulated waste will be used to provide additional information regarding the treatment process (e.g. to define QGCR boundaries for constituents that are not contained in the specified waste tanks at levels that could potentially adversely affect glass quality, refer to Section 2 of Appendix C). The combined information from the subset of tanks specified by contract and the simulated waste will be used to ensure acceptable glass compositions may be produced for waste tanks yet to be characterized. It may be necessary to revisit the delisting and LDR treatability variance prior to processing wastes not currently scoped by the WTP Contract.

Because of known variations in the tank contents, the tanks have been categorized into envelopes that represent the constituent makeup of the wastes. R&T is being conducted based on the constituent concentration of these envelopes. Table 1-3 lists the envelopes and the associated tanks that fall within each envelope that will be evaluated through the R&T program.

The physical boundary (constituent concentration range) for the entire population of wastes in all tanks is represented by the contents of the combined constituents of the various envelopes. The envelopes that are described in Section 1.5, which represent those tanks listed in the contract specifications, represent the populations (range of constituents) currently undergoing testing within R&T. Note that by the time the LAW waste gets to the melter, the distinction between Envelopes A, B, and C largely disappears because of incidental blending. Data developed from the performance evaluation of materials representative of Envelopes A, B, and C feed (pretreated waste and simulants) will be used to support decisions regarding land disposal of ILAW. Data from the performance of Envelope D wastes and simulants of those tank wastes will support decisions related to the delisting strategy for IHLW destined for deep geologic disposal. Because of the concern over exposure to laboratory personnel associated with sampling of actual tank waste and the resulting glass form, much of the R&T program will be based upon the development of simulated wastes. The performance of these simulants will provide the primary basis for evaluating the performance of the waste glass.

As noted above, this DQO process is intended to establish the criteria and parameters for the sampling program that will provide data to support petitions for a treatment variance and delisting. To the extent that the contents of these tanks are representative of subsequent tank waste, the results of these analyses may support future compliance determinations for other tanks.

The current approach for the final waste-form verification is described above. In order to verify the WTP treatment technology, R&T will generate test glass produced from feed envelopes, as previously described in Section 1.5, using both simulants and active waste. The test glass from the R&T envelopes serve as the boundary for the data generated from this DQO process, and will define the qualified glass composition region (QGCR).

4.3 Temporal Boundaries

4.3.1 Timeframe for Decision Making

The criteria established from this DQO process will initially apply to the generation of data prior to the startup of the WTP. These data will support petitions to regulators relating to LDR and delisting compliance for treated tank waste (ILAW and IHLW). These data requirements will be refined as information is generated through the R&T process, key operations parameters, and as indicator constituents are identified.

4.3.2 Timeframe for Data Collection

Successful implementation of the DQOs will require integration with the R&T testing program through test specifications that will implement the data collection requirements, along with the appropriate quality assurance (QA) and quality control (QC) requirements. During R&T, constituent concentrations will be measured before and after vitrification in order to provide data pertinent to decisions. EPA SW-846 (EPA 1997) holding times will generally be applicable to the simulated waste and corresponding vitrified products. For radioactive waste samples, information gathered through the Regulatory DQO implementation process will be used to adjust SW-846 prescribed holding times, if appropriate.

Data collection must be completed in time to support petition development during fiscal year 2003, which is a contractual requirement for the WTP. It is intended that DQO implementation will be prior to commissioning and operations.

4.4 Practical Constraints

Practical constraints must be considered to facilitate the optimization of data collection activities. The following subsections qualitatively describes various project constraints.

4.4.1 Financial/Schedule Constraints

R&T activities support both design- and compliance-related decisions from the same budget. For this reason, it is vital for the WTP to implement the R&T testing program in a cost-effective fashion, so that there remains a sufficient contingency funding for analysis of unanticipated problems and alternative designs.

Handling and sampling of radioactive material warrant special precautions and considerations (e.g., conducting work processes in accordance with the ALARA principles, radiation monitoring, reduced sample sizes etc.) that eventually result in higher costs relative to non-radioactive material testing. Accordingly, the focus of the R&T testing will be with simulated non-radioactive wastes. It is anticipated that only a limited amount of radioactive waste testing will be required for confirmation. In addition, the bulk of R&T testing will be on a small scale, with limited large-scale tests for assessment of scaleup issues.

As previously discussed, the R&T testing program has a very compressed schedule. R&T testing to support both compliance and design must be completed so that all necessary design changes are incorporated in time to support WTP construction. Additionally, once a test melter is removed from service, re-start is not possible.

Cost and schedule considerations are drivers for maximizing waste loading in the glass. Neglecting impacts to capital and miscellaneous operations costs, and accounting only for those costs directly related to the volume of glass produced, there is a direct relationship between the annual volume or metric tons of glass produced and the associated costs. There is, however, an inverse relationship between the waste loading in the glass produced and cost (higher waste loading results in lower cost). Figure 4-1 illustrates this inverse relationship, and how reductions in the waste loading result in increased costs for waste treatment.

It can be argued that the nominal glass production rate (volume or weight per-unit-time) can be increased to offset operations costs, maintenance costs aside. The current baseline design (24590-DB-ENG-01-001) for a HLW melter has contingency to allow for a 100 % increase in the nominal throughput (from 1.5 MTG/day to 3 MTG/day). Conceivably, reductions in waste loading can be accommodated by increasing throughput, and annual operations costs, as a function of annual canister production, may appear to decrease, since more glass would be produced. However, since the waste loading is reduced, the actual cost-per-unit of waste treated would actually increase. Additionally, assuming a 30 % nominal waste loading, a decrease to as low as 11 % could result in the need for glass production at capacity, with elimination of any contingency melter downtime. Decreased waste loading beyond that point would push the completion of processing the initial candidate tanks beyond the target date of 2018.

In summary, waste loading is a key factor to be balanced with project economics, as well as processability. Reductions in waste loading will ultimately result in increased quantities of glass and associated costs, and potential impacts to the WTP processing schedule. Furthermore, increased glass production is counter to policies of waste minimization, and would eventually impact disposal facility storage capacity.

4.4.2 ALARA Constraints

Radioactive waste poses health hazards to all personnel required to handle the material. In addition, to keep these hazards minimal, special handling precautions are taken to shield personnel from exposure. Equipment, such as gloveboxes, hoods, and remote manipulators, are often employed. These physical limits pose logistical challenges to the analytical facility, which ultimately increase sample handling and analytical error. Measurements made at the Savannah River Technology Center (CCN 030691) have indicated that dose rates as high as 2 rem/hour/gram whole body (gamma) for a 100 gram sample of Hanford IHLW. The DOE radiation annual dose limit would be met by handling this sample for only 3 minutes. The size reduction required to comply with the laboratory dose limits for contact handled samples (5 mRem/hour whole body - gamma) results in a final sample size of only 2.5 grams for IHLW. Both ILAW and IHLW glasses give beta (extremity) dose rates in excessive amounts unless shielded. A 1/2 inch thick high-density polyethylene plate can shield about 95-98 % of the beta dose. Only a very small portion of glass can be removed from behind the shielding for analysis. The beta radiation dose is very dependent on geometry, orientation and shielding. Beta radioactivity is difficult to predict and/or manage. Beta radiation from only the outer few millimeters of the sample surface can be released into the environment, however, grinding to increase surface area, as required for TCLP analysis, will increase the beta emissions. The dose limits specified in 10 CFR 835 often require that sample sizes be reduced below the SW-846 requirements, in order to lower dose. This sample-size reduction can result in elevated detection limits (DLs). Since detection limits need to support decisions, this is a valid consideration and a very real constraint to effective data collection.

4.4.3 Simulants

The analytical work planned in association with this DQO will be based on the use of inactive simulants. Joint NRC and EPA guidance on testing requirements for mixed wastes support reliance upon non-radioactive simulants. The guidance emphasizes the use of simulant materials as long as they are “chemically identical to the mixed waste and faithfully represent the hazardous constituents in the waste mixture” (EPA/NRC 1997).

Historically, glass development testing reveals that minor constituents are not generally composition affecting unless there is very strict performance criteria associated with them such as a very low numeric performance standard. Generally, the glass composition is not affected dramatically (e.g., glass durability is not impacted) until compound concentration exceeds 0.5 percent by weight. Use of simulants provides a cost-effective means of verifying this assertion prior to glass production with real waste.

Spiked simulants used will likely have to represent both bounding conditions and nominal operating conditions. Simulant requirements are detailed in Appendix F of this document. Simulant formulations for nominal feeds are compared directly to TFCOUP data (CHG 2000) and/or characterization data (as it becomes available) to ensure representiveness.

Simulants will be required for both LAW and HLW within each of the sub-envelopes previously identified. Spikes will be added as necessary to create “bounding simulants” that represent wastes with uncharacteristically high levels of regulated constituents. Likewise, a range of spiked simulants will be required to fully define the qualified glass composition region (QGCR) for some of the COPCs that potentially leach from the glass at or near the ALs.

Testing with simulants spiked with metals, however, has the following limitations:

- Characterization of the waste feed being simulated and spiked must be well known
- To compensate for variations in waste feed, and the limited availability of characterization data, a number of statistically designed simulants may be required. Statistically designed simulants are those simulants designed to mimic the potential extremes of waste feed concentration on a per constituent basis. They are typically designed to cover that portion of the glass composition region that overlaps, but may not necessarily include the waste feed as described by available tank characterization data. Statistically designed simulants are custom designed to populate that portion of the QGCR not otherwise represented by nominal feeds and thus, comparison to tank data is not necessarily appropriate for statistically designed simulants.

Additionally, another approach to minimizing the impact of limited characterization data to simulant design is to design experiments with the constituents of interest, and their impact to vitrification, in mind. Spiking constituents well beyond their reasonably anticipated concentration will provide information that can be used to bound the acceptable level of constituent concentration for a given QGCR. Such an approach may also warrant the development of multiple QGCRs in order to optimize waste loading as well as compensating for potential variability in the melter feed. This will be discussed in greater detail in subsequent sections of this document.

- Unexpected complications associated with the real waste feed may not be represented by a spiked simulant.
- Combined or competing effects of the real waste feed may not be represented by a spiked simulant.

Laboratory observations reported in discussions with WTP personnel have indicated potential problems with spiking the LAW simulants to the more extreme concentrations. Generally, as the solubility level for an inorganic spike is approached, the spiked inorganic drops from solution, effectively settling out such as would be expected in HLW waste. Solubility limits will bound the amount of COPCs that can be spiked into simulated LAW feed. It will be incumbent upon the WTP to ensure that solubility limits of simulated LAW are representative or bounding of those indicated by the COPC concentration in real pretreated LAW. This will primarily be done by comparing the simulant formulation directly with existing waste analysis data to ensure simulants are valid for use according to their intended purpose.

Simulant evaluations for tank waste representativeness will be performed on a case by case basis. Since the QGCR will include extremes and intermediate concentrations of the range of pretreated tank waste constituent levels, simulant results are useful in expanding the glass composition database regardless of their degree of representativeness. Section 7 and Appendix E of this DQO describe the details of a research program to develop TCLP response models. The models will quantify the synergistic effects of the waste constituents in the vitrification process. Until these effects are quantified, it would be premature to specify criteria for simulant representativeness. Likewise, the uncertainties of those models will be quantified, and will provide input for the analysis of simulant representativeness. For example, as explained in Appendix E, a linear regression coefficient is multiplied by the concentration of the constituent of interest for a given simulant/glass composition. In cases where data indicate that coefficient is very low, variations of melter feed constituent concentration may have little to no detectable impact on glass TCLP durability. In such cases, it would not be appropriate to consider a precise comparison of simulant to actual pretreated tank waste a valid measure of representativeness for that particular constituent. The reverse may be true for those constituents shown to have a dramatic effect on TCLP durability with increased concentration. In such situations, a precise comparison of simulant to pretreated tank waste may be required to ensure simulant representativeness for the constituent of interest. The degree of precision required will be an output of the model uncertainty analysis.

4.4.4 Spike Levels, Solvents, and Solubility Limits

Spike levels are constrained by solubility and by the solvent used. Spike levels should generally not be above solubility limits, as inorganics tend to precipitate from the LAW fraction of the waste, effectively becoming HLW components, which are normally removed through ultrafiltration. Spike material shelf life and stability should be considered, as well as ease of handling and toxicity.

4.4.5 Model Performance/Uncertainty

Models are used to determine the glass former chemicals (GFCs) required for a given feed stream. Model performance and uncertainty is a constraint in that the R&T process is an iterative one by which models are used to predict GFCs for the waste, tests are run, uncertainties assessed, and additional testing performed, until desired confidence around the QGCR is attained. Fortunately, the extensive history of glass testing can be used to provide a basis for initial assessment of uncertainty about the model. However, it is not possible to remove all uncertainty. Models developed from fewer data are prone to a greater level of uncertainty. The WTP can accept this consequence for those constituents of less concern (constituents with little impact to glass quality); however, for constituents shown to approach limits when subjected to TCLP, many data points may be required in order to minimize composition model uncertainty.

4.5 Scale of Decision

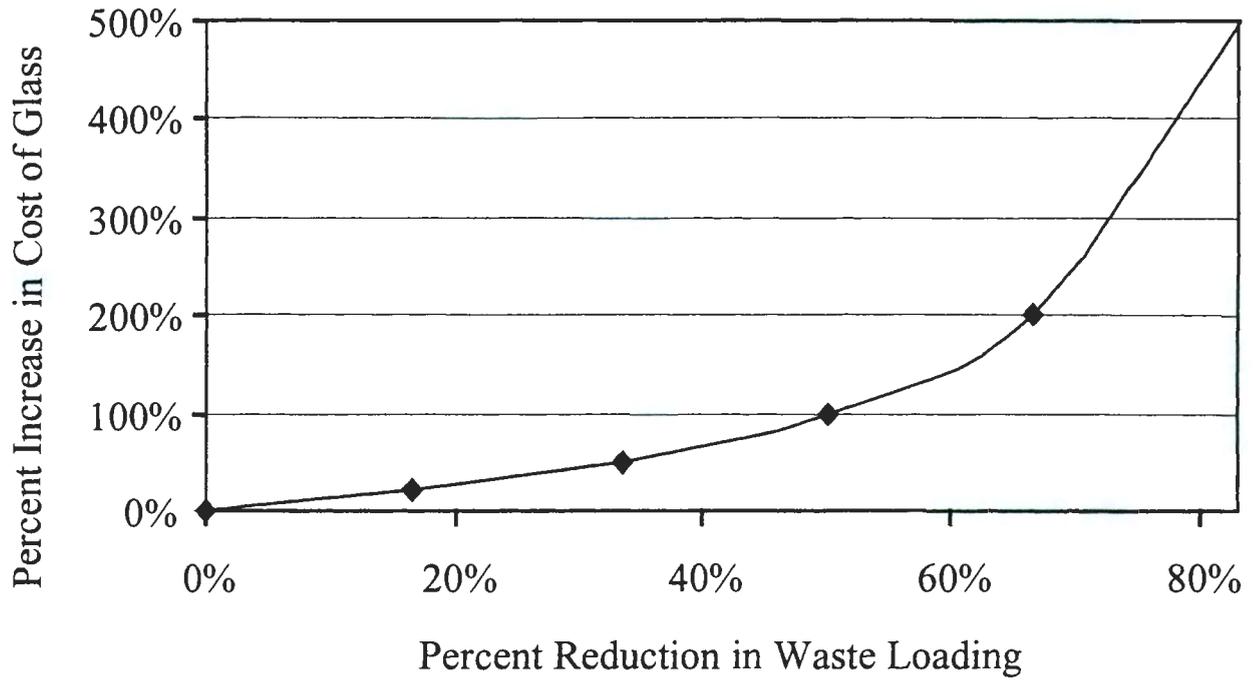
The scale of the decision is the extent of decision applicability with regards to an “exposure unit”, and is whatever serves to bound the decision with respect to a physical or time boundary. An exposure unit is a segment of the population corresponding to the conceptual site model, such that the data collected can be applied to make a decision regarding that exposure unit.

There are two scales of decision for the entire project. The first is the scale that applies to R&T, and that is the subject of this DQO; the second scale is that ultimately used once the R&T work is completed, and delisting and LDR petitions are generated.

For the R&T process, the scale is the set of concentration boundaries that represent each envelope of waste based on the COPCs, glass formers, and modifiers.

The ultimate boundary for both delisting and LDR is the QGCR, which will be generated based on the results from the modeling and data collection from the R&T work described in this DQO.

Figure 4-1 Percent Cost Increase vs. Waste Loading Reduction



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5 Step 5 - Decision Rule

The purpose of step 5 of the data quality objectives (DQO) process is to define the statistical parameter and associated statistic of interest (for example, population mean and 90th percent upper-confidence interval), specify the action level, and integrate outputs from the previous DQO steps into a single statement that describes a logical basis for choosing among alternative actions.

5.1 Statistical Parameter and Associated Statistic of Interest

A one-sided, 90th percent upper-confidence level (90 % UCL) of the mean is the recommended statistic of interest. A 90 % UCL is consistent with the original draft of the *Waste Treatment Plant Waste Analysis Plan* (24590-WTP-RPT-ENV-01-003). This plan has since been modified to reflect a sampling program that would be consistent with the outcome of the land disposal restrictions (LDR) and delisting petitioning processes; however, the 90 % UCL has been retained as a DQO to ensure any statistically based sampling approach will adequately address the decision to be made. Chapter 1 of SW-846 recommends the one-sided 90 % UCL. Step 6 provides additional discussion of the applicable statistics.

The contaminant distribution in the concentrate receipt vessel (CRV), as represented by the simulant, and glass (populations of interest), is assumed to be homogenous due to the substantial amount of blending and treatment that occurs in the waste-feed pretreatment process.

5.2 Action Levels

Action levels (ALs) are required to make an evaluation as to whether the data generated through the research and technology (R&T) program demonstrate that treated waste forms will meet regulatory criteria. Action levels to support these decisions for delisting and LDR compliance were presented in Section 3.2. The output from the delisting risk assessment software (DRAS), which summarizes the delisting ALs, is provided in the last two columns of Table 3-6.

As noted elsewhere in this DQO, there are no set criteria established in the LDR program to measure the suitability of an alternative treatment technology. The proposed treatment, however, must "minimize threats to human health and the environment posed by land disposal of the waste" (40 CFR 268.44(h)). In order to conduct a screening of the treated wastes and simulants against this standard, the concentrations of the constituents of potential concern (COPCs) in the glass forms will be compared against the relevant criteria found in Tables 3-4 and 3-6. Although the delisting concentrations found in Table 3-6 are, in some cases, higher than universal treatment standard (UTS) limits for compounds found in Table 3-4, the DRAS output concentrations consider health-based exposures, and are an appropriate standard for consideration when evaluating the threat to human health and the environment. For many of these constituents, concentrations from glass samples may well be lower than both the DRAS and the UTS limits; however, if results are higher than the UTS value, but lower than the DRAS limit, the delisting standard will provide the basis for a decision whether or not to proceed with a petition for the LDR treatability variance. As discussed elsewhere in this DQO, these decisions will be made based primarily on the results of the testing of waste formulations using simulants and their resulting glass form.

The action limits for delisting are based on the EPA required DRAS modeling. The action limits for LDR are based on minimizing threats to human health and the environment posed by land disposal of the waste

and allows the project to propose alternate treatment standards. Data will be evaluated against the DRAS levels and the LDR Universal Treatment Standards (UTS). However, should the results be above the UTS and below the DRAS, the delisting standards will serve as the action level.

5.3 Decision Rules

The decision statements (DSs) from step 2 are reformatted in Table 5-1 into decision rules (DRs), based on the inputs and boundaries established in steps 3 and 4.

5.4 Action Levels and Estimated Quantitation Limits

Table 5-2 lists the lowest potential ALs for delisting as determined from Table 3-6 and the anticipated estimated quantitation limits (EQLs) for the simulant, tank waste, and in the glass. The EQL must be based on a documented factor, multiplied by the method detection limit (MDL). The EQL and MDL must be determined per Chapter 1, SW 846 methods. The Regulatory DQO requires the development of MDLs, EQLs, and finally a consistent approach for presenting experimental EQLs in tank waste.

The EQLs presented in Table 5-2 for the waste are consistent with the approach discussed and agreed upon by DOE and regulators in test plans that implement the Regulatory DQO. The simulant EQLs presented are reporting levels from a standard commercial environmental laboratory, and are based on recent analysis performed on inactive simulants. The EQLs presented for the active waste (as derived from ongoing Regulatory DQO work) represent anticipated EQLs that result from the limited sample size and dilution typically needed for analysis of the high-sodium/high-ion radioactive tank waste. The EQLs presented for the TCLP extract (be it vitrified simulant or waste) represent those EQLs anticipated for a buffered acetic acid solution. This is feasible since the glass matrix of the vitrified simulant/waste will immobilize most of the interfering constituents. Table 5-2 is presented to provide information to indicate potential problems and limits for the analytical methods, given the issues associated with the analysis of a high-sodium/high-ion radioactive matrix. Optimally, the EQL should be below the AL if undetected or if estimated analytical results are to be used to support decision making relative to the decision rules of this DQO. These issues are discussed in the subsections that follow.

Each column in Table 5-2 is discussed below. The values presented are from work in progress and are not currently available in other documentation. They are considered "draft" and are subject to change.

Columns A and B. The Chemical Abstracts Service (CAS) number and the compound names are from Table 3-1.

Column C. This column indicates the anticipated analytical method, along with associated preparation and leach methods and the relevant matrix. Actual preparation and analytical methods may vary from the particular SW-846 methods shown, but will be SW-846 methods. The final preparation and analytical methods used will be consistent with the data use. Matrix cleanup may be required in certain situations. For the total metals analysis of the glass, the 3052 method is specified and this method is a total digestion of the glass. Method 3052 will provide higher results than the 3050B method. Method 3050B is a nitric acid dissolution of the surface. Method 3052 presumably provides data on total glass composition for regulated inorganics of interest and is suitable for validation of TCLP response models, however, most total metals for EPA delistings are analyzed using 3050B. Other methods, such as ASTM methods, may be required for total glass dissolution, and their use will be evaluated in the event of incomplete dissolution using SW-846 method 3052. However, for simplicity's sake, the ASTM methods have not

been evaluated in Table 5-2 below. There may also be situations where preparation by method 3050B is used to facilitate comparison of glass performance to other waste forms typically prepared by method 3050B; thus, method 3050B is in Table 5-2.

Column D. The AL is from 40 CFR 268.48, Table Universal Treatment Standards (UTS). Note that limits are expressed in the concentration in the leachate (mg/L).

Column E. The AL is from Table 3-6, which listed the limit based on the lower value from either the DRAS/MCLs, or toxicity characteristic (TC) limit (Column E). Note that these are expressed in the concentration in the leachate (mg/L).

Column F. The Environmental Protection Agency (EPA) allows measuring totals in the waste and mathematically accounting for the percent moisture and the ratio of the leachate to waste ratio of 20:1 (EPA 1993c). The Department of Ecology also allows the use of total analyte values to obtain a bounding TCLP value. This column presents the TCLP limit (Column E) multiplied by 20 to compensate for the leachate ratio, and assumes 100 % solids. Multiplying the AL by 20 derives an equivalent value for determining compliance as obtaining the total result and dividing the result by 20 for waste with 100 % solids.

Columns G. The data presented are EQLs for analysis of the simulated melter feed. The EQLs are typically 10 times the method detection limit (MDL). Although inactive, the feed contains both simulated waste and glass formers, and is high in ionic content, thus the analyses are subject to matrix interferences. Actual EQLs will vary depending on simulated waste properties.

Column H. The data presented are estimated quantitation limits (EQLs) for analysis of the supernatant by the methods specified. The EQLs are typically 10 times the method detection limit (MDL), multiplied by a typical dilution factor. Occasionally, sample dilution is also required to compensate for matrix interference effects from the high sodium and high ion content of the waste. Actual EQLs will vary, depending on waste properties.

The EQLs for the waste are based on results of the Regulatory DQO. In most cases, the EQLs are based on 10 times the MDL for a water matrix, multiplied by a waste dilution factor. However, the EQLs presented for silver, arsenic, antimony, selenium, thallium, and vanadium are based on replicate waste measurements with an associated MDL computed in accordance with 40 CFR 136, Appendix B. Final Regulatory DQO data will be available in a report to be published in the future, at the conclusion of the Regulatory DQO analytical program.

Column I. The data presented are estimated quantitation limits (EQLs) for analysis of the centrifuged tank solids by the analytical methods specified. The EQLs for waste solids are based on results of the Regulatory DQO. Note that in most cases, the EQLs are based on 10 times the MDLs in spiked clean sand, multiplied by a waste dilution factor. However, the EQLs presented for arsenic, selenium and vanadium are based on replicate waste measurements with an associated MDL computed in accordance with 40 CFR 136, Appendix B. Digestions were performed based on Battelle analytical procedure PNL-ALO-129, which is based on the SW-846 solid waste digestion method 3050, using HNO₃-HCl-based digestion. The TC limits and DRAS modeling are based on the EPA acid digestion methods.

Cyanide EQLs are questionable. The analytical method is known to have sporadic recovery for the tank waste matrix.

Implementation of the Regulatory DQO is ongoing. Final Regulatory DQO data will be available in a report to be published in the future at the conclusion of the Regulatory DQO analytical program.

Column J. The data presented are anticipated EQLs for a modified acid digestion process, and are presented to provide information pertinent to the selection of the appropriate analytical method. The EQLs are based on results of the Regulatory DQO. Like the data in column H, in most cases the EQLs are based on 10 times the MDLs in spiked clean sand multiplied by a waste dilution factor. However, the EQLs presented for arsenic, antimony, beryllium, selenium, thallium, and vanadium are based on replicate waste measurements with an associated MDL computed in accordance with 40 CFR 136, Appendix B. Digestions were performed based on a modification of Battelle analytical procedure PNL-ALO-129, which is based on the SW-846 method 3050, using a more aggressive HNO₃-HCl-based digestion than that used for derivations of Column I EQLs. Details are described in Battelle test plan TP-RPP-WTP-023 (Wagner 2001).

Columns K & L. The data presented represent anticipated EQLs for the analysis of TCLP leachate from both vitrified material made of simulant and active waste. TCLP leachate is essentially buffered acetic acid solution. Based on experience to date with actual vitrified tank waste, the TCLP leachate is far less radioactive than the glass from which it was derived (in both ILAW and IHLW leachate). The EQLs of Column K were provided for the standard TC analytes by a commercial laboratory. Since the radioactive components tend to not leach from the glass, the anticipated EQLs shown in Column L are identical to those shown in Column K. Note that the reports referenced in Appendix B provide data from analysis of glass and provide MDLs for these analyses. There is some question as to whether these values are EQLs or MDLs and whether additional information on the method of determining and reporting these limits must be obtained.

Column M. The anticipated listed in Column M were obtained from a commercial laboratory and are based on totals analysis of actual vitrified simulant. They are shown to illustrate the additional sensitivity to be gained from performing a "totals" analysis for some COPCs instead of a TCLP extraction and analysis.

Note the footnotes that accompany Table 5-2. The EQLs presented are anticipated and are based on a culmination of the most recent information available at the time of table development. Actual active waste EQLs will likely be tank dependent, as will simulated feed (dependent upon the make-up of the simulant and loading). Table 5-2 is presented for two basic purposes; 1) indicate constituents for which EQLs are unlikely to be low enough to support regulatory evaluations, and 2) present information to be considered in order to specify constituent spike levels that would facilitate detection in a simulated feed or glass total analysis. The table also provides a quantitative example of the difference between analysis of active waste and glass, verses that of inactive simulated feed and the resulting glass.

Comparison of EQLs to the Action Levels

The data provided indicate that the typical EQL for TCLP leachate analysis for the glass will support decisions. The delisting values used for comparison in Table 5-2 are the lowest of the MCL (times DAF), DRAS computed value, or toxicity characteristic, and may not represent the final delisting levels established by the EPA and Ecology. Comparison of the EQL to the proposed delisting levels

summarized in Table A indicates that this achieving meaningful EQLs would still be an issue for some constituents. There are numerous cases (particularly for the solids) from the table where EQLs for waste analysis are well above action levels (comparison of columns E and F to columns H through J). Thus, analysis of the waste for total metal content will not provide data that will support decisions regarding whether it is practical to discard a particular metal from further consideration because it is simply not present in the waste at levels of concern. The data in columns H through J also indicate that, due to the dilution required to reduce sample radioactivity, non-radioactive simulants will be needed to assess the degree of immobilization achievable by vitrification for those waste streams containing relatively low concentrations of constituents. However, it is anticipated that achieving meaningful EQLs for glass TCLP leachate will not be a problem.

Requirement

Table 5-2 indicates that the EQL (TCLP analysis) for antimony and thallium may exceed the potential delisting limit, as derived from the lower of the MCL or DRAS computed delisting limit (note that none of the anticipated EQLs exceed the corresponding toxicity characteristic or UTS). Nonetheless, to the extent feasible, the requirement for this DQO is that the EQL, as applied to a specific sample (sometimes called the sample reporting limit), be below the AL for the glass. The data generated to support the petition must be based on calculations of the MDL and EQL per Chapter 1 of SW-846, and must be well documented. For a given sample, the sample reporting limit must be calculated. The sample reporting limit uses the EQL and takes into account the dilutions and, as applicable, percent solids, for a given sample. Note that for glass, the percent solids is zero. Without the sample reporting limit, one cannot assess whether the analytes are measured at a level low enough to assess whether the AL is exceeded. However, EQLs for active wastes may be significantly higher than those that may be obtainable for simulants, and sufficiently high that they may not be useable for developing delisting or LDR correlations. If neither an EQL nor a sample specific reporting limit can be achieved that is below the AL, this analytical limitation must be resolved in discussions between DOE and the regulators. In cases where the technology and the matrix will not allow detection below the AL, it is proposed that the EQL be the AL, and that non-detect results will indicate compliance with action limits.

Table 5-1 Decision Rule (DR)

#	Decision Rule (DR)
DR #1	If the data generated through the R&T process show that IHLW meets health-based delisting criteria, then an upfront, technology-based conditional delisting petition will be submitted, or else additional data to reduce uncertainty or explore alternative methods to achieve disposition of IHLW will be developed.
DR #2	If the data from vitrified LAW are adequate to support a petition to designate vitrification as an alternate treatment standard, then a petition will be submitted, or else additional data to reduce uncertainty or comply with LDR regulations will be developed.

Table 5-2 AL Versus Anticipated Estimated Quantitation Limits ⁽¹⁾

A	B	C	D	E	F	G	H	I	J	K	L ⁽²⁾	M	
CAS#	Name	Preparation & Analytical Methods	Action Levels			EQL ⁽⁶⁾ in simulated melter feed mg/kg	Raw Waste Anticipated EQLs			Vitrified Material TCLP Leachate Anticipated EQLs		Vitrified Material Totals	
			UTS ⁽³⁾ mg/kg, unless noted as mg/L TCLP	Lowest Predicted Delisting TCLP Leachate ⁽⁴⁾ (see Table 3-6) mg/L	Total ⁽⁵⁾ Analysis mg/kg		EQL in waste supernatant mg/L	EQL in waste solids (typical) mg/kg	EQL in waste solids (modified acid digestion) mg/kg	EQL ⁽⁶⁾ in Simulated ILAW & IHLW TCLP Leachate mg/L	EQL in Active ILAW & IHLW TCLP Leachate mg/L		EQL ⁽⁶⁾ in the Simulated ILAW & IHLW Total Analysis of Glass mg/kg
7429-90-5	Aluminum ⁽⁷⁾	SW-846 Method 3052 (glass prep for totals analysis)	no limit	no limit	N/A	20	18	52	69	0.5	0.5	20	
7440-36-0	Antimony ⁽⁷⁾		1.15 mg/L TCLP	0.412	8.24	TBD	16	170	39	0.5	0.5	6.0	
7440-38-2	Arsenic		5.0 mg/L TCLP	0.03	0.6	TBD	15	190	230	0.5	0.5	1.0	
7440-39-3	Barium		21 mg/L TCLP	58.6	1170	TBD	0.53	4.4	5.9	10	10	20	
7440-41-7	Beryllium		1.22 mg/L TCLP	1.33	26.6	TBD	0.034	0.36	1.3	0.5	0.5	0.5	
7440-43-9	Cadmium		0.11 mg/L TCLP	0.451	9.02	TBD	1.9	48	10	0.1	0.1	0.5	
7440-70-2	Calcium ⁽⁷⁾		no limit	no limit	N/A	500	not determined	not determined	not determined	10	10	500	
7440-47-3	Chromium		SW-846 Method 3050B (feed prep for totals analysis)	0.60 mg/L TCLP	5	100	1.0	0.71	14	23	0.5	0.5	1.0
7440-50-8	Copper ⁽⁷⁾			N/A	8420	168,000	TBD	1.8	24	40	0.5	0.5	2.5
7439-92-1	Lead		SW-846 Methods 1311/3010A (TCLP/prep for extract)	0.75 mg/L TCLP	5	100	0.3	12	200	95	0.5	0.5	0.3
7440-02-0	Nickel	11 mg/L TCLP		22.6	452	4.0	6.5	96	43	0.5	0.5	4.0	
7723-14-0	Phosphorus	N/A		no limit	N/A	30	12	140	190	2	2	30	
7440-09-7	Potassium ⁽⁸⁾	N/A		no limit	N/A	500	not determined	not determined	not determined	10	10	500	
7782-49-2	Selenium ⁽⁷⁾	5.7 mg/L TCLP		1	20	TBD	18	210	160	0.25	0.25	0.5	
7440-22-4	Silver	SW-846 Methods 6010B or 6020 (analysis)	0.14 mg/L TCLP	3.07	61.4	TBD	2.5	12	21	0.5	0.5	1.0	
7440-23-5	Sodium ^(8,9)		N/A	no limit	N/A	500	44	350	600	N/A ⁽⁹⁾	N/A ⁽⁹⁾	500	
7440-28-0	Thallium ⁽⁷⁾		0.20 mg/L TCLP	0.106	2.12	TBD	11	68	170	0.2	0.2	1.0	
7440-62-2	Vanadium ⁽⁷⁾		N/A	16.9	338	TBD	2.0	49	26	0.1	0.1	5.0	
7440-66-6	Zinc	N/A	225	4500	40	3.5	190	11	0.5	0.5	2.0		
7439-97-6	Mercury	7470A/7471A (prep & analysis)	0.025 mg/L TCLP	0.0651	41.30	TBD	0.031	2.02	N/A	0.02	0.02	0.033	
57-12-5	Cyanide (Amenable) ⁽¹⁰⁾	9013 (solids leach) followed by 9010B (distillation)/ analysis by 9012A or 9012A (distillation and automated analysis) for preparation of glass	30	N/A	N/A	TBD	N/A	N/A	N/A	TBD	N/A	TBD	

Table 5-2 AL Versus Anticipated Estimated Quantitation Limits ⁽¹⁾

A	B	C	D			E	F	G	H			I	J	K	L ⁽²⁾	M
CAS#	Name	Preparation & Analytical Methods	Action Levels			EQL ⁽⁶⁾ in simulated melter feed mg/kg	Raw Waste Anticipated EQLs			Vitrified Material TCLP Leachate Anticipated EQLs		Vitrified Material Totals				
			UTS ⁽³⁾ mg/kg, unless noted as mg/L TCLP	Lowest Predicted Delisting TCLP Leachate ⁽⁴⁾ (see Table 3-6) mg/L	Total ⁽⁵⁾ Analysis mg/kg		EQL in waste supernatant mg/L	EQL in waste solids (typical) mg/kg	EQL in waste solids (modified acid digestion) mg/kg	EQL ⁽⁶⁾ in Simulated ILAW & IHLW TCLP Leachate mg/L	EQL in Active ILAW & IHLW TCLP Leachate mg/L		EQL ⁽⁶⁾ in the Simulated ILAW & IHLW Total Analysis of Glass mg/kg			
57-12-5	Cyanide (Total) ⁽¹⁰⁾	9013 (solids leach) followed by 9010B (distillation)/ analysis by 9012A or 9012A (distillation and automated analysis) for preparation of glass. Leachate for delisting only-1311/9010B/9012A or 1311/9012A	590	10.8	216	TBD	2.8	0.28	N/A	TBD	N/A	TBD				

- 1 All EQLs are subject to change based on laboratory method updates or matrix effects (e.g. dilution). The waste EQLs (Columns H through J) are estimates based on Regulatory DQO (unless otherwise noted) and are typically the lowest calibration standard multiplied by the total dilution factor.
- 2 Limits based on radioactive waste matrix analyses. EQLs for active glasses are speculative, and matrix is assumed to be low-level acetic acid TCLP leachate with minimal matrix effects.
- 3 Vitrification (HLVIT) is the selected LDR treatment standard for arsenic, barium, cadmium, chromium (total), lead, mercury, selenium, and silver. UTS apply to metals not covered by HLVIT.
- 4 Refer to Table 3-6. Value shown is the lowest of MCL×DAF, DRAS computed level, or toxicity characteristic - for direct comparison to potential detection limits.
- 5 The "total" analysis is calculated as 20 times the predicted TCLP concentration anticipated for delisting leachate.
- 6 With exceptions for nonstandard analytes in footnote 7, EQLs in simulated waste and inactive vitrified material are based on commercial laboratory reporting limits, courtesy Severn Trent Laboratories, Inc., Knoxville, TN.
- 7 Non-standard analyte. TCLP is not typically performed for these compounds/elements as they are not on the Toxicity Characteristic list. EQL provided is speculative based on method performance with compounds of similar chemical group. Special EQL/MDL data are required based on SW 846 Chapter 1.
- 8 These metals are likely to exceed linear range if analyzed by ICP Trace instrument. As long as EQLs are met and the concentration measure is within the instrument's linear range, any metal analysis may be performed by ICP or ICP/MS.
- 9 Sodium is used in the preparation of the TCLP extraction fluid. It is not appropriate to analyze for this element in a TCLP leachate.
- 10 For cyanide (total and amenable) in non-radioactive simulant, distillation of a 10 g sample for 1 hr and 15 minutes is required by LDR regulations.

N/A = not applicable

TBD = To be Determined by the laboratory. To date, no analysis for this constituent has been performed for this matrix.

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6 Step 6 - Decision Error

The purpose of step 6 is to discuss decision errors that are possible when making decisions based on sample data, and to set tolerable limits (in terms of probabilities) on these decision errors.

6.1 Decision Errors

Generally, decision rules are written as if the true state of nature is known. Since toxicity characteristic leaching procedure (TCLP) leachate data from ILAW and IHLW glass are the focus of this data quality objective (DQO), the decision rules in step 5 are written to describe how decisions would be made if true mean TCLP leachate concentrations for all constituents of potential concern (COPCs) could be determined without any error. However, in order to know the true mean TCLP leachate concentration, all possible samples must be collected and analyzed without error. Clearly, this is not possible. Time and money prevent every possible sample from being analyzed and sampling, analytical, and handling errors are always present.

Since the true mean TCLP leachate concentration for a COPC cannot be known, decisions are made based on sample means, which are used to represent the true mean TCLP leachate concentration. Sample data represent incomplete information (because not every possible sample was analyzed) and have uncertainty associated with it that results from various sources of error. Therefore, it is possible to make an incorrect decision when using sample data. There are two basic types of decision errors that are possible:

1. Incorrectly deciding that the true mean TCLP leachate concentration is less than the action level (AL), when in fact it is greater than the AL. This type of error is referred to as an alpha (α) or Type I error (when using the null hypothesis, as discussed below). Making this error would result in applying for delisting when in fact it is not appropriate to do so. The primary risk of this type of error is sending glass to the federal high-level waste repository as delisted waste when it does not meet the delisting criteria. The risks and hazards of making this error are incorporated into the delisting risk assessment software (DRAS) model, which is used for developing delisting criteria (see Section 3.2.1 for details). As inputs, the DRAS model uses the chemicals to be delisted and the risks and hazards associated with appropriate exposure pathways. Using these inputs, the DRAS model back-calculates the TCLP leachate concentrations that will be used as ALs for the input chemicals. These ALs are described in step 5. They were selected based on the total mass of waste disposed in the landfill, and on the most conservative health-based limits.
2. Incorrectly deciding that the true mean TCLP leachate concentration is equal to or greater than the AL when it is actually less than the AL. This type of error is referred to as a beta (β) or Type II error (when using the null hypothesis, as discussed below). Making this type of error would result in not applying for delisting when it is appropriate to do so. The consequences of making this type of error are that immobilized waste is treated as though it did not meet delisting requirements, when in fact it does. The primary risks of this type of decision error are to schedule, budget, and waste loading. This error would mean that the waste cannot go to the federal high-level waste repository for disposal and that other disposal options would need to be developed, or adjustments to waste loading and GFCs would be required to develop a compliant vitrified glass form.

6.2 The Null Hypothesis

Since it is not known (and cannot be known) whether the true mean TCLP leachate concentration is above or below the AL, an initial assumption about the true mean TCLP leachate concentration is made. This assumption is maintained unless and until there is overwhelming evidence that it is not true and should be rejected. This initial assumption is called the null hypothesis. It is standard practice to phrase the null hypothesis in terms of the opposite of the claim that the investigation hopes to demonstrate. In other words, if the investigation hopes to demonstrate that the true mean TCLP leachate concentration is below the AL, then *the null hypothesis is that the true mean TCLP leachate concentration is equal to or greater than the AL*. Setting the null hypothesis in this fashion means that strong evidence is required to reject this initial assumption and to support the investigation's claim. So for this DQO, the null hypothesis will be that the true mean TCLP leachate concentration (for all COPCs) is equal to or greater than their corresponding AL. The other approach - that is, stating the null hypothesis so that it must be confirmed (glass TCLP < action limits) - can be done; however, the statistics required to bound error tolerance and determine the sampling requirements are more complex. This would be analogous to gathering data to demonstrate that the null hypothesis cannot be disproved (e.g., collect data showing it cannot be proved that the null hypothesis is false).

Note that the conceptual model (Section 1.7) is in agreement with the demonstration of concept data in Appendix B, but conflicts with the null hypothesis presented. The fact that the null hypothesis is in apparent conflict with the conceptual model is typical for a DQO. This is because the null hypothesis (glass TCLP > action limits) is stated so that the data obtained can be used to disprove that hypothesis. This approach lends itself to more precise error control, as discussed below.

6.3 Controlling Decision Error Probabilities

In order to understand how decisions are made with sample data and how decision errors are managed or controlled, it is instructive to first discuss how decisions would be made in an "ideal world", where all possible samples are taken and measured without error. This ideal decision rule is depicted in Figure 6-1. Here the probability of making a correct decision is 100 %, and the probability of making a decision error is 0 %. This is illustrated by the bold line, which indicates that the probability of deciding that the true mean TCLP leachate concentration exceeds the AL is 0 % when the true mean is actually below the AL, or 100 % when the true mean is actually above that AL.

Such ideal decision error probabilities are unachievable because decisions are based on sample data that are merely representative of a true condition and have uncertainties associated with them. However, through the use of statistical methods, the probabilities of making decision errors can be controlled. To do so, tolerable decision error probabilities need to be specified. In other words, with what probability can the two types of decision errors be tolerated?

For this investigation, an α or Type I, error rate of 0.10 is proposed. Setting α to a fixed value is a means of controlling the probability of making a Type I error. This error probability will be achieved by requiring the $(1-\alpha)$ % upper-confidence limit (UCL) of the true mean (or 90 % UCL) to be less than the AL in order to justify delisting. A discussion of why the use of such a confidence interval criterion meets the α requirement is included in Appendix E. A very simplified, shorthand equation that represents this concept is:

$$\text{Mean TCLP Leachate Concentration} + \text{Uncertainty} < \text{AL}$$

In this shorthand equation, the mean TCLP leachate concentration comes from the sample data. Using the 90 % UCL specified above, the uncertainty is factored in with the mean concentration so that a comparison to the AL can be made. If the sum of these two values (TCLP Leachate Mean + Uncertainty) is less than the AL, then there is a low (and tolerable) probability of making a Type I decision error.

$$\text{Mean TCLP Leachate Concentration} + \text{Uncertainty} = 90 \% \text{ UCL}$$

Figure 6-2 is used to illustrate the concepts of α and β , and is an expanded version of Figure 6-1. In Figure 6-2, the horizontal axis represents potential values for the true mean TCLP leachate concentration. On this axis, the AL is taken to be 1.0, so the value 0.8 on the axis indicates 80 % of the AL, while 1.2 indicates 120 % of the AL. The vertical axis gives the probability of deciding that the true mean TCLP leachate concentration exceeds the AL. If the true mean TCLP leachate concentration is at the AL, there is a probability α of making a Type I error. If the true mean is greater than the AL, α appropriately decreases. In Figure 6-2, the β error rate is set to 0.20 as the lower bound of the gray region (LBGR). The probability of deciding that the glass does not qualify for delisting when it actually does is limited to 20 %. The probability of making a β error must be defined for some specific value below the AL. In this example, this value is 60 % of the AL. This is the point at which making a β error is controlled or limited to 20 % (for example, at 60 % of the AL, the probability of making a Type II error is 20 %). This point is referred to as the LBGR. If the true mean TCLP leachate concentration falls below the LBGR, β decreases because the true mean is moving away from the AL. Note, however, that between the LBGR and the AL (within the Gray Region) the β error rate climbs steeply. The gray region represents a range of values where it is not deemed necessary to control the incorrect decision that delisting criteria are not met because the true mean is so close to the AL. In qualitative terms, as the true mean TCLP leachate concentration approaches the action level, the severity of Type II error consequences begin to outweigh the severity of Type I error consequences, thus the project is willing to accept less control of Type II error probability.

Note: Figure 6-2 applies to the Case 1 statistical analysis that is discussed in step 7. Additional graphics will be introduced as appropriate to the discussion of other statistical analyses.

For this DQO, α is set at 10 % to correspond to a $(1-\alpha) = 90 \%$ upper confidence limit. An initial approximation of $\beta = 20 \%$ will be assumed for illustrative purposes (refer to Figure 6-2). However, for Type II error assessment of analytical data, β will not be established at this time. Justification lies in the fact that a beta error would lead to the false conclusion that glass leach properties do not meet the relevant action limits, and the QGCR would be decreased to compensate and assure production of a compliant glass form. The consequences of an erroneously reduced QGCR could lead to limits that would eventually manifest themselves as increased waste volume and costs. However, adherence to delisting and LDR criteria would still be assured (because the Type I error is alpha error controlled). Evaluation of beta error and corresponding sample requirements will be performed for those cases in which research data indicates that glass leach properties (the 90 % UCL of the TCLP results) just exceed the relevant action limits, and the corresponding reduction in QGCR could warrant production cost increases that exceed the cost of additional research, and/or result in unnecessary processing restrictions and potential feed limits.

The discussion above of decision error probabilities leads to a general decision criterion for being able to reject the initial assumption (the null hypothesis) that the mean TCLP is equal to or greater than the AL:

- If the 90 % UCL estimate of the true mean TCLP leachate concentration is less than the AL, then there is sufficient evidence to reject the initial assumption and conclude with high confidence that the true mean TCLP leachate concentration is below the AL.

Required sample sizes for achieving these combined α and β error probabilities are discussed in step 7 of this DQO.

Figure 6-1 Ideal Decision Rule

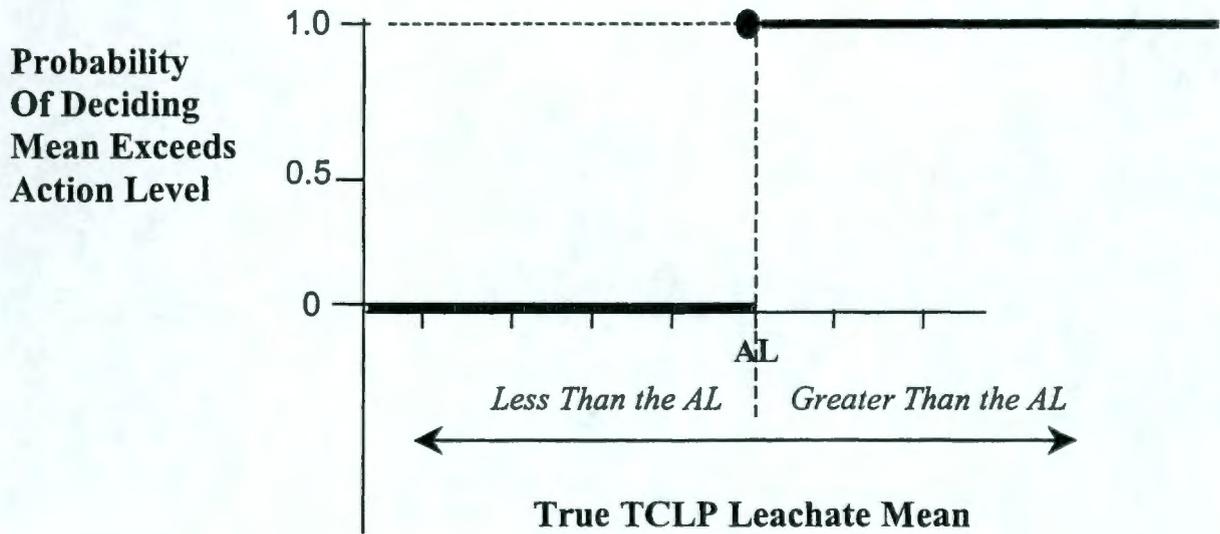
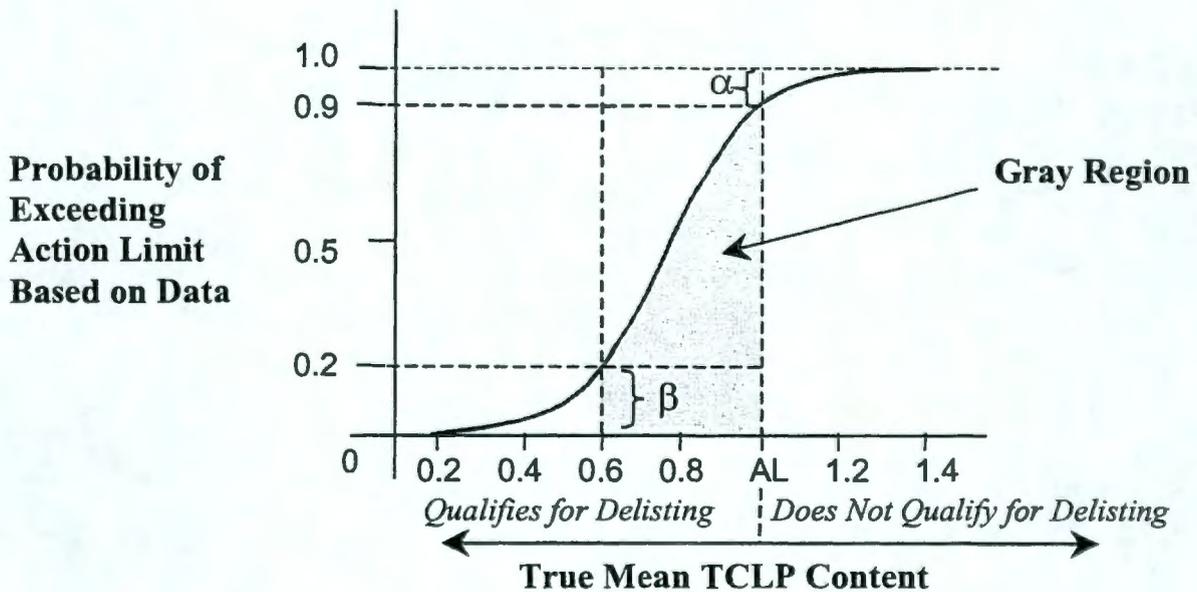


Figure 6-2 Decision Rule/Probability Graph



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7 Step 7 - Optimize Design

The purpose of step 7 is to develop a resource-effective sampling and analysis design for generating data that are expected to satisfy the data quality objectives (DQOs). Organics and metals, in general, are treated during vitrification as described in the previous sections and appendices of this document. Organics are generally eliminated from the feed through thermal destruction and volatilization. Metals are treated primarily by immobilization and stabilization in the waste matrix, although some metals may be eliminated through volatilization. These mechanisms lead to the conclusion that data gathering efforts must consider and accommodate the mechanisms that produce a compliant waste form. The testing of organics in the glass is unwarranted since organics do not survive the vitrification process. However, data for immobilized metals from previous tests have shown that leachability is an intrinsic glass property and that further testing is warranted. Some metals are likely to be bound within almost any glass composition of interest, while other, more leachable constituents require narrower ranges of glass formulations to sufficiently immobilize waste constituents.

This section presents a phased approach for testing glasses to determine whether they qualify for delisting and a LDR treatability variance. For ease of discussing these glass-testing phases, constituents of potential concern (COPCs) are broken into two different groups. These include:

- Metals with a low likelihood of leaching at levels approaching the action level (AL)
- Metals with a higher likelihood of leaching at levels approaching the AL

The general approach to testing is described in Section 7.1 below. Section 7.2 describes the statistical basis for the minimum test design requirements presented in Section 7.4.

7.1 Phased Approach to Testing

Metals are broken down into two categories, based on their release rates from glass. The categories presented below are based on two considerations - (1) the release rates discussed in Appendix C to this document, and (2) the action levels (ALs) for specific metals relative to the release rate (i.e., higher release rates may be acceptable for metals with a higher action level).

- Non-leachable metals. Metals in this category have very slow release rates that generally result in mean TCLP leachate concentrations well below their corresponding ALs. These are generally the elements that have slow, irregular or retarded intrinsic release rates as discussed in Appendix C. Also in this category are metals that have inherently low concentrations in the glass - again, resulting in mean TCLP leachate concentrations well below the ALs. It is expected that all ILAW metals, and some IHLW metals, will fall into this category. Metals tend to precipitate out when spiked into LAW at high levels, in effect, making the feed more like HLW. Consequently, it is anticipated that the leachable metals will not exist at high, problematic concentrations in the ILAW.
- Leachable metals. Metals in this category have higher release rates than non-leachable metals, resulting in higher TCLP leachate concentrations. These are generally the elements that have advanced intrinsic release rates as discussed in Appendix C. This can include some slow and retarded elements that are present at high concentrations in the leachate with respect to their action level. The TCLP leachate mean is likely to be near the AL. In addition, metals at high concentrations in the glass, even with the reduced release rates, may fall into this category.

Testing glasses to determine whether they qualify for delisting will follow a phased approach. A general outline of this phased testing approach is presented below. This outline is followed by a more detailed discussion of the statistical methods that will be used to analyze the data from each testing phase. Each phase in the approach has a corresponding statistical analysis, which is introduced in detail in Section 7.2, and discussed in detail in Appendix E.

In the first phase of glass testing, a small number of glasses (probably 1 to 3) will be spiked with all metal COPCs in order to identify those metals that can affect glass quality from a regulatory perspective. The results from this testing will support the development of glass formulation models and determination of potential feed restrictions or blending requirements. The experimental parameters NBO, M3T, BM3, and M1M12 (DOE/CH9601, refer to Appendix C) are at extremes representing that portion of the glass composition region of interest which would bound glass formulation. A "high" spiking level will be chosen for each metal, relative to the waste feed composition and the corresponding AL. Each glass will be tested independently, and a mean TCLP leachate concentration will be established for each metal within each glass. The 90 % upper-confidence level (UCL) estimate of the true mean TCLP leachate concentration will also be calculated for each metal. See the discussion below of the Case 1 statistical analysis for more details. If the 90 % UCLs for all metals are below their corresponding ALs, then the glass meets the proposed delisting conditions. If only a few isolated UCLs exceed their ALs, a qualitative decision will be made concerning the next appropriate analytical step. The criteria will include considerations such as:

- How far the constituent is above the limit
- How many other COPCs met the limits
- Frequency of failure occurrence (how many times the COPC exceeded the limit)

Other criteria may also be applied as appropriate. In most circumstances, cases where a UCLs exceed their ALs will lead to the development of a more complex TCLP leachate model; the second phase of testing will be skipped and the third phase will be implemented (e.g., the Case 3 example described in Step 7 of the DQO).

In the second phase of testing, only the metals that "failed" the first round of testing would be spiked into the glass. Metals used in this second phase of testing are now, by definition, leachable metals. These leachable metals will be spiked into a glass at multiple spiking levels to better characterize resulting TCLP leachate values as a function of COPC levels. The phase two testing plan may also be able to demonstrate that TCLP delisting requirements can be met simply by restricting the COPC levels to lower values; that is, by imposing waste loading restrictions.

In the second phase of testing, the exact spiking levels used will depend on information gained from the first phase. Therefore, it is not possible to pre-specify what spiking levels will be used in this phase. In all likelihood, the second phase of glass testing will involve only one glass that represents extreme or bounding conditions of the Glass Composition Region of Interest. However, it is possible that several glasses may be tested. TCLP leachate data from this testing phase will be analyzed using the Case 2 statistical strategy discussed below. This type of analysis is called regression modeling. As with the first testing phase, if all of the 90 % UCLs for the leachable metals fall below their corresponding ALs, then the glass meets the proposed delisting conditions. While there is some question as to whether this phase of testing and its related statistical approach will actually be needed, it is useful in this discussion, as it

demonstrates the mathematical bridge between the statistical methods used in the simpler “non-leachable metals” case, and the more complex “leachable metals” case.

There are two situations in which the third phase of testing may be used. It may be used if most of the non-leachable metals “fail” the first phase of testing, or if the second phase of testing does not clearly demonstrate a contaminant loading which will meet delisting or LDR action levels in the finished glass product. In either case, the third phase involves simultaneously analyzing multiple glasses with multiple spiking levels of metals. This analysis involves a very complex modeling process in n-dimensional space, (i.e., a space in which glass compositions composed of “n” components are represented as points). Data from this phase of testing will be analyzed using the Case 3 statistical strategy discussed below. The results of this analysis could indicate the need for restricting waste loading or for further reducing the glass composition to a more restricted qualified glass composition region (QGCR).

Each glass testing phase or strategy introduces several sources of variability or uncertainty into the data. In the first two strategies, the glass composition is not being varied, so possible sources of variability include:

- Variability between different batches of the same type of glass (processing variability)
- Variability within one specific batch of glass (sampling variability and/or heterogeneity)
- Variability due to handling and analytical methods (analytical variability)

Note, however, that the goal of the first two glass testing strategies is not to develop estimates of these separate sources of variability in order to come up with a more efficient testing strategy. Rather, the goal is to include all of these sources of variability in the calculation of the UCLs. In the first two sampling strategies, all three sources of uncertainty causing the measured TCLP leachate results to vary are captured in the UCL. Therefore, for those cases where the QGCR sufficiently bounds the melter feeds, if the UCL meets the criterion for delisting, further testing can be suspended, because all sources of variance have been factored into the UCL. If further testing is required, then the third phase of glass testing will be required. In those cases where the melter feed does not fit the QGCR, additional glass development work may be required. The goal of this phase is to identify and estimate sources of excessive variability, so methods can be designed to reduce their impact.

7.2 Statistical Data Analysis Cases

The statistical basis for the three-tiered approach to inorganics testing is described below. These statistical models are introduced in general terms in this section and discussed in technical detail in Appendix E. Stated succinctly, these cases are:

- Case 1: Experimental TCLP leachate results are analyzed for each glass composition individually and for a single COPC spiking level.
- Case 2: Experimental TCLP leachate results are analyzed for each glass composition individually, with multiple COPC spiking levels.
- Case 3: Experimental TCLP leachate results are analyzed for multiple glass compositions simultaneously at multiple COPC spiking levels.

Each of the glass testing phases for metals (Cases 1, 2, and 3) requires an increasingly sophisticated statistical model to analyze the data that results from that testing phase. The third case is the most

complex. The second is a simplification of the third case, and the first case is a further simplification of the second case. These statistical models are introduced in general terms in this section and discussed in technical detail in Appendix E. The similarities between the cases and additional technical detail are given in Appendix E. The somewhat different UCL expressions associated with each case are all special cases of a more general methodology that is explained in Appendix E.

For Case 1, sample sizes required to meet specific levels of α , β , and width of the gray region (Δ) (as defined in Section 6.3) can easily be calculated using standard statistics. Therefore, the calculation of required sample sizes can be predetermined for this case. However, the calculation of sample sizes for Cases 2 and 3 do not “fit” so easily into the standard DQO framework because of the increasing complexity of the statistical analyses used in these last two cases. In fact, without information gained from a Case 1 analysis, it is merely an academic exercise to try and determine what sample sizes will be required. Additional information on sample size requirements for Cases 2 and 3 is presented in Appendix E.

7.2.1 Case 1: Experimental TCLP leachate results are analyzed for each glass composition individually, and for a single COPC spiking level

For this case, the $(1 - \alpha) \%$ UCL (Expression 1) for the mean TCLP leachate concentration is used as the decision criteria. To qualify for delisting, this UCL must be less than the AL. This decision criteria guarantees with high confidence that when the criteria are met, the underlying true mean is indeed less than the associated AL. The UCL is given by

$$\bar{x} + t_{\alpha, n-1} s/n^{1/2} \quad (1)$$

Here \bar{x} and s are the usual sample mean and standard deviation computed from a sample size n , and $t_{\alpha, n-1}$ is the $1 - \alpha$ percentile of a t -distribution with $n - 1$ degrees of freedom. This UCL would be compared to the associated AL to decide whether the delisting criterion is met. This approach is precisely the context of the typical DQO application.

Required sample sizes for specified α and β decision error tolerances, along with an estimate of the underlying standard deviation, can be readily computed using a standard formula based on the assumption of underlying normal distributions of TCLP leachate concentrations. This formula, with a minor modification to accommodate the use of relative standard deviations, was used to generate Table 7-1.

For Table 7-1, the α error rate is fixed at 0.10. The β error rate is set at 0.10, 0.20, and 0.30 in consecutive blocks of the table. The lower bound of the gray region (LBGR) (expressed as a percentage of the AL) is varied from 0.20 to 0.95. Finally, three values of the relative standard deviation (σ/μ) (that is, standard deviation divided by mean) are used: 0.25, 0.50, and 0.75.

For a specific example of how to read this table, assume that an α error rate of 0.10 and a β error rate of 0.2 are required when the LBGR is 60 % of the AL. Further, assume that historical data indicate that relative standard deviation of TCLP leachate concentration values is 50 %. Table 7-1 indicates that, in order to meet the conditions set for α , β , and the LBGR, a sample size of six or more is required.

Note that when the LBGR becomes 1.0 (100 % of the AL) or greater, the glass does not meet the proposed delisting criterion, and β errors are no longer of concern. At this point, the error rate of concern

is α , but that is already controlled through the use of a confidence limit criterion. As the β level increases, the sample sizes needed to achieve that error level can be seen to decrease.

7.2.2 Case 2: Experimental TCLP leachate results are analyzed for each glass composition individually with multiple COPC spiking levels

Those COPC metals whose Case 1 UCLs are not clearly below their respective ALs will be further investigated in the second phase of glass testing by using linear regression methods. In order to conduct this phase of glass testing, a glass will be spiked with multiple levels of each COPC metal. In all likelihood this phase of glass testing will involve only one glass that represents an extreme or bounding condition of the glass composition region of interest. However, it is possible that several glasses may be tested. If several glasses are used, each will be tested and analyzed separately.

Figure 7-1 is used to illustrate, in general, how the second phase of glass testing will be conducted, and how the resulting data will be analyzed. The horizontal X-axis indicates the COPC metal spiking levels in the glass. The vertical Y-axis indicates the TCLP leachate levels that result from testing the glass. For the sake of discussion, assume that in the first testing phase, a given COPC metal was spiked at level X_4 in Figure 7-1 below. Three samples were taken and analyzed, yielding three slightly different TCLP leachate levels (represented by the three points on the graph for spike level X_4). Further, assume that the 90 % UCL calculated using these data was above (or uncomfortably close to) the COPC's AL. To move into the second phase of glass testing, additional spiking levels of this metal must be chosen. In this example, four additional spiking levels were chosen—one above, and three below, the original spiking level of X_4 . At each spiking level, three samples are collected and analyzed. The 15 resulting data points (three samples from each of five spiking levels) would be used for the Case 2 regression analysis. Another way to describe this process is to say that there are "m" spiking levels with "n" samples taken and analyzed at each level. In Figure 7-1 below, $m = 5$ and $n = 3$.

Now, assume that the line on the graphs represents the true underlying linear relationship between the COPC metal spiking level and the TCLP leachate level. The statistical equation for this relation is denoted as $Y = \beta_0 + \beta_1 X$. Note that β_0 here is the y-intercept and β_1 , the slope. These regression parameters should not to be confused with the decision error probability β discussed earlier.

The estimate of the mean TCLP leachate level for this metal can be refined by considering it as a function of the spiking level in the glass. For each potential spiking level along the X-axis, the estimated TCLP leachate mean becomes the height to the line on the graph. However, this line represents the true relationship between the spiking levels and the TCLP leachate levels. Since this true relationship cannot be known, it must be estimated from sample data. Any time true values are estimated, there are uncertainties associated with those estimates. These uncertainties are given by the following expression, which calculates the UCL limit for a regression line (illustrated in Figure 7-2).

$$(\hat{\beta}_0 + \hat{\beta}_1 X_0) + t_{\alpha, n-2} s/n^{1/2} [1/m + (X_0 - \bar{x})^2/\Sigma (X_i - \bar{x})^2]^{1/2} \quad (2)$$

The initial expression in parentheses ($\hat{\beta}_0 + \hat{\beta}_1 X_0$) is the height to the estimated regression line at any particular value X_0 along the horizontal axis. The set of all such predicted values for values of X_0 gives the indicated "estimated mean line". The remainder of the expression in Expression 2 is the uncertainty that is added to the mean estimate to provide a $(1-\alpha)$ % UCL for the mean at value X_0 . The sum Σ in this expression is over all the COPC spiking values used in the study. The set of all such confidence limits for

all values X_0 gives the curved line indicated in Figure 7-2. Note that the uncertainty expression in Expression 2 ($t_{\alpha, n-2} s/n^{1/2} [1/m + (X_0 - \bar{x})^2/\Sigma (X_i - \bar{x})^2]^{1/2}$) depends on the particular COPC spiking levels (X_i) used in the experiment.

There are three points of interest on this graph (X_0 , X_1 , and X_2). The narrowest gap between the estimated mean line and the UCL line occurs at the value $X_0 = \bar{x}$, the mean of the spiking values over all glass samples tested. Why this occurs can be observed in Expression 2. When $X_0 = \bar{x}$, the latter term in the uncertainty is zeroed out, leaving an expression for the UCL that is very similar to Expression 1 in Case 1.

Next, notice point X_2 . If the AL is as indicated on the vertical axis in the figure, the indicated value X_2 is the minimum COPC level whose corresponding TCLP leachate mean is at or below the AL. However, to meet the UCL delisting criteria, it is not sufficient for the estimated mean to be below the AL. Instead, the corresponding UCL must be below, as well. This condition is satisfied for the COPC levels between 0 and X_1 . This range of spiking levels is denoted as the acceptable range of COPC spiking levels because the UCLs that correspond to these levels fall at or below the AL. Therefore, if this criterion were to be applied in order to meet delisting, glass COPC levels would have to be confined to this acceptable region, possibly through waste loading restrictions.

7.2.3 Case 2: Sample Size Requirements

Discussion of required sample sizes is considerably more complex in this case. Unlike Case 1, sample sizes will now depend on experimental design features. The range of spiking levels chosen for Case 2 will depend on the results from the Case 1 analyses. In general, a few spiking levels would be chosen that are expected to give TCLP leachate results bracketing the AL and the LBGR discussed in Case 1 (for example, $\beta = 0.2$ at $LBGR = 0.6 \times AL$).

The expression of the UCL for Case 2 is a function of the values of these spiking levels. Because of this function, definitive sample size calculations for Case 2 metals will best be accomplished after those metals have been identified through the Case 1 investigation, and the general range of additional spiking levels are determined. Sample size calculations can then be derived specifically for that range of spiking levels to determine the number of intermediate spiking levels (m levels total) and number of TCLP analyses (n) at each level to meet the final α , β , and the LBGR criteria already selected.

An example sample size table could be generated here to show the process, but it would have to be based on restrictive assumptions regarding the underlying experimental design, and would be expected to have little use at this time. Sample size computations, when used in similar statistical analysis of other data sets, have typically resulted in a need for 12 to 20 data points to support computing a UCL with the desired error tolerance.

7.2.4 Case 3: Experimental TCLP leachate results are analyzed for multiple glass compositions simultaneously at multiple COPC spiking levels

The purpose of the second phase of glass testing is to try and refine the estimate of the mean and the UCL by taking advantage of any linear relationship between spiking levels and TCLP leachate levels. If this strategy does not provide sufficient information to define a QGCR, then phase three glass testing will be implemented. In this phase of testing, multiple glass compositions with multiple COPC spiking levels are analyzed simultaneously-in contrast with the first two phases, where glasses were analyzed separately.

Data from the third phase of testing will be analyzed using the Case 3 data analysis strategy described here and in Appendix E.

This case is completely analogous to Case 2, but now a model is fit to "k" glasses, at "m" spiking levels, with "n" glass samples used at each of the $m \times k$ glass/spiking level combinations. For this experimental design, the UCL becomes

$$\hat{P}_0 + t_{\alpha, mk-p} s/n^{1/2} [X_0(X'X)^{-1}X_0']^{1/2} \quad (3)$$

X is the design matrix, with each row of X representing a glass/spiking level combination considered in the study. Since each glass/spiking level combination generates n glass analyses, the rows of X actually come in $m \times k$ groups, with each group consisting of n rows of the same glass/spiking constituent values. This model is explained more thoroughly in Appendix E.

Like Case 2, \hat{P}_0 is the estimated mean for a new glass/spiking level combination X_0 . The standard deviation, s , is an uncertainty estimate, and $t_{\alpha, mk-p}$ the appropriate t-distribution value. The remainder of the expression is part of the uncertainty that depends on the experimental design through $(X'X)^{-1}$, and on X_0 , a newly proposed glass/spiking level of interest. Again, this approach is completely analogous to the similar components of the UCL in Case 2. To meet UCL delisting criteria, model results could be used to either impose waste load restrictions, or to further reduce the glass composition to a smaller QCGR.

7.2.5 Case 3: Sample Size Requirements

Derivation of required sample sizes for k , m , and n , for given α and β , the point $P \times AL$ at which β applies, for given μ , σ , and X_0 , becomes even more complex in this case. Not only does the estimated uncertainty depend on the X_0 of interest, but so, too, does the estimated mean. In addition, these computations, as in Case 2, would depend on the experimental design to be used, as well, and that will be best known after Case 1 or Case 2 results are established.

Again, some significant simplifications could be assumed regarding the many experimental design features in order to generate a sample size table for k , m , and n that would be analogous to that in Case 1. The utility of such an exercise is again questionable. In actual applications, the information gained through Case 1 and Case 2 analyses will contribute vital information regarding the added investigation needed in this full-blown model-based application. At that time, sample sizes can be better estimated. Experience suggests that 40 to 60 glasses should be sufficient to make a reliable delisting decision.

7.2.6 Case Comparison

The UCLs for the three cases are shown below, so the similarities can be noted. As stated earlier, a more thorough explanation of how the expressions are all based on the same underlying model is given in Appendix E. Note for each UCL, there is an initial estimated mean value to which an uncertainty expression is added. That uncertainty consists of a t-distribution value, and a variability estimate s divided by $n^{1/2}$, where n is the number of replications used. Cases 2 and 3 also include expression in their uncertainties that are functions of the experimental design used, and of X_0 , the point in the experimental design range for which mean, uncertainty, and UCL estimates are of interest.

$$\begin{array}{lll}
 \text{Case 1:} & \bar{x} & + t_{\alpha, n-1} s/n^{1/2} \\
 \text{Case 2:} & (\hat{\beta}_0 + \hat{\beta}_1 X_0) & + t_{\alpha, m-2} s/n^{1/2} [1/m + (X_0 - \bar{x})^2 / \sum (X_i - \bar{x})^2]^{1/2} \\
 \text{Case 3:} & \hat{\rho}_0 & + t_{\alpha, mk-p} s/n^{1/2} [X_0(X'X)^{-1}X_0']^{1/2}
 \end{array}$$

Note, again, that in each case, the α error level is controlled through the use of the UCL criterion. β level errors can be readily characterized, along with their influence on sample sizes, in the standard DQO application of Case 1. For Cases 2 and 3, such computations are considerably complicated by the nature of the experimental design. The most practical approach is to eventually use Case 1 results to derive an appropriate Case 2 experimental design and associated sample size requirements and, similarly, to use Case 1 and Case 2 results to derive appropriate Case 3 experimental design and sample size requirements.

7.3 Summary of Step 7

Table 7-2 summarizes the information presented in step 7. The first column lists the two general COPC types. Each type of COPC is associated with one (or more) experimental designs, which together comprise the phased approach to glass testing, listed in column 2. Each experiment may be repeated one or more times with different glasses, resulting in multiple experiments being run (column 3). Each experimental design is also associated with a specific statistical analysis; these are listed in column 4. The last four columns present numbers that pertain to one repetition of a given experiment. The total number of samples given for the non-leachable metals represents the current recommendation, and is well-grounded with the knowledge gleaned from previous experimental data. The numbers given for leachable metals, Cases 2 and 3, are "best guess" estimates because these numbers will actually be determined after information from Case 1 has been evaluated.

The testing discussed in Table 7-2 will be performed via multiple test plans that will be written by Bechtel National, Inc. (BNI), with assistance from research and technology (R&T) testing facilities, as appropriate.

7.4 Testing Requirements

Typically, a DQO is followed by a test plan (as an attachment or stand-alone document) indicating the actual requirements for implementation of the data collection process(es) required to support the quality assurance needs and decisions established by the data quality objectives specified by the DQO. As discussed, this DQO results in an iterative testing program by which a graded approach to testing allows research to focus on those COPCs that are shown to have a greater impact to glass quality. Accordingly, it would not be appropriate to develop a specific test plan at this time for inclusion, however, there is a recognized need for decision-maker concurrence on the actual scope of a testing program developed in response to the data quality objectives specified by this document. The sub-sections that follow describe the minimal requirements for a testing program to be developed in response to this DQO.

The testing requirements identified below will be implemented through multiple test iterations. Figure 7-3 provides a simplified diagram that summarizes the role of this test effort in the WTP's strategy for LDR/Delisting DQO implementation. Data generated will support development of a petition for a treatability variance for ILAW and IHLW, and a petition for an upfront conditional delisting of IHLW. Data shall be obtained on crucible and bench-scale unit operations. Data generated will be sufficient to support establishment of acceptable operating conditions of the equipment, permit development efforts and technical discussions with regulatory agencies.

As part of the test scope, researchers shall plan and conduct laboratory or small-melter research activities that are required to support the LDR and delisting activities. It is anticipated that multiple tests will be needed to address the objectives of this DQO document. Each test may address only a limited set of objectives, as clearly indicated in the associated test plan. Because of the nature of the graded approach to testing, data will be required across successive campaigns regardless of the glass composition being processed.

The need for inorganics testing is fairly well defined in this DQO. The inorganics testing program will identify and confirm the non-leachable and leachable inorganics using a graded testing program and development of TCLP response models for leachable inorganics (e.g., multiple feed concentrations and glass samples). Data sufficient to demonstrate non-leachable inorganics are not a concern from a LDR/delisting compliance perspective will be needed. The testing program will also identify leachable inorganics and limiting concentrations which may reduce the QGCR. The graded testing approach will require collection of sufficient data in accordance with the Case 1, Case 2 (if needed), and Case 3 sampling scenarios as described above. Ultimately, the testing will be used to develop and validate TCLP response models for leachable inorganics, and will support glass formulation and waste loading predictions.

7.4.1 Case 1: Non-Leachable Inorganics Testing

The Case 1 experimental approach is warranted in those cases where data for the target constituents, when processed at the maximum reasonable COPC concentration, results in constituent leachate concentrations that are below the action limit. This experimental approach is a starting point for evaluating COPCs whose propensity for leaching may be somewhat insensitive to the concentration of other components in the glass within the composition region of interest. A glass composition for testing TCLP response at the limit of glass composition space shall be developed and utilized so that it can be shown that non-leachable inorganics will be sufficiently immobilized. The experimental parameters NBOT, M3T, BM3, and M1M12 will be adjusted to bound the QGCR of interest. The feed compositions shall be based (as appropriate) on the projected pre-treated waste composition (including non-regulated organics and chelators), adjusted for the addition of recycle waste contributions, and should represent a potential "worst case" feed composition from an inorganics immobilization perspective (e.g., relatively high boron release rate). Glass former additions shall be appropriate to the glass composition required for this test. A minimum of one LAW simulant and a minimum of one HLW simulant will be processed under the Case 1 test regime.

Spike solution(s) or oxides will be prepared at the required spiking levels. Spiking compounds (test compounds) are identified in Table 7-3. Spiking levels for LAW should be relatively high (maximum possible for the envelope definition), but not exceed solubility limits such that the LAW simulant becomes more appropriate as a representation of HLW. The spiking levels should exceed the action levels for TCLP leachate concentrations in Table 7-3 by at least 2 orders of magnitude ($>100\times$) for HLW for those COPCs whose action limits equate to less than 0.5 % by weight.

A crucible melt campaign to support creation of a glass(es) using feed or a glass composition spiked with Table 7-3 inorganics will be implemented. Glass samples shall be collected and correlated with glass composition data so that constituent leachability data can be obtained. Minimal requirements for routine test samples (excluding quality control samples) are identified in Table 7-4. Additional samples may be identified in the test plan where needed. The decision to proceed with more in-depth testing (Case 2 or Case 3 below) shall be based on considerations such as:

- How much the constituent concentration is above the limit
- How many other COPCs met the limit
- Frequency of failure occurrence (how many times the COPC exceeded the limit)

Other criteria may also be applied as appropriate. Assessment of the data will be performed to confirm that assumption that Case 1 target constituents, when processed at the maximum reasonable COPC concentration, result in constituent leachate concentrations that are well below (at least an order of magnitude) the action limit, regardless of other components in the glass composition. This assessment shall be performed with consideration given to historical experimental results (for instance, compared to results from other similar experiments).

7.4.2 Case 2: Leachable Inorganics Testing

Where the 90 % UCL for Case 1 testing approaches the action limit of Table 7-3 for the corresponding COPC, additional testing may be required to develop a linear response model for the glass composition of interest. The Case 2 experimental approach is warranted in those cases where data indicate that constituent leachate concentrations are influenced primarily by the concentration of the COPC of interest. If this is not the case, then the Case 3 approach is required in order to sufficiently quantify and model TCLP response for a variety of glass compositions.

The Case 2 testing regime will require a similar potential "worst case" glass composition as that used in Case 1 testing. Spike solution(s) or glass compositions at the required COPC spiking levels (minimum of 4 spike levels, more if appropriate) will be prepared and tested. Any spiking compounds (test compounds) identified in Table 7-3 that "failed" the Case 1 testing campaign will be spiked into the glass. These leachable inorganics will be spiked into glass at multiple spiking levels to better characterize resulting TCLP leachate values as a function of COPC concentration in the melter feed. The exact spiking levels used will depend on information gained from previous testing, therefore, it is not possible to pre-specify what spiking levels will be used in this test campaign. It is anticipated that the highest spike level used will result in a 90 % UCL of leachate concentration (for replicate samples) that equals or just slightly exceeds the action level of Table 7-3.

A crucible melt campaign to support creation of a glass(es) using glass composition(s) spiked with the appropriate Table 7-3 inorganics will be implemented. At least three TCLP glass samples for each spiking level will be collected for correlation to their respective glass formulations. Information shall be collected so that "before" and "after" processing data can be obtained. Minimal requirements for routine test samples (excluding quality control samples) are identified in Table 7-4. Additional samples may be identified in the test plan where needed.

If data indicate a dependence of TCLP leachate concentrations on glass composition for a particular or multiple COPCs, and the corresponding TCLP leachate concentrations (90 % UCL) approach the action limits, additional testing in accordance with the Case 3 test approach below will be required. The decision to proceed with more in-depth testing (Case 3) shall be based on considerations such as:

- How well the constituent concentration in the melter feed represents variable feed concentrations
- How much the constituent concentration is above the limit
- How many other COPCs met the limit

- Frequency of failure occurrence (how many times the COPC exceeded the limit)

Other criteria may also be applied, as appropriate. The data will be used to verify that constituent leachate concentrations are influenced solely by the concentration of the COPC of interest, regardless of other components in the glass composition. This assessment shall be performed with consideration given to historical experimental results (e.g., compared to results from other similar experiments).

7.4.3 Case 3: Leachable Inorganics Testing

Where the 90 % UCL for Case 1 or Case 2 testing approaches the action limits of Table 7-3 for the corresponding COPC, additional testing is required to develop an TCLP response model for the glass composition region of interest. The Case 3 testing approach involves simultaneously analyzing multiple glasses with multiple spiking levels of inorganics. This analysis involves a very complex modeling process in n-dimensional space. The results of data analysis will be used to refine QGCRs for the waste types simulated.

A variety of glass compositions (15 minimum) that both encompass and bound the QGCR will be developed and tested. The experimental parameters NBOT, M3T, BM3, and M1M12 will be adjusted to represent the boundaries of the applicable QGCR, as well as representing nominal or target glass formulations. The glass formulation approach will be consistent with the standard approach to experimentation to support waste form qualification activities and modeling currently underway for QARD compliance.

Glass compositions containing compounds (test compounds) identified in Table 7-3 that “failed” the Case 1 or Case 2 testing campaign will be tested. These leachable inorganics will be spiked in multiple glass formulations at multiple concentration levels to better characterize resulting TCLP leachate values as a function of waste loading (feed concentration). The exact spiking levels and corresponding glass formulations used will depend on information gained from previous testing, therefore, it is not possible to pre-specify what spiking levels will be used in this test campaign. It is anticipated that the highest spike level used will result in a 90 % UCL of leachate concentration that equals or just slightly exceeds the action level of Table 7-3.

A crucible melt campaign to support creation of glasses using glass formulations containing various concentrations of the appropriate Table 7-3 inorganics will be implemented. At least one TCLP glass sample for each glass composition will be collected. Information shall be collected such that “before” and “after” processing data can be obtained and TCLP response can be modeled. Minimal requirements for routine test samples (excluding quality control samples) are identified in Table 7-4. Additional samples may be identified in the test plan where needed.

7.5 Remaining Issues

Not all issues identified in this DQO effort can be adequately addressed through the R&T testing program. To support the development of delisting and land disposal restrictions (LDR) variance petitions, a technical document has been written to support the assertion that the multiple extraction procedure (MEP) is not applicable to vitrified waste.

The technical logic establishing why the MEP is not an appropriate test for assessing vitrified waste is included Appendix G and will be included as supporting information for the petition. The information provided explains how vitrification differs from chemical stabilization and how matrix dissolution and

diffusion mechanisms of glass differ from the breakdown of buffering capacity in stabilized (cementitious) waste forms.

As previously discussed, although this DQO provides a list of organic COPCs, the destruction and volatilization of organics compounds has been demonstrated in previous experiments conducted by the WTP. The EPA publication, *Vitrification Technologies for Treatment of Hazardous and Radioactive Waste* (EPA 1992), states that “the destruction of organic constituents occurs primarily via pyrolysis in the melt and combustion in the plenum” (Section 4.2.3, 2nd paragraph, p. 4-9). The EPA handbook explains how organics degrade to form mainly combustion products such as CO₂, H₂O, and HCl. The handbook also provides data indicating that organics destruction in excess of 99.99 % is common. This is further substantiated by test results presented in Appendices B and H of this DQO.

Table 7-1 Table of Sample Sizes for Case 1 when α Is Fixed at 0.10

False-Negative Error Tolerance (β)	Proportion of Action Level (LBGR as % of AL)	Relative Standard Deviation (σ/μ)		
		0.25	0.50	0.75
0.1	0.2	2	2	3
	0.4	2	4	6
	0.6	3	8	16
	0.8	10	35	76
	0.9	38	150	335
	0.95	157	626	1406
0.2	0.2	2	2	3
	0.4	2	3	5
	0.6	3	6	13
	0.8	7	25	55
	0.9	27	105	235
	0.95	110	434	976
0.3	0.2	2	2	3
	0.4	2	3	5
	0.6	2	5	10
	0.8	6	19	42
	0.9	21	78	174
	0.95	81	318	714

Table 7-2 Summary of Sampling Design for Delisting/LDR

				Numbers Are per Experiment ^(a)			
COPC Type	Experimental Design	# of Experiments ^(b)	Statistical Analysis	# of Glasses (k)	# of Spiking Levels (m)	# of Samples per Glass, per Spiking Level Combination (n)	Total # of Samples: N=k×m×n
Non-leachable Metals	One Glass with One Spiking Level	1-3	Case 1	1	1	6	6
Leachable Metals	One Glass with Multiple Spiking Levels	1-3	Case 2	1	4-5	3	12-15
	Multiple Glasses with Multiple Spiking Levels	1	Case 3 ^(c)	15-60	1	1	15-60

(a) Cases 2 and 3 are estimates; actual k, m, and n will be calculated based on non-leachable metals (Case 1) results.

(b) Note that the number of experiments (column 3) is not necessarily the same as the number of glasses tested per experiment (column 5). In instances where glasses are analyzed separately (non-leachable metals/Case 1, and leachable metals/Case 2), the number of experiments is the same as the number of glasses tested per experiment. But in Case 3, an experiment is run using multiple glasses. Here, the number of experiments run and the number of glasses per experiment are not the same.

(c) Although 15 to 60 glasses with one spike level are specified, interpretation is that glass composition will be varied by any combination of base glass formulae and spike levels. As a result, 15 to 60 unique glass compositions will be required to support the Case 3 statistical approach.

Table 7-3 Metals and Anions Proposed as COPCs for Testing ⁽¹⁾

CAS#	Metal	Release Rate (see § 1.6.5)	IHLW Action Level ⁽²⁾ TCLP Leachate	ILAW Action Level ⁽²⁾ TCLP Leachate
57-5-12	Cyanide	unknown	11.5 mg/L	590 mg/kg (total) ^(a) 30 mg/kg (amenable)
7429-90-5	Aluminum	Slow/Irregular	NA	NA
7440-36-0	Antimony	Retarded	0.659 mg/L	1.15 mg/L
7440-38-2	Arsenic	Slow/Irregular	3.08 mg/L	HLVIT ⁽³⁾
7440-39-3	Barium	Advanced	100 mg/L	HLVIT ⁽³⁾
7440-41-7	Beryllium	unknown	1.22 mg/L	1.22 mg/L
7440-43-9	Cadmium	Advanced	0.48 mg/L	HLVIT ⁽³⁾
7440-70-2	Calcium	Advanced	NA	NA
7440-47-3	Chromium	Slow/Irregular	5.00 mg/L	HLVIT ⁽³⁾
7440-50-8	Copper	Advanced	29200 mg/L	NA
7439-92-1	Lead	Retarded	5.00 mg/L	HLVIT ⁽³⁾
7439-97-6	Mercury ⁽⁴⁾	unknown	0.200 mg/L	HLVIT ⁽³⁾
7440-02-0	Nickel	Advanced	11.0 mg/L	11.0 mg/L
7723-14-0	Phosphorus	unknown	NA	NA
7440-09-7	Potassium	Advanced	NA	NA
7782-49-2	Selenium ⁽⁴⁾	unknown	1.00 mg/L	HLVIT ⁽³⁾
7440-22-4	Silver	Advanced	3.07 mg/L	HLVIT ⁽³⁾
7440-23-5	Sodium	unknown	NA	NA
7440-28-0	Thallium	Retarded	0.200 mg/L	0.200 mg/L
7440-62-2	Vanadium	unknown	16.9 mg/L	NA
7440-66-6	Zinc	Advanced	225 mg/L	NA

NA = Not applicable, no limit established (maximum analytical estimated quantitation limit (EQL) or minimum detection limit should correspond to limits published in SW-846)

⁽¹⁾ Table excerpted from LDR/Delisting DQO, Table 3-7 and Table 5-2.

⁽²⁾ Action level presented serves as the target level for the maximum analytical EQL or applicable reporting limit (RL), target EQLs/RLs shall be less than (3 to 5 times below) the action levels shown. Concentrations greater than the MDL, but less than the EQL/RL shall be reported and qualified as estimated values.

⁽³⁾ Vitrification is the LDR technology-based standard (40 CFR 268.40). Target analytical EQLs shall equate to the UTS (40 CFR 268.48) on an opportunistic basis.

⁽⁴⁾ COPC is toxicity characteristic limited. Action level is the toxicity characteristic (40 CFR 261.24).

^(a) Total cyanide does not require preparation per TCLP. Analysis is of glass product

Table 7-4 Summary of Minimum Inorganics Testing Routine Samples ⁽¹⁾

Sample Type or Purpose	Number or Type of Glass ⁽²⁾ (k)	Number of TCLP Samples per Glass, per Spike Level (# of replicate samples, n)	Total Number of Samples Per Experiment (Total # of samples, N)
Case 1: Non-leachable COPCs Single spike level (m)	ILAW glass IHLW glass	6	6
Case 2: Leachable COPCs 4 to 5 Spike levels (m)	IHLW glasses ⁽²⁾	3	12 to 15
Case 3: Leachable COPCs Single spike level (m)	15 to 60 IHLW glasses ⁽³⁾	1	15 to 60

⁽¹⁾ Collect quality control samples in accordance with Section 3, Tables 3-6 and 3-11, in addition to routine samples. Test plan may identify additional requirement (summary above represents minimum requirements). Number of samples shown are estimates; actual k, m, and n will be calculated based on non-leachable inorganics (Case 1) results.

⁽²⁾ Additional glass compositions may be required if needed to bound the glass composition region of interest.

⁽³⁾ Experiment scope will be increased to include ILAW if there are COPCs which are shown to be leachable in Case 1.

Figure 7-1 Example of Case 2 Statistical Approach

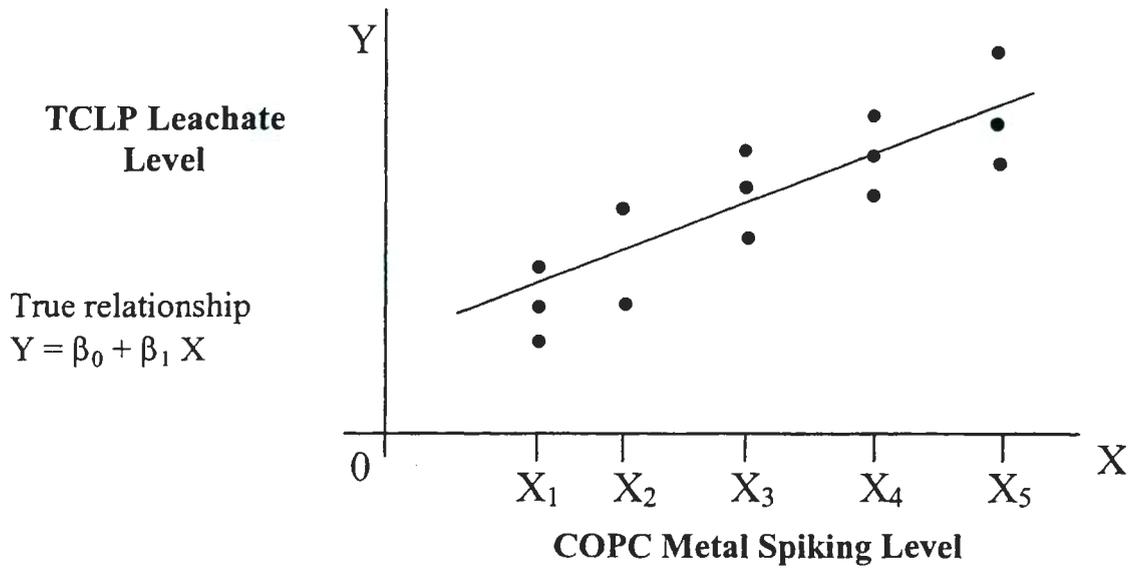


Figure 7-2 Uncertainty Evaluation of Case 2

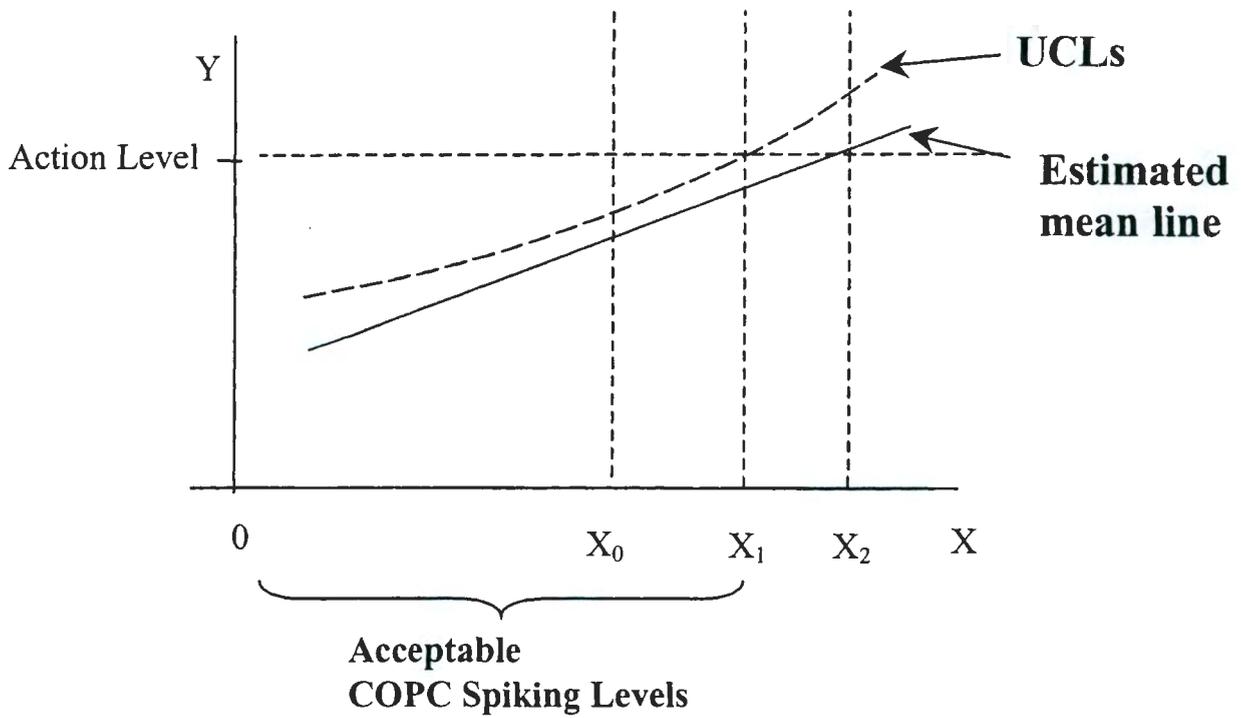
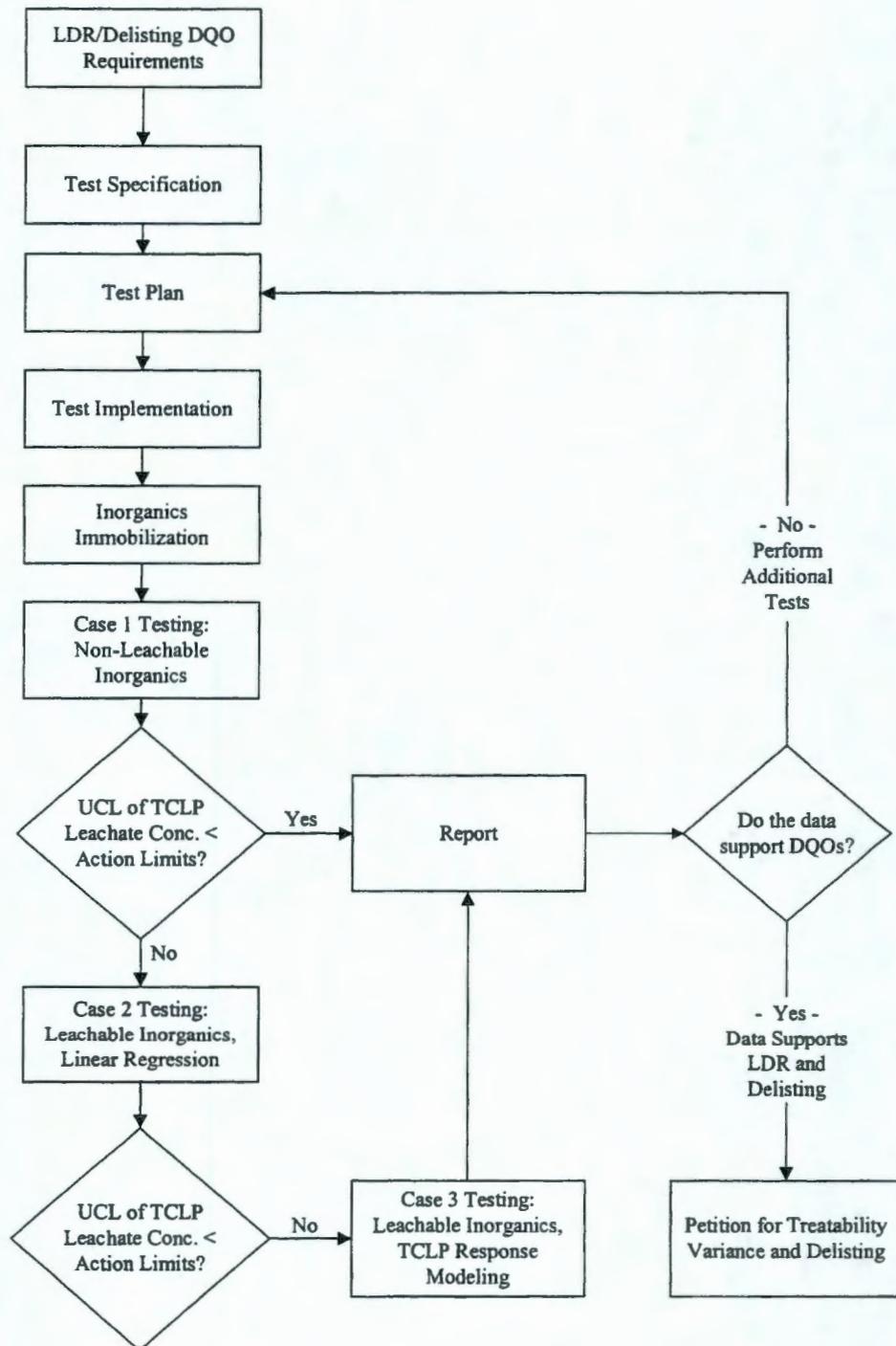


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Appendix A

Waste Treatment Plant Description

Appendix A

Waste Treatment Plant Description

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Appendix A

Waste Treatment Plant Description

The following discussion presents an overview of the waste treatment processes at the Hanford Tank Waste Treatment and Immobilization Plant (WTP). The information presented describes the WTP design at the time of development of this document. This information is not controlled, and the reader should refer to the current version of the *WTP Dangerous Waste Permit Application* for the most up to date information on the WTP design. Figure A-1 presents a simplified process flow diagram (PFD) of the WTP treatment processes.

1 Pretreatment

The WTP will store and treat waste feed from the Hanford Site double-shell tank (DST) system in the pretreatment plant. The pretreatment plant will separate the waste into two feed streams for the low-activity waste (LAW) and high-activity waste (HLW) melters. The feed will be processed through ultrafiltration to separate the solids. The processes in the pretreatment plant will condition feed and remove cesium, technetium, strontium, transuranic (TRU) compounds, and entrained solids.

The pretreatment plant is designed to prepare the LAW and HLW feeds for vitrification through the following activities:

- Receive and store HLW and LAW feeds from the Hanford Site double-shell tank (DST) system unit
- Separate cesium, technetium, strontium, and TRU radionuclides from the waste feed
- Segregate solids into the HLW feed stream
- Concentrate and neutralize the separated radionuclides
- Adjust the concentration of the waste
- Collect and monitor liquid effluents
- Blend waste fractions to optimize treatment steps

1.1 Waste Feed Receipt Process System (FRP)

Feed will be transferred from the DST system unit via any one of three co-axial underground transfer pipelines into the feed receipt tanks. The waste feed receipt process system (FRP) receives waste from the DST system and pretreatment waste processing, facilitates sampling of the waste, provides lag storage, and transfers the waste feed for subsequent treatment within the pretreatment plant. Feed receipt tanks are designed to perform the following functions:

- Receive feed from the DST system unit and waste from other WTP facilities
- Store untreated and treated waste
- Transfer the waste

The waste receipt vessels are of steel construction. Each tank is equipped with pulsejet mixers to mix the vessel contents and suspend solids. Reverse flow diverters are provided for each vessel to transfer the

waste, and each is equipped with an auto-sampling system to allow confirmation of the individual tank waste characteristics. All waste receipt vessels are vented to the pretreatment vessel vent process system (PVP).

1.2 Waste Feed Evaporation Process System (FEP)

The primary functions of the waste feed evaporation process system (FEP) are to receive waste from the waste feed receipt process system (FRP) and miscellaneous recycle streams, to evaporate a portion of the feed (reducing the volume and increasing the sodium concentration), to transfer the waste to the ultrafiltration process system (UFP), to condense the overhead vapors and transfer the condensate to the radioactive liquid waste disposal system (RLD), and to vent non-condensable gases to the pretreatment vessel vent process system (PVP) for treatment. The FEP is composed of two evaporator trains arranged in parallel. The waste feed evaporators are forced-circulation units operating under a vacuum to reduce the operating temperature. Each evaporator feed vessel has a pulsejet agitation system to provide mixing and to prevent settling of solids. The waste feed from the feed vessels is pumped continuously to the evaporator.

The vapor stream will be condensed to a liquid in a three-stage system consisting of a primary condenser, an intercondenser, and an aftercondenser. Condensate from this system will pass to a process condensate pot, from which it will be either transferred to the process condensate collection system or recycled. Non-condensable gases from the aftercondenser pass through the demister, which removes entrained droplets and are then routed to the PVP for treatment.

1.3 Ultrafiltration Process System (UFP)

The ultrafiltration process system (UFP) separates the concentrated waste feed from the evaporator system into a high solids stream, referred to as the HLW stream, and a solids-free stream, the LAW stream. Waste is received from the waste feed evaporator system into the evaporator concentrate buffer vessels of the UFP system, and transferred, in batch modes, into the ultrafilter feed vessel.

The waste stream is fed from the ultrafilter feed vessels to the ultrafilters, which are long bundles of permeable tubes. Chemicals are added into the ultrafilter feed vessels to precipitate the TRU elements, primarily strontium, contained in the waste feed stream, so that they form solid particles, which will then be separated into the HLW stream during the ultrafiltration process. The concentrated solids stream, or HLW feed stream, is transferred to the HLW lag storage vessels of the HLW lag storage and blending system (HLP), and then on to the HLW vitrification process. The liquids pass through the permeable ultrafilter surface, while the solids are retained. The solids-free stream is now designated as the LAW feed stream, which is then routed to the three permeate hold vessels prior to further processing.

1.4 HLW Lag Storage and Blending Process System (HLP)

The HLW lag storage and blending process system (HLP) receives the HLW feed stream from the UFP. It stages this high solids slurry prior to transfer and subsequent processing in the HLW vitrification plant. The system also provides for blending of cesium and technetium recovered from the LAW treatment process into the HLW feed stream prior to transfer to the HLW vitrification plant.

1.5 Cesium Ion Exchange Process System (CXP)

Permeate from ultrafiltration will be transferred to the cesium ion exchange process system (CXP) to remove cesium from the LAW feed stream. The CXP uses four columns operating in series. At any given time, only three of the ion exchange columns are operating in the loading cycle, with the fourth column in standby, or undergoing elution/rinse/conditioning or resin replacement. The order of the columns may be rotated in series so that any of the columns may be in the lead position.

The concentration of cesium in the feed stream is monitored prior to, and following, each ion exchange column. When cesium is detected above an established setpoint, the lead A column is removed from service for regeneration or spent-resin replacement. Afterwards, it becomes a lag column in the next loading cycle. Cesium is removed from the resin with nitric acid. The cesium-loaded nitric acid is then routed to the nitric acid recovery process system (CNP), with the cesium ultimately processed in the HLW melter.

1.6 Cesium Nitric Acid Recovery Process System (CNP)

The cesium nitric acid recovery process system (CNP) recovers nitric acid that was previously used in resin bed regeneration for cesium ion exchange, for reuse. In addition, this system concentrates and transfers to storage the cesium extracted from the ion exchange system for incorporation into the HLW melter feed.

1.7 Technetium Ion Exchange Process System (TXP)

The primary function of the technetium ion exchange process system (TXP) is to remove technetium from the LAW feed stream. This is accomplished using a series of ion exchange columns containing a resin that preferentially extracts technetium. The TXP uses four columns operating in series, and is operated similarly to the CXP (including column regeneration and eluant management). The eluate from the resin bed regeneration is collected and transferred to the technetium eluant recovery process system (TEP) for recycling. Treated LAW is transferred to the treated LAW collection vessels.

1.8 Technetium Eluant Recovery Process System (TEP)

The technetium eluant recovery process system (TEP) recovers water from the eluate that was previously used for technetium ion exchange resin bed regeneration so that it may be reused. In addition, this system concentrates and transfers to storage the technetium extracted from the ion exchange system for incorporation into the HLW melter feed.

1.9 Treated LAW Evaporation Process System (TLP)

The treated LAW evaporator is a forced-circulation unit, operating under a vacuum to reduce the operating temperature. The treated LAW evaporation process system (TLP) will receive waste from the treated LAW collection vessels following technetium removal, and will receive and neutralize submerged bed scrubber purge from LAW vitrification. The TLP will also be available to condense the overhead vapors and transfer the condensate to the radioactive liquid waste disposal system (RLD). Additionally, off-specification effluent may be received from the plant wash and disposal system (PWD). The primary purpose of the TLP is to evaporate a portion of the LAW feed (reducing the volume and increasing the sodium concentration), and transfer the waste to the treated LAW concentrate storage process system (TCP).

The treated LAW evaporator is a forced-circulation unit operating under a vacuum to reduce the operating temperature. The TLP consists of a single evaporator train composed of two LAW submerged bed scrubber (SBS) receipt vessels, an evaporator separator vessel with demisters, a reboiler, a recirculation pump, overhead condensers, and an evaporator condensate pot. The recirculation pump maintains a high flow rate around the evaporation system. The recirculation pump transfers the waste through the reboiler and back into the separator vessel. The recirculating waste stream is prevented from boiling in the reboiler tubes by maintaining sufficient hydrostatic head to increase the boiling point above the temperature of the liquor in the reboiler.

As the liquid travels through the reboiler, the hydrostatic head diminishes, and flash evaporation occurs as the flow enters the separator vessel. The liquid continues to flash, and the vapor and liquid streams are separated. The liquid stream circulates in this closed loop (becoming more concentrated), while the vapor stream passes to the evaporator overhead system which contains a multi-stage condenser system. The non-condensables pass through the demister and are then routed to the pretreatment vessel vent process system (PVP) for treatment. The concentrated waste stream produced by the TLP is pumped continuously out of the evaporator system, and is discharged to the treated LAW concentrate buffer vessel.

1.10 Treated LAW Concentrate Storage Process System (TCP)

The primary functions of the treated LAW concentrate storage process system (TCP) are to receive treated waste from the pretreatment process, to provide buffer storage capacity, and to transfer waste to the LAW vitrification plant.

1.11 Plant Wash and Disposal System (PWD)

The primary function of the plant wash and disposal system (PWD) is to receive, store, and transfer effluent. It will collect plant wash, drains, and acidic or alkaline effluent from the pretreatment plant. Effluents will be recycled to the waste feed evaporation process system (FEP).

1.12 Radioactive Liquid Waste Disposal System (RLD)

The RLD system primarily receives effluent from the caustic scrubber purges from the LAW vitrification facility via PWD, waste feed evaporator system (FEP), and the treated LAW evaporator system (TLP), these effluents being the condensed vapors removed from the waste streams. Liquid effluents from the systems will be recycled or discharged to the Hanford Site liquid effluent retention facility (LERF) and then transferred to the effluent treatment facility (ETF).

1.13 Pretreatment Plant Vessel Vent Process System (PVP)

The PVP will treat two offgas streams. One stream will be from pretreatment vessel vents (tanks and other vessels), and the other stream will be exhaust from reverse flow diverters and pulsejet mixers. Following treatment in the PVP, the offgas streams will proceed to the process vessel vent extraction (PVV), where the streams will be routed through dual-stage HEPA filtration and radiological monitoring, prior to being discharged through the pretreatment plant stack.

2 Vitrification

The following subsections provide detailed descriptions of the melter units and processes.

2.1 LAW Melter System

The LAW vitrification plant will consist of several process systems designed to perform the following functions:

- Hold pretreated LAW waste
- Convert blended LAW waste and glass formers into molten glass
- Provide melter offgas treatment systems
- Provide immobilized low-activity waste (ILAW) container handling systems
- Provide ILAW container finishing systems
- Provide storage areas for ILAW containers
- Provide supporting equipment for the melter
- Provide miscellaneous waste handling systems
- Provide LAW vitrification plant ventilation systems

2.1.1 LAW Melter Feed

The LAW melter feed consists of the following systems:

- LAW Concentrate Receipt Process System (LCP)
- LAW Melter Feed Process System (LFP)
- Glass Former Reagent System (GFR)

These systems are shown in the schematic in Figure A-2.

The LCP and LFP prepare feed for the LAW melters to produce a vitrified product. The LAW concentrate will be transferred from the pretreatment plant to the feed concentrate vessels (LCP). Process control samples will be collected from these vessels and analyzed to determine the glass former formulation. After glass former addition and blending with pretreated LAW, the combined feed stream is fed into the melter where it is vitrified. This is described in greater detail below.

Each melter feed system consists of a LAW concentrate receipt vessel, a feed preparation vessel, and a melter feed vessel. The LCP includes all the LAW concentrate receipt vessels (CRV). The LFP includes the melter feed preparation vessel (MFPV) and the melter feed vessel (MFV) for each of the three melters. The LAW concentrate will then be transferred from the LCP to the LFP, where it will be mixed with glass formers from the LAW glass former feed hoppers. This will form a uniform slurry, which will be transferred to the LAW melter feed vessels, and then to the melters.

The glass former compounds required to produce a glass composition within the QGCR will be predetermined using a glass formulation algorithm to determine the glass former compound additions

needed to attain the nominal operating composition for the waste type being processed. The glass-forming chemicals that are expected to be used include silica, alumina, boric acid, calcium silicate, ferric oxide, lithium carbonate, magnesium silicate, zircon sand, and zinc oxide. Individual glass former compounds will be transferred from storage silos to individual hoppers fitted with load cells. Transfer of each glass former compound will be terminated when the calculated amount of each glass former compound is received in the corresponding hopper. Glass former compounds from the individual hoppers will then be transferred to a single blending hopper fitted with a load cell. The combined weight of glass former compounds will be verified (within measurement uncertainty) against the sum of the weights of the individual glass former compounds.

The glass former compounds will be blended and transferred to the GFR in the LAW vitrification building. The GFR contains the glass former feed hoppers that hold blended glass formers and sucrose. Each feed hopper is equipped with a pneumatic blending head at the base of the hopper to re-blend the glass former feed. The feed hoppers are equipped with load cells to weigh the glass formers to confirm that the material in the upstream blending silo is conveyed to the feed hoppers and to confirm that the glass formers are transferred out of the feed hoppers to the MFPV. The glass formers are gravity-fed with a rotary feeder into the MFPV, where the blended glass formers are mixed with the waste. The pretreated LAW feed in the MFPV will be continuously stirred by means of a mechanical agitator as the batch of glass former compounds are added from feed hopper. The hopper will be equipped with load cells to confirm that the correct mass of glass former compounds was transferred. Once blended, the melter feed slurry will be transferred from the MFPV to the MFV. From the MFV, the blended material is fed to the melter (to the LMP) continuously.

2.1.2 LAW Melter Process System (LMP)

The purpose of the LMP is to convert a blended slurry of liquid LAW feed and glass former additives into molten glass. The glass is discharged from the melter into metal containers, where it cools to form the immobilized low-activity waste (ILAW).

The current design of the LAW melter is a rectangular tank, lined with refractory material, with an outer steel casing. An additional outer steel casing with access panels will provide local shielding and containment. Each melter has a nominal design capacity of 10 metric tons of glass production per day. Based on experience with other vitrification systems, the anticipated operating temperature of the melter will be in the range of 950 °C to 1,250 °C. The actual operating temperature and residence time will be determined based on the results of research and technology (R&T) testing of waste forms. The temperature will be sufficient to ensure the removal of volatile and semi-volatile organic constituents from the waste matrix, as well as ensuring the proper mixing of waste constituents with the glass-forming materials.

The melter will be maintained under a vacuum to prevent escape of contaminants. Consumable melter parts will be replaced through access panels. The melters will be transported in and out of the gallery on a rail system.

The refractory package is housed in a steel shell, which provides containment for the molten glass. Active cooling on the exterior of the melter is provided by water jackets. The intermediate loop containing the water jacket will be a closed system that isolates the water circulating through the water jacket from the water in the cooling water loop circulating to the cooling tower. Any radioactive material leaking into the intermediate loop cooling water will be prevented from becoming an inadvertent discharge via the cooling tower. This system is designed for plenum temperatures of up to 1,100 °C.

Each LAW melter will use two independent discharge chambers. Molten glass is pumped by an airlift from the bottom of the melter pool, through a riser, into a discharge chamber, and poured into an ILAW container. The ILAW is then allowed to cool, forming a highly durable borosilicate glass waste form within the container.

Feed will be introduced to the melter as a slurry through nozzles in the melter lid. The LAW feed will be heated by passing an electrical current between electrodes in the glass pool, through a process known as joule-heating. The water and volatile feed constituents in the slurry will evaporate, leaving behind a layer of material known as the cold cap. New slurry will be added at about the same rate as the cold cap dissolves, maintaining the quantity of cold cap material at a steady level. Waste feed components that remain in the cold cap will undergo chemical reactions, be converted to their respective oxides, and dissolve in the melt. Air bubblers may be used to mix and agitate the molten glass.

After filling, the container will remain positioned at the glass pour seal head to recover residual glass discharges from the pour trough and provide initial cooling of the poured glass. Steam, volatile feed constituents, and decomposition products will be released as offgas during the vitrification process. This offgas, along with air from in-leakage, purges, and injections, will be routed to the LAW melter offgas treatment systems.

2.2 HLW Vitrification Plant

The HLW vitrification plant will consist of several process systems designed to perform the following functions:

- Hold pretreated HLW slurry
- Convert blended HLW slurry and glass formers into molten glass
- Treat melter offgas
- Handle IHLW canisters
- Store IHLW canisters
- Provide supporting equipment in the melter cave
- Handle miscellaneous waste
- Provide HLW vitrification plant ventilation systems

2.2.1 HLW Melter Feed

The HLW melter feed consists of the following:

- HLW Cave Receipt Process System (HCP)
- HLW Melter Feed Process System (HFP)

These systems are shown in the schematic in Figure A-2.

The HCP receive HLW feed slurry from the pretreatment plant. An analysis of the waste determines a glass additive formulation for the conversion of the waste to glass. The HCP contents are then transferred to the HFP and mixed with glass formers to form a uniform blend, and provide a blended feed to the

HLW melters. The glass additives specified in the formulation are weighed and mixed with the waste. This slurry will be transferred to the HLW melter feed vessel (MFV) and then to the HLW melter process system (HMP).

Like the LAW processing, the glass former compounds required to produce a glass composition within the QGCR will be predetermined using a glass formulation algorithm to determine the glass former compound additions needed to attain the nominal operating composition for the waste type being processed. Individual glass former compounds will be transferred from storage silos to individual hoppers fitted with load cells. The glass-forming chemicals expected to be used include silica, boric acid, calcium silicate, ferric oxide, lithium carbonate, and sucrose. Transfer of each glass former compound will be terminated when the calculated amount of each glass former compound is received in the corresponding hopper. Glass former compounds from the individual hoppers will then be transferred to a single blending hopper fitted with a load cell. The combined weight of glass former compounds will be verified (within measurement uncertainty) against the sum of the weights of the individual glass former compounds.

The glass former compounds will be blended and transferred to a glass former compound feed hopper in the HFP. In the HFP, waste from the HCP is transferred to the MFPV for blending with the appropriate glass formers. The mixture in the MFPV will be vigorously agitated to form a well-mixed melter feed slurry. The slurry will then be transferred to the MFV. The volume of slurry transferred will be confirmed by level measurements in the sending and receiving vessels. The slurry from the MFV will then be transferred on a continuous basis to the melter for vitrification.

2.2.2 HLW Melter Process System (HMP)

The primary functions of this system are to convert blended waste slurry and glass formers into molten glass, deliver molten glass to HLW canisters, fill the canisters with molten glass waste, and monitor and control glass waste level during waste filling.

The current design of the HLW melter is a rectangular tank lined with refractory material, with an outer steel casing. It has four compartments: a glass tank, two discharge chambers, and a plenum just above the glass tank. The tank is lined with refractory material designed to withstand corrosion by molten glass.

The HLW melter system consists of two HLW melters. Each of the two HLW melters has a nominal design capacity of 1.5 metric tons of glass waste per day. Based on experience with other vitrification systems, the anticipated operating temperature of each melter will be in the range of 950 °C to 1,250 °C. The actual operating temperature of the melters will be determined based on the results of R&T testing of waste forms. The temperature will be sufficient to ensure the removal of volatile and semi-volatile organic constituents from the waste matrix, as well as ensuring the proper mixing of waste constituents with the glass-forming materials.

The HLW melters will use two independent discharge chambers. Discharge will be achieved by transferring the molten glass from the bottom of the melter pool through a riser, from which it will be poured into a stainless steel IHLW canisters. Glass waste transfer will be accomplished through air lifting. The IHLW will then be allowed to cool, forming a highly durable borosilicate glass waste form.

The HLW melters will receive blended melter feed, consisting of glass formers and HLW feed slurry from the HLW melter feed vessel. The melters will be maintained at a negative pressure to the melter cave to ensure that any air leaks are inward. The melter caves will also be maintained at a negative air

pressure to the operating areas. The melters will be refractory-lined rectangular tanks with an outer steel casing. A water-cooled jacket will surround the exterior of the refractory to maintain a thermal gradient in the refractory material for corrosion control, to suppress outward migration of glass, and to reduce the heat load in the process cell.

The feed will be heated by passing an electrical current between two electrodes in the glass pool, through joule-heating. Feed will be introduced to the melter as a slurry. The water and volatile feed constituents will evaporate from the slurry to leave behind a layer of material known as the cold cap. New slurry will be added at about the same rate as the cold cap dissolves, maintaining a steady quantity of cold cap material. Waste feed components that remain in the cold cap will undergo a chemical reaction, be converted to their respective oxides, and dissolve in the melt. Air injectors may be used to mix and agitate the molten glass.

Steam, entrained particulates, decomposition products, and volatile feed constituents will be released as offgas during the vitrification process. The offgas, along with air from in-leakage, purges, and injections, will be routed to the HLW melter offgas treatment system.

It is anticipated that the design will incorporate an interface between the melter process, monitoring system, and integrated control system, to ensure consistency in the process of wastes, and that each batch of glass is processed to meet the needs for its specific constituent load. The details of this interface are being refined as part of the design process.

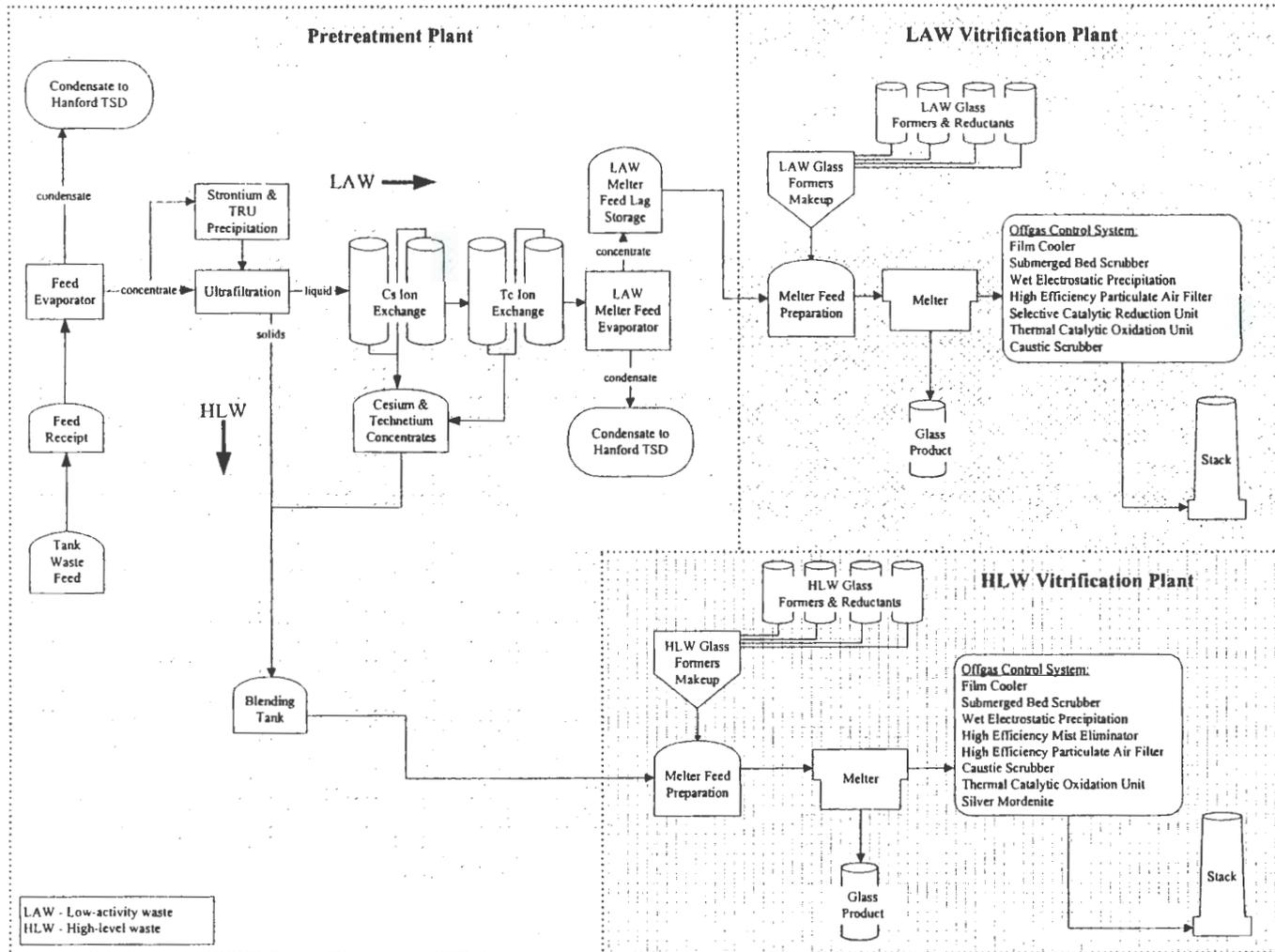
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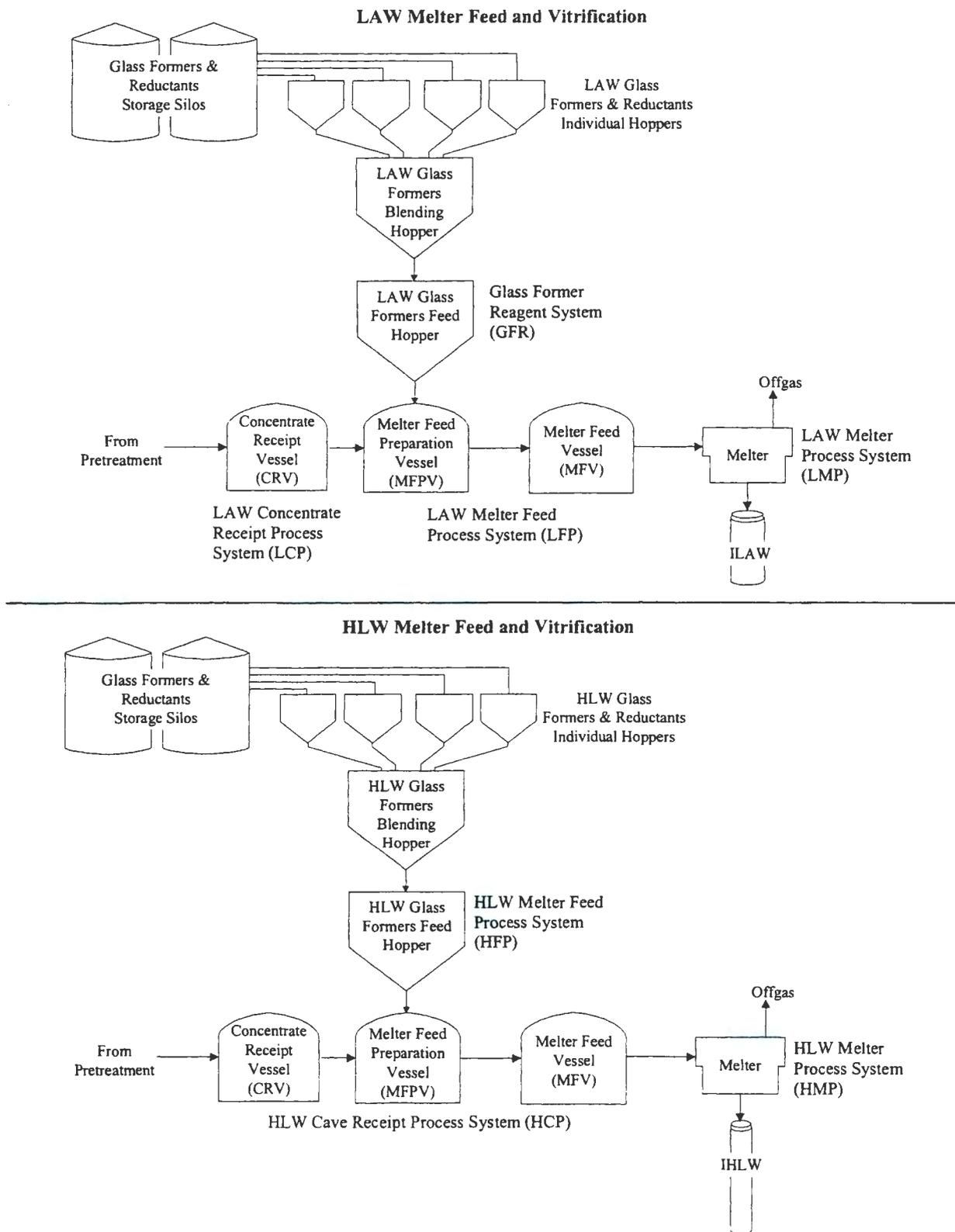
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Figure A-1 Simplified Waste Treatment Plant Flow Diagram



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Figure A-2 Simplified Melter Feed and Vitrification Schematic



Appendix B

Existing WTP Research Data and Activities Demonstrating the Concept of Vitrification

Appendix B

Existing WTP Research Data and Activities Demonstrating the Concept of Vitrification

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1 Introduction

The River Protection Project - Waste Treatment Plant (WTP) has conducted a number of analyses to determine the constituent makeup of Hanford tank waste, the intermediate products from pretreatment, and the glass resulting from vitrification of tank waste and simulated waste. The results of these analyses are summarized in this appendix. A general summary is provided in the introduction of each sub-section, with details provided below. References are provided in the write-up for each data summary, which will direct the reader to the source documents if additional information is desired.

The tables presented in these summaries provide data only for those constituents that were found in the samples; it is not the intent of this appendix to provide all of the analytical results from this extensive body of research. So, for example, if a constituent of concern was detected in supernatant from a specific tank feed sample, that constituent will be listed at the detected concentration, even if it was not found in the solids sample or glass sample from that feed stream. In addition, for each analysis, an attempt was made to provide a detection limit (DL) for the method that was used to evaluate that sample. None of the referenced analyses were performed according to strict SW-846 protocols, except where noted. For these, MDLs were not determined in accordance with Environmental Protection Agency (EPA) procedures. The referenced values should be considered an overall estimate of method performance, but not in the traditional meaning of a true detection limit. The data presented are research data, and are included to demonstrate the concept that vitrification is capable of immobilizing inorganic waste constituents. These data do not represent the data required to demonstrate LDR and delisting compliance. Data collected as part of the implementation of this DQO will be used for compliance demonstrations.

Data summarized below are flagged with modifiers U, J, and B. "U" indicates that the compound was not detected. "J" indicates that the compound or analyte has been detected, but concentrations are less than the DL, and are likely to have greater than a 15 % error in precision, accuracy, or both. "B" indicates that the compound or analyte was detected in the blank. Compounds flagged with a "B" were evaluated by the "5/10 Rule" for inclusion in the summary tables. The 5/10 rule is described in the Environmental Protection Agency Functional Guidelines for Data Validation of Organics (EPA 1991). If concentrations of common lab contaminants (methylene chloride, bis-2ethylhexyl phthalate, for example) in the sample exceeded blank concentrations by a factor of 10, results were included in the table. If unlikely lab contaminants in the sample exceeded blank concentrations by a factor of 5, results were included in the table. Contaminants detected in both the blank and the corresponding samples in approximately the same concentrations were not included in the results.

The summaries provided here identify the purpose of the tests for each data set, as described in the report of analytical results, the analyses performed along with any issues associated with those specific analyses or results, and any conclusions that could be made based on the results. As noted above, results have been grouped according to the corresponding waste envelope associated with a given sample. A discussion of results for the feed material (tank waste) is provided first, followed by a discussion of any available analysis for vitrified product from that feed material. The purpose for the analyses, as provided below, reflects the intent of the sampling and analysis as described in the relevant report. Results from analysis of surrogate and simulant materials are provided at the end of this appendix.

2 Tank Waste Characterization

The WTP contract defines four waste envelopes based on their constituent makeup. The following discussion presents the results of analyses that have been conducted to evaluate the composition of feed materials from Hanford DSTs, and the glass product from some of these feeds.

For LAW, the analytical results from crucible-scale tests are evaluated, and revised compositions are generated in order to optimize the properties of the glass. The formulations are therefore “actively designed”, rather than “statistically designed”. The actively designed approach is better suited to quickly and efficiently identifying acceptable solutions in the face of evolving constraints, whereas the statistically designed approach generally provides more even coverage of the composition space of interest once that region can be specified.

For the HLW, the analytical results from crucible-scale tests are evaluated, and revised compositions are generated in parallel with the development of statistically designed matrices of glasses, which are also generated and characterized. Earlier work covered an extremely wide composition range that was defined by the tank waste remediation system waste specifications, and the incorporation of LAW pretreatment products and entrained solids into the HLW feed stream. More recent work, in contrast, has had the benefit of a more refined contractual waste loading specification, and places more emphasis on formulations based on estimates of the compositions of wastes found in candidate waste tanks. For the HLW, Envelope D solids were blended with the projected products from LAW pretreatment, consistent with WTP design.

The model descriptions, descriptions of the relative impact of varying oxides on glass quality, and leachate prediction model equations are discussed in Appendix C.

Some or all of the following analyses were performed for each waste form:

- TC Metals following the TCLP extraction, were analyzed by inductively coupled plasma (ICP),
- Total inorganic, organic, and total carbon (TIC/TOC/TC)
- Inorganic and organic anions,
- Volatile organic analysis (VOA)
- Semi-volatile organic analysis (SVOA)
- Polychlorinated biphenyls (PCBs)
- Headspace analysis
- Radiochemical analyses

Detection limits (DLs) for specific analytes of interest varied, depending on the procedures used for preparing the samples for analysis, required dilutions for “as low as reasonably achievable” (ALARA), safety considerations, and the magnitude of interfering analytes. These detection limits, therefore, do not necessarily qualify as method detection limits (MDLs) as defined by SW-846. However, MDLs will be determined for water based on SW 846 or EPA 40 CFR 136, Appendix B protocols and adjusted for dilution of the TCLP extract being analyzed. Note that the MDLs/EQLs for the TCLP leachate (buffered acetic acid solution) are likely to be the same as those reported for water (with adjustments for dilution, if necessary). However, for inactive work, the MDLs/EQLs will be established by the subcontracted commercial laboratory. Section 5 provides action levels that translate into EQLs which will be specified

for testing facilities whose test plans are subject WTP approval before testing. Likewise EQLs have not been established for the analyses used. Analytical laboratories have reported DLs based upon evaluation of overall method performance and analytical instrument response. Where DLs have been provided with the laboratory data, these values are included in the "DL" column, although it is likely these values are closer to EQLs. Not all data reports included a DL for the analyses.

Some research laboratories reported results below their reported DL; these typically represent values for constituents detected by the analytical instrument, but at concentrations below the instrument calibration range. Determination of MDLs and EQLs is beyond the scope of the analytical work presented here, and is part of the Regulatory DQO, which is currently being implemented under a different project scope. For these reasons, all detected compounds of interest, and not just those detected above DLs, are summarized in the tables. Metals results, however, are limited to regulated toxic constituents. Radionuclide data are not included because these constituents are not subject to delisting or LDR criteria.

2.1 LAW Envelope A Results

Laboratory personnel collected and analyzed samples from tank waste, intermediate feed material, and glass product from Tanks 241 AW-101, 241-AP-101, and 241-AN-103 to evaluate the makeup of the feed and effectiveness of the various process steps to remove or otherwise stabilize constituents in the Envelope A materials.

TC metals analyses indicate concentrations in the feed materials for chromium, lead, arsenic and mercury at levels that exceed the regulatory threshold. Due to ALARA concerns, and the low regulatory threshold for selenium, it was not possible to determine accurately whether selenium exceeds the regulatory threshold in the feed materials.

Several volatile organic compounds (VOCs) were found in samples from the Envelope A feed and intermediate stage materials. These include 1-4 dioxane, acetone, and tetrahydrofuran found at concentrations above the DLs in the supernatant materials from AW-101.

Organic anion analysis resulted in detectable concentrations for oxalate, formate, and acetate in feed samples from multiple sources. Although acetate is reported, acetate co-elutes with glycolate and requires the use of an alternate column for separation from glycolate, which was not done by the laboratory. Therefore, the analytical results may be indicative of primarily glycolate, primarily acetate, or a combination of both anions.

Headspace analyses were performed on supernatant samples from AW-101; methanol was detected below the DL. Ethanol was detected in the blank and samples at approximately the same concentrations, and is likely due to contamination.

Analysis of glass samples from the treated Envelope A materials, found no TC metals at concentrations that exceed the TC limits, indicating that these constituents are either removed from the feed during pretreatment, or effectively bound within the glass matrix.

No detectable concentrations of VOC or SVOCs were found in AW-101 glass samples. The analysis of glass product did not include an evaluation for organic anions.

No volatile organics, semi-volatile organics, PCBs, dioxins, or furans were detected in the glass samples from Envelope A product generated from treatment of feed from AW-101 and AN-103. No glass product

analyses were available for product from AP-101. A small quantity of cyanide was detected in the AW-101 glass sample; however, the quantity detected in the glass is near the DL, and the actual presence of cyanide in the glass is questionable.

None of the TC metals analytical results exceeded TC limits (Fiskum 2000; TRPT-W375-00012, Urie et al. 1999; Ferrara, Ray, Kubilius, and Crawford 2001; Urie et al. 2001; Hay et al. 2000; 83). Details are provided below.

2.1.1 Tank AW-101

2.1.1.1 Waste Characterization

Summary: Pacific Northwest National Laboratory (PNNL) analytical staff mixed 30 jars of waste material from Tank AW-101 to provide a single composite sample. The composite was homogenized and sub-sampled for inorganic, radiochemical, and organic analyses. Results were reported for the "supernatant" fraction and the "wet centrifuged solids" fraction.

Purpose: The organic analysis results obtained from the "as received" tank waste materials will be used to support permitting activities, and to provide limited characterization information for subsequent process testing.

Analyses: Organic analyses of the feed materials consisted of volatile organic analysis (VOA), semi-volatile organic analysis (SVOA), polychlorinated biphenyls (PCBs) and pesticides, dioxins and furans, oxalate, formate, acetate, and acrylate by ion chromatography (IC), ethanol, methanol, 2-propanol, 1-propanol, n-butanol, triethylamine, tert-butanol, and 2-butanol by headspace analysis. More limited analysis was conducted for the glass product.

Discussion of Analytical Results

TCLP Metals Analysis: The results from total metals analysis for the feed and glass product are included in Table B-2. The toxicity characteristic leaching procedure (TCLP), SW-846 Method 1311, was not performed on AW-101 waste materials for toxic metals. Estimated toxicity characteristic (TC) metals concentrations were calculated from the following information:

- The total analysis concentrations of the TC metals in supernatant
- The total analysis concentrations of TC metals from acid digestion of the solids (assuming all metals would be leached 100 % using Method 1311)
- The density of the supernatant
- The centrifuged wet weight % solids

The calculations assumed a 100 g initial sample size for processing. The acid digestion results are considered to be conservative, because the nitric-hydrochloric acid digestion is significantly more rigorous than the TCLP acetic acid leaching. The EPA published memos allowing the use of the total analysis versus the analysis of the leachate in 1993 and 1994 (EPA 1994). The results of analysis indicate that the AW-101 feed waste materials may have TC metals concentrations that exceed the regulatory threshold, specifically for arsenic, chromium, mercury, and lead (Table B-1). Due to the dilutions required to support as low as reasonably achievable (ALARA) concerns, and the low regulatory threshold for selenium, it could not be determined if selenium in the waste feed exceeds the regulatory threshold.

Organics: Table B-2 includes the volatile, semi-volatile, PCB, and pesticide compounds that were detected through analysis of the feed and glass product. As cited in Table B-2, there were a limited number of volatile, semi-volatile, PCBs and pesticide compounds found in the feed materials. It should be noted, however, that, because the samples were homogenized and centrifuged, the volatile analysis is not valid.

Headspace analysis was performed on supernatants only. Methanol was detected below the DL in a sample from AW-101 (that is, methanol was detected, but the uncertainties associated with quantification at such a low level result in an "estimated" quantity for a result). Ethanol was detected in the blank and samples at approximately the same concentrations, and is likely due to contamination; therefore, ethanol concentrations were not included in Table B-2. Again it should be noted, that, because the composite sample of the feed was homogenized and centrifuged before analysis, the results for volatile analysis are not valid.

Organic anion analysis resulted in detectable concentrations for oxalate, formate, and acetate. These results are summarized in Table B-2. Although acetate is reported, acetate co-elutes with glycolate, and requires the use of an alternate column for separation from glycolate, which was not done by the laboratory. Therefore, the analytical results may be indicative of primarily glycolate, primarily acetate, or a combination of both anions.

References:

Klinger, G. S., et al. 2000. *Organic Analysis of AW-101 and AN-107 Tank Waste*, Battelle, Pacific Northwest Division, PNWD-2461.

Urie, M.W., et al., 1999. "Inorganic and Radiochemical Analysis of AW-101 and AN-107 Tank Waste," PNWD-2462, BNFL-RPT-008, Rev. 0. Pacific Northwest National Laboratory, Richland, Washington.

2.1.1.2 Glass Product Analysis

Summary: The WTP retained PNNL to produce, test, and characterize vitrified immobilized low-activity waste (ILAW) waste forms from an Envelope A low-activity waste (LAW) sample from Tank 241-AW-101.

Purpose: An objective of this work was to provide analytical data that can be used to support designation of the ILAW product for dangerous waste characteristics, dangerous waste criteria, and dangerous waste sources generated from the processing of AW-101 pretreated waste. The analyses also provide data to demonstrate compliance with applicable land disposal restrictions (LDR) criteria. The testing and characterization are being conducted to aid in planning for treatment and eventual disposition of Hanford tank waste.

Analyses: The LAW glass sample was either analyzed directly (VOA and cyanide (CN)), extracted (SVOA, PCB, dioxins, and furans), or leached (TCLP) prior to analysis.

Discussion of Analytical Results: Table B-2 identifies the analytes detected in the glass sample. No volatile organics, semi-volatile organics, PCBs, dioxins, or furans were detected in the AW-101 glass sample.

No cyanide was detected in the AW-101 process blank, yet a small quantity of cyanide was detected in the AW-101 glass sample. The quantity detected in the glass is near the DL, however, and the actual presence of cyanide in the glass is questionable (Table B-2).

The AW-101 glass sample was leached and the TCLP leachate was analyzed for TC metals (As, Ba, Cd, Cr, Pb, Se, Ag). None of the TC metals analytical results exceeded TC limits.

Reference:

Urie MW et al. 2001. *Regulatory Analysis on Glass Product from AW-101 and AN-107 LAW Pretreated Wastes*, WTP-RPT-005, Rev. 0. Pacific Northwest National Laboratory, Richland, Washington, USA, February 2001.

Conclusions

Overall, the results indicate that the glass produced by the vitrification method is resistant to leaching and does not contain volatile or extractable organic compounds above target levels for this waste form. The AW-101 glass product contained no substantial levels of target analytes, although some analytes were detected above the analytical DL.

2.1.2 Tank 241-AP-101

2.1.2.1 Waste Characterization

Summary: WTP transmitted five supernate samples from Hanford waste Tank 241-AP-101 to Battelle for analysis. The samples were collected at five different depths within the tank, and mixed together to provide a single composite sample. The composite was homogenized, and representative sub-samples were collected for inorganic, radioisotopic, and organic analyses. No settled solids were visible in the samples; therefore, solids were not characterized. All samples were clear, yellow liquid with no visible settled or suspended solids. All analyses were run in triplicate, and the average results from the three runs are summarized in Table B-3. No analytical results were available for glass product from 241-AP-101.

Purpose: The waste in Tank 241-AP-101 has been identified as a potential candidate for LAW Envelope A feed. Samples were provided to PNNL for analysis and testing to evaluate the waste composition and ability to process the waste. The results of the analyses will be used to assess the waste composition relative to the contract limits defined in contract Specification 7 for Envelope A.

Analyses: The characterization of the 241-AP-101 composite feed samples included the following analyses: total metals by inductively coupled plasma (ICP), radioisotopic analyses, ion chromatography (IC) for inorganic and organic anions, density, total inorganic carbon (TIC), total organic carbon (TOC), toxicity characteristic (TC), mercury, free hydroxide, ammonia, cyanide, and polychlorinated biphenyls (PCBs).

Discussion of Analytical Results: Detected analytes (excluding radioisotopes) are summarized in Table B-3.

Inductively Coupled Plasma (ICP) Metals: Boron was present in the preparation blank at 40 %, and arsenic at 10 %, of the sample concentration, indicating the sample boron and arsenic concentrations could be biased high by the digestion method. Matrix spike recoveries were low for silver (35 %), barium

(30 %), and lead (65 %). Low recoveries are attributed to the presence of sulfate or carbonate in the sample. Low silver recoveries are attributed to the small amount of hydrochloric acid used in sample preparation, causing some silver chloride precipitation. The phosphorous concentration is virtually identical to the phosphate concentration, indicating the phosphorous is primarily present as phosphate.

Anions by IC: The reported acetate concentration represents the summation of acetate and glycolate, as both ions co-elute under the sample analysis conditions. The reported fluoride result (average 2900 µg/ml) represents the maximum concentration due to overlap of the IC peak with acetate and formate. The acetate and formate were quantified on the organic IC system, the sum of these two analytes is 2840 µg/ml. This result indicates that very little fluoride is present in 241-AP-101.

Organics: No PCBs (detection limit of 1.4 µg/L) were detected in the samples. No other organics characterization work was performed.

Conclusion: The 241-AP-101 composite sample met all contract limits (molar ratio of analyte to sodium or ratio of becquerels of analyte to moles of sodium) defined in Specification 7 for Envelope A, as provided in tank waste remediation system privatization contract DE-AC27-96-RL133008. No glass product analyses were received for Tank 241-AP-101.

Reference:

Fiskum, S. K. 2000. *Inorganic and Radioisotopic, and Organic Analysis of 241-AP-101 Tank Waste*. PNWD-3046, BNFL-RPT-046, Rev. 1. Battelle, Pacific Northwest Division, Richland, Washington.

2.1.3 Tank 241-AN-103

2.1.3.1 Waste Characterization

Summary: The Savannah River Technology Center (SRTC) received and chemically characterized a whole tank composite sample from Hanford waste Tank 241-AN-103. Prior to characterization, the sample was diluted to approximately 5 molar (M) sodium concentration. The SRTC analyzed the filtered supernatant liquid, the total dried solids of the sample, and the washed insoluble solids obtained from filtration of the sample.

Purpose: The SRTC was contracted to provide pretreatment development and testing services to support the vitrification of Hanford tank waste. The tank samples allow for testing of the pretreatment processes with actual waste samples. The characterization data provide a basis for developing pretreatment processes, determining reagent requirements, and developing physical design parameters for the pretreatment plant.

Analyses: Analyses conducted on tank sample 241-AN-103 included anions by IC (also fluoride and chloride by ion selective electrode [ISE]), total metals by ICP, potassium and mercury by cold vapor atomic absorption (CVAA), and radioisotopic analyses by gamma energy analysis (GEA), inductively coupled plasma-mass spectroscopy (ICP-MS), and alpha counting spectroscopy.

Discussion of Analytical Results: The composite sample from AN-103 was derived by combining 12 extruded samples. The composite sample was thoroughly mixed and split into two samples; one was diluted to approximately 5 M sodium concentration and analyzed. The second sample was set aside. After completing the first set of tests, the second sample was diluted to approximately 5 M sodium

concentration, combined with the balance of the diluted first sample, and the analyses were repeated. Table B-4 includes a summary of analytes of interest that were detected in these samples. The report contains no discussion of quality control (QC) samples.

Reference:

Hay, M. S., et al. 2000. *Chemical Characterization of an Envelope A Sample from Hanford Tank 241-AN-103*, BNF-003-98-0248, Rev. 0. Savannah River Technology Center, Aiken, South Carolina.

2.1.3.2 Glass Product Analyses

Summary: A sample of waste from Hanford Tank 241-AN-103 was shipped to the Savannah River Site, where it was pretreated to remove the majority of radionuclides, and then vitrified. Pretreatment and vitrification were conducted using laboratory-scale methods of the approach that is planned for the WTP. Results of analysis indicate that the glass was close to target composition.

The report contains no discussion of QC samples.

TCLP analysis, performed on a supernate sample from AN-103 that was pretreated and vitrified, showed that the waste would not designate as characteristic waste.

Purpose: SRTC was asked to perform demonstrations of the proposed vitrification process using both nonradioactive samples in the form of waste simulants, and radioactive samples from the Hanford Tank Farms. A regulatory analysis was performed of the glass waste form that was produced from the pretreatment and vitrification of a supernate sample from Tank 241-AN-103. The results in the referenced report are from analysis of a glass waste form that was produced through six vitrification tests. Three tests were performed with a non-radioactive simulant, and three were performed with pretreated samples of supernate from 241-AN-103.

Analysis: For VOA, samples were broken with a mortar and pestle to fit into a 40 ml vial. For other analyses, the material was ground into particles smaller than 0.9 cm in diameter. Samples were analyzed for volatile organics, IC organics, methanol, semi-volatiles, pesticides and PCBs, dioxin and furan, TCLP, miscellaneous physical properties, and radionuclides. It must noted, however, that because the sample was broken using a mortar and pestle, any volatiles that may have been in the sample may no longer be there.

Discussion of Analytical Results: Although some of the results from TCLP analysis were higher than expected, the results indicate that the glass waste form did not possess the characteristics of dangerous waste. The waste form was not ignitable, reactive, or toxic and did not contain cyanide above regulated levels.

Cyanide was not detected in the samples or the blanks. Although the detection limits used in the analysis were limited due to the quantity of sample available, the values used are well below the LDR criteria for total (590 mg/kg) or amenable (30 mg/kg) cyanide.

The results of TCLP analysis were at least an order of magnitude below Universal Treatment Standards (UTS) for all constituents except barium. Even barium, however, was less than one-eighth of the UTS value.

Although four volatile organic constituents (toluene, acetone, tert-butanol, and octamethyl cyclotetrasiloxane) were found in the samples using Method 8260B, the concentrations at which they were detected (between 3 and 7 µg/kg) are below what is typically considered quantitative (less than ten times the detection limit). With the exception of acetone, all of these compounds were also found in the field blank. The presence of these compounds is believed to be due to sample contamination.

Method 8015 analysis showed methanol concentrations below the detection limit (0.1 mg/kg) for all samples and blanks, except for one process blank. This result is expected to have been due to contamination, although the source is not known. Semi-volatile organic compounds (SVOCs) were looked for using Method 8270 °C. Target compounds were not detected at concentrations above approximately 500 µg/kg for the group.

PCB analysis was conducted using Method 8082; none of the Aroclors were detected in the samples at concentrations above 150 µg/kg.

Two dioxins and one furan were reported as present in concentrations above method detection limits. All of these compounds, however, were found at similar or higher concentrations in all process and field blanks.

Reference:

Ferrara, D., Ray, R., Kubilius, W., and Crawford, C. 2001. *Results from Analyses of a Hanford Envelope A Radioactive Glass Waste Form*. SRT-RPP-2-001-000266, WSRC-TR-2001-00109, Rev. 1. Savannah River Technology Center, Aiken, South Carolina.

2.2 LAW Envelope B Results

Tank wastes evaluated for Envelope B included materials from Tank 241-AZ-102. Envelope B supernatant contained low levels of metals, such as aluminum and phosphorus, but a relatively high concentration of chromium. The supernatant from these feed materials also contained relatively high concentrations of sulfate. Potassium, iron, aluminum, chromium, and silicon also were present at significant concentrations in the total dried solids. In contrast, iron and aluminum dominate the composition of the dried insoluble sludge solids. The insoluble solids also consist of lesser amounts of cadmium, zirconium, nickel, sodium, and silicon. (Note the insoluble solids associated with Envelope B are actually Envelope D feed.) TC limits for Envelope B (AZ-102 supernatant, see Table B-5) were exceeded for chromium. It is uncertain if TC limits for lead or mercury were exceeded because the analytical quantitation limit is above the TC limit. Cadmium was not detected above TC limits.

The TOC value in Envelope B exceeds the organic carbon derived from the sum of the formate and oxalate by nearly an order of magnitude. These results indicate the potential presence of a significant organic carbon source besides the formate and oxalate, however, organic analysis only included formate, oxalate, and TOC.

No glass product sample results are available for treated Envelope B materials (Brooks et al. 2000; Hay and Bronikowski 2000). Details are provided below.

2.2.1 Tank 241-AZ-102

2.2.1.1 Waste Characterization

Summary: The SRTC received and chemically characterized a sample from Hanford waste Tank 241-AZ-102. The sample, containing supernate (designated Envelope B), and a small amount of sludge solids (designated Envelope D), was analyzed as received. The filtered supernatant liquid, the total dried solids of the sample, and the washed insoluble solids obtained from filtration of the sample were analyzed. No glass product was sampled from this waste form.

Purpose: The SRTC was contracted to provide pretreatment development and testing services to support the vitrification of Hanford tank waste. The tank samples allow for testing of the pretreatment processes with actual waste samples. The characterization data provide a basis for developing pretreatment processes, determining reagent requirements, and developing physical design parameters for the pretreatment plant.

Analyses: Analyses conducted on tank sample 241-AZ-102 included anions by IC (also fluoride and chloride by ISE), total metals by ICP, potassium and mercury by CVAA, and radioisotopic analyses by GEA, ICP-MS, and alpha-counting spectroscopy.

Discussion of Analytical Results: Data from selected analytes of interest found in the waste are summarized in Table B-5. The analytical results for the filtered supernatant indicate the sample is a relatively dilute salt solution with a sodium concentration of 2.77 M. ICP analysis indicates the supernatant contains low levels of other metals, such as aluminum and phosphorus, but a relatively high concentration of chromium. The supernatant also contains a relatively high concentration of sulfate. A high sodium content is also evident in the solids samples. Other metals with significant concentrations in the total dried solids include potassium, iron, aluminum, chromium, and silicon. In contrast, iron and aluminum dominate the composition of the dried insoluble sludge solids. The insoluble solids also consist of lesser amounts of cadmium, zirconium, nickel, sodium, and silicon.

The TOC value exceeds the organic carbon derived from the sum of the formate and oxalate by nearly an order of magnitude. The TOC results indicate the potential presence of a significant organic carbon source besides the formate and oxalate. The report does not include a discussion of QC samples.

Table B-5 includes the data for both the supernate and solids portions of the samples from 241-AZ-102, although these fractions correspond to different waste envelopes (B and D, respectively). This information is repeated in the summary of results for Envelope D, which is presented later in this Appendix.

Reference:

Hay, M. S., and Bronikowski, M. G. 2000. *Chemical Characterization of an Envelope B/D Sample from Hanford Tank 241-AZ-102*, BNF-003-98-0249, Rev. 0. Savannah River Technology Center, Aiken, South Carolina.

2.3 LAW Envelope C Results

Envelope C analyses were performed for feed wastes from Tanks AN-107 and AN-102. Calculated concentrations for TCLP metals indicate that the AN-107 waste feed materials may contain TC metals

concentrations that exceed the regulatory threshold, specifically chromium, cadmium, arsenic, and lead. Due to the dilutions required to support ALARA concerns and the low regulatory threshold for selenium, it could not be determined if selenium exceeds the regulatory criteria in the feed.

Organic anion analysis resulted in detectable concentrations for oxalate, formate, and acetate. Although acetate is reported, acetate co-elutes with glycolate, and requires the use of an alternate column for separation from glycolate; therefore, the analytical results may indicate primarily glycolate, primarily acetate, or a combination of both anions.

Headspace analyses were performed on supernatant samples from AN-107. Methanol and triethylamine were detected in the sample at concentrations below the DL. Ethanol was detected in the blank and samples at approximately the same concentrations, and is likely due to contamination.

Analysis also was performed on a glass sample of treated waste from AN-107. Although a limited number of volatiles, semi-volatiles, PCBs, pesticides, dioxins, and furans were present at detectable concentrations in the feed materials, analysis of glass product showed only the presence of 2-butanone (MEK) in the product from the AN-107, at a concentration below the DL, and well below the UTS for that compound. The presence of MEK is likely the result of laboratory contamination.

None of the samples from the Envelope C glass product were found to have TC metals at concentrations that exceed regulatory criteria (Urie et al. 1999; Urie et al. 2001; Hay, Bronikowski, Hsu, and White 2000; Klinger, et al. 2000). Details are provided below.

2.3.1 Tank 241-AN-102

2.3.1.1 Waste Characterization

Summary: The SRTC received and chemically characterized an approximately 14.25 L sample from Hanford waste Tank 241-AN-102. Prior to characterization, the sample was diluted to approximately 6 M sodium concentration. The filtered supernatant liquid, the total dried solids of the sample, and the washed insoluble solids obtained from filtration of the sample were analyzed. No analysis was performed on a glass sample from this waste.

Purpose: The SRTC was contracted to provide pretreatment development and testing services to support the vitrification of Hanford tank waste. The tank samples allow for testing of the pretreatment processes with actual waste samples. The characterization data provide a basis for developing pretreatment processes, determining reagent requirements, and developing physical design parameters for the pretreatment plant.

Analyses: Analyses conducted on tank sample 241-AN-102 included anions by IC (also fluoride and chloride by ISE), total metals by ICP, potassium by atomic absorption and mercury by CVAA, and radioisotopic analyses by GEA, ICP-MS, and alpha-counting spectroscopy. Organic analyses consisted of EDTA and HEDTA by ion-pair chromatography; organic acids (citrate, glycolate, formate, and acetate) were analyzed with ion-exclusion chromatography.

Discussion of Analytical Results: A sample designated as "Small C" was obtained from the composite of the first shipment. Approximately 1.5 L of the first shipment composite was diluted with approximately 750 ml of 0.01 M NaOH, producing 2.25 L of an approximately 6 M sodium solution. The resulting Small C sample was then filtered. Samples of the total dried solids of the diluted Small C

sample, the filtered supernatant liquid, and the insoluble solids were collected during filtration and analyzed. Table B-6 provides results for selected analytes of interest.

Reference:

Hay, M. S., Bronikowski, M. G., Hsu, C. W., and White, T. L. 2000. *Chemical Characterization of an Envelope C Sample from Hanford Tank AN-102*, BNF-003-98-0250, Rev. 0. Savannah River Technology Center, Aiken, South Carolina.

2.3.2 Tank 241-AN-107

2.3.2.1 Waste Characterization

Summary: PNNL analytical staff mixed 17 jars of LAW Envelope C waste material from Tank 241-AN-107 to provide a single composite sample. The composite was homogenized and sub-sampled for inorganic, radiochemical, and organic analyses. Results were reported for the “supernatant” fraction and the “wet centrifuged solids” fraction.

Purpose: The results of organic analysis obtained from the “as received” tank waste materials will be used to support permitting activities, and provide limited characterization information for subsequent process testing.

Analyses: Organic analyses consisted of VOA, SVOA, PCBs and pesticides, dioxins and furans, oxalate, formate, acetate, and acrylate by IC, ethanol, methanol, 2-propanol, 1-propanol, n-butanol, triethylamine, tert-butanol, and 2-butanol by headspace analysis.

Discussion of Analytical Results

TCLP Metals Analysis: The TCLP, SW-846 Method 1311, was not performed on 241-AN-107 waste materials for toxic metals. The estimated TCLP metals concentrations (Table B-7) were calculated from the following information:

- The total analysis concentrations of the TC metals in supernatant
- The total analysis concentrations of TC metals from acid digestion of the solids (assuming all metals would be leached 100 % using Method 1311)
- The density of the supernatant
- The centrifuged wet weight % solids

The calculations assumed a 100 g initial sample size for processing. The acid digestion results, found in Table B-8, are considered to be conservative, because the nitric-hydrochloric acid digestion is significantly more rigorous than the TCLP acetic acid leach. The EPA published memos in 1993 and 1994 allowing the use of total analysis versus analysis of the leachate (EPA 1993). The results indicate that the 241-AN-107 waste materials may contain TC metals concentrations that exceed the regulatory threshold, specifically chromium, cadmium, arsenic, and lead. Due to the dilutions required to support ALARA concerns, and the low regulatory threshold for selenium, it could not be determined if selenium exceeded the threshold for this analysis.

Detected compounds for volatile organic compounds (VOCs), SVOCs, PCBs, pesticides, dioxins, and furans are summarized in Table B-8. Although a limited number of volatiles, semi-volatiles, PCBs, pesticides, dioxins, and furans were present at detectable concentrations in the feed materials, analysis of the 241-AN-107 glass product showed only the presence of 2-butanone (MEK), at a concentration below the DL (Sample 46J $\mu\text{g}/\text{kg}$; DL=50 $\mu\text{g}/\text{kg}$), and well below the UTS for that compound (36 mg/kg for non-wastewaters). Glass product analysis is discussed below. Because the feed sample was homogenized before analysis, results of volatile analysis should not be considered representative of actual concentrations.

Organic anion analysis resulted in detectable concentrations for oxalate, formate, and acetate, as summarized in Table B-8. Although acetate is reported, acetate co-elutes with glycolate, and requires the use of an alternate column for separation from glycolate; therefore, the analytical results may indicate primarily glycolate, primarily acetate, or a combination of both anions.

Headspace analysis was performed on supernatants only. Methanol and triethylamine were detected in the 241-AN-107 sample below the DL. Ethanol was detected in the blank and samples at approximately the same concentrations, and is likely due to contamination; therefore, ethanol concentrations were not included in Table B-8.

Reference:

Klinger, G. S., et al. 2000. *Organic Analysis of AW-101 and AN-107 Tank Waste*, Battelle, Pacific Northwest Division, PNWD-2461.

Urie, M. W., et al. 1999. *Inorganic and Radiochemical Analysis of AW-101 and AN-107 Tank Waste*, PNWD-2462, BNFL-RPT-008, Rev. 0. Pacific Northwest National Laboratory, Richland, Washington.

2.3.2.2 Glass Product Analyses

Summary: PNNL was retained to produce, test, and characterize vitrified ILAW waste forms from an Envelope C LAW sample from Tank 241-AN-107.

Purpose: An objective of this work is to provide analytical data that can be used to support designation of the ILAW product for dangerous waste characteristics, dangerous waste criteria, and dangerous waste sources generated from the processing of 241-AN-107 pretreated waste. The analyses are also used to provide data that demonstrate compliance with applicable LDR criteria. The testing and characterization are being conducted to aid in planning for treatment and eventual disposition of Hanford tank waste.

Analyses: The LAW glass sub-samples were either analyzed directly (VOA and CN), extracted, or leached prior to analysis (SVOA, PCB, TCLP, dioxins and furans).

Discussion of Analytical Results: Analytes detected in tank waste feed or glass product are summarized in Table B-8. The compound 2-butanone (MEK) was detected in the 241-AN-107 glass sample, but was not detected in the sample duplicate. Concentrations of 2-butanone (MEK) were below the DL (Sample 46J $\mu\text{g}/\text{kg}$; DL=50 $\mu\text{g}/\text{kg}$), and well below the UTS for that compound.

No SVOCs, PCBs, dioxins, furans, cyanide, or sulfide were detected in any of the glass samples.

The 241-AN-107 glass sample was leached and the TCLP leachate was analyzed for TC metals (As, Ba, Cd, Cr, Pb, Se, Ag). None of the TC metals exceeded TC limits.

Reference:

Urie MW et al. 2001. *Regulatory Analysis on Glass Product from AW-101 and AN-107 LAW Pretreated Wastes*, WTP-RPT-005, Rev. 0. Pacific Northwest National Laboratory, Richland, Washington, USA, February 2001.

Conclusions

Overall, it appears from the results that the glass produced by the vitrification method is resistant to leaching and does not contain volatile or extractable organic compounds above target levels for this waste form. The 241-AN-107 LAW glass products contained no substantial levels of target analytes, although some analytes were detected above the analytical DL.

2.4 HLW Envelope D Results

Feed samples have been analyzed to characterize Envelope D wastes from Tanks C-104, C-106, AY-102, AZ-101, and AZ-102. The initial dewatering steps, as well as dilute caustic washing, appear to remove a majority of the sodium, potassium, and the anions from the Envelope D feed materials. During the caustic leaching, aluminum, phosphorus, silicon, and chromium also were removed, as well as additional potassium. During the course of washing and leaching, most of the soluble anions measured by ion chromatography (IC) were washed from the solids, with small amounts of chloride, phosphate, sulfate, and fluoride remaining.

Where TCLP analysis SW-846, method 1311, was not performed on feed samples, TCLP concentrations were estimated based on total metals analysis. Estimated TCLP metals concentrations from feed materials indicate that the C-104 waste may have TC metals concentrations that exceed the regulatory threshold, specifically for cadmium, chromium, mercury, and lead. Due to the dilutions required to support ALARA concerns, and the low regulatory threshold for selenium, it cannot be determined if selenium exceeds the threshold.

The TOC values in the feed materials for C-104 and AZ-102 exceed the organic carbon derived from the sum of the formate and oxalate by nearly an order of magnitude. The TOC results indicate the potential presence of a significant organic carbon source in the feed, beside the formate and oxalate.

Although the presence of Aroclors was evident, a substantial degradation of the expected response pattern was observed. The presence and approximate quantity of PCBs in the solids sample were confirmed using mass spectrometry, however, the concentration of PCBs in the supernate was not adequate for confirmation by mass spectrometry. Further investigation is necessary to accurately determine the quantity of PCBs present in these samples.

Samples of glass product from C-104 and AZ-102 have been analyzed for regulated constituents in the treated waste. No volatile compounds were detected in glass samples. One semi-volatile compound, bis(2-ethylhexyl)phthalate, was detected in both samples at concentrations less than the DL (Sample 730J/110J $\mu\text{g}/\text{kg}$, DL=1000 $\mu\text{g}/\text{kg}$). Bis(2-ethylhexyl)phthalate is a common plasticizer, however, and its presence may be due to contamination during sample processing.

No PCBs, dioxins, or furans were detected in any of the glass samples.

Sulfide was not detected in HLW glass samples. Cyanide was detected in glass from C-104 at a level approximately two times the DL, but still well below the UTS criteria. At this level, and with no cyanide detected in the C-104 duplicate, the presence of cyanide in the C-104 HLW glass is questionable.

None of the TC metals results from the HLW glass samples exceeded TC limits (Battelle 2000; Goheen et al. 2001; Evans et al. 2001; Hay and Bronikowski 2000; Fiskum et al. 2000). Details are provided below.

2.4.1 Tank 241-C-104

2.4.1.1 Waste Characterization

Purpose: Characterization of the “as received” tank waste materials was conducted to provide key characterization information for processing, and to provide limited information to support permitting activities and envelope characterization.

Analyses: Inorganic analyses consisted of total metals by ICP (acid digestion and KOH fusion digestion), radiochemical analyses, ICP/MS (radionuclides), total uranium, anions by IC, mercury, CN, ammonia, TOC, TIC, and total carbon, pH and OH-, and flashpoint. Organic analyses consisted of VOA, SVOA, PCBs, pesticides, dioxins and furans, oxalate, formate, acetate and acrylate by IC, ethanol, methanol, 2-propanol, 1-propanol, n-butanol, triethylamine, tert-butanol, and 2-butanol by headspace analysis.

Findings/Discussion:

TCLP Metals Analysis: The TCLP, SW-846 Method 1311, was not performed on 241-C-104 waste materials for toxic metals. The estimated TCLP metals concentrations (Table B-9) were calculated from the following information:

- The total analysis concentrations of the TC metals in supernatant
- The total analysis concentrations of TC metals from acid digestion of the solids (assuming all metals would be leached 100 % using Method 1311)
- The density of the supernatant
- The centrifuged wet weight % solids

The calculations assumed a 100 g initial sample size for processing. The acid digestion results, provided in Table B-10, are considered to be conservative because the nitric-hydrochloric acid digestion is significantly more rigorous than the TCLP acetic acid leach. The results indicate that the 241-C-104 waste materials may have TC metals concentrations that exceed the regulatory threshold, specifically cadmium, chromium, mercury, and lead. Due to the dilutions required to support ALARA concerns and the low regulatory threshold for selenium, it cannot be determined if selenium exceeds the threshold.

ICP Metals Analysis: Approximately 35 metals were analyzed by ICP. Supernatant samples were acid digested prior to analysis, while the wet centrifuged solids fraction were acid digested, as well as fusion digested. The analyte concentrations reported for the wet centrifuged solids prepared by acid digestion agree reasonably well with the results from KOH-KNO₃ fusion. Two analytes, Si and Zr, are exceptions; their concentrations are significantly lower in the data generated from acid digestion preparation. The

fusion preparation is much better than acid digestion in dissolving Si and Zr compounds; thus, concentrations derived from the fusion preparation are considered more reliable for Si and Zr. Analytes of interest are included in Table B-10.

Note that current EPA methods for metals digestion use acid digestion, which by design does not completely dissolve the entire particle. It digests metals on the surface. Fusion digestions are complete digestions of the entire material and have been used in the uranium processing and mining industries to provide a complete material digestion.

TOC/TIC Analyses: The analyses of the 241-C-104 supernatant and solids samples were performed by the hot persulfate wet oxidation method and the furnace oxidation method. Under normal conditions, the furnace method and hot persulfate method should provide equivalent TC results. The supernatant results demonstrated good agreement between the furnace and hot persulfate methods, but there was significant disagreement between the methods for the centrifuged solids. The TC results from the furnace method are nearly twice the level measured from the hot persulfate method. The disagreement suggests that the carbon compounds (most likely organic carbon compounds) are not well decomposed by the hot persulfate method. Matrix spike recoveries (although within acceptance criteria) were also lower for the hot persulfate method.

Anion Analysis: The oxalate results reported from the inorganic IC analysis are provided for information only. The reported fluoride results must be used with caution. Because the IC column and parameters used have insufficient resolution, fluoride cannot be isolated from acetate and formate. It is unlikely the levels of fluoride quantified are present in the 241-C-104 tank waste; because both acetate and formate could be present, the fluoride results should be used with reservation.

VOA and SVOA: Table B-10 summarizes detected volatile and semi-volatile compounds.

PCBs: GC/ECD analysis of the residue from the solid samples resulted in quite complex chromatograms. Although the presence of Aroclors was evident, substantial degradation of the expected response pattern was observed. The presence and approximate quantity of PCBs in the solid sample were confirmed using mass spectrometry. The concentration of PCBs in the supernate was not adequate for confirmation by mass spectrometry. Although the two analytical methods agreed within a factor of two, the PCB results should be considered qualitative. While the GC/MS data confirm the presence of PCBs, it was not intended to provide adequate quantitation based on this calibration. Further investigation is necessary to more accurately determine the quantity of PCBs present in these samples.

Organic Anions: Acetate co-elutes with glycolate under typical analytical conditions and requires the use of an alternate column for separation from glycolate. Without this separation, it is not possible to state whether or not the observed peak contains only acetate, only glycolate, a combination of both anions, or a possible contaminant.

References

Fiskum, S. K., et al. 2000. *Inorganic and Radiochemical Analysis for 241-C-104 Tank Waste*, BNFL-RPT-043, Rev. 0. Battelle, Pacific Northwest Division, Richland, Washington.

Evans, J. C., et al. 2001. *Organic Analysis of C-104 Tank Waste*. WTP-RPT-008, Rev. 1. Pacific Northwest National Laboratory, Richland, Washington.

2.4.1.2 Glass Product Analyses

Summary: PNNL was retained to produce, test, and characterize vitrified IHLW waste from an Envelope D high-level waste (HLW) sample from Tank 241-C-104. A pretreated tank sludge sample, along with a HLW process simulant (identified as the HLW process blank), were prepared as melter feeds for vitrification. The pretreated sludge was converted to HLW glass.

Purpose: An objective of this work is to provide analytical data that can be used to support hazardous waste delisting petitions for immobilized HLW forms (IHLW) generated from processing of 241-C-104 waste, as well as providing data that demonstrate compliance with applicable LDR criteria. The testing and characterization are being conducted to aid in planning for treatment and eventual disposition of Hanford tank waste.

Analyses: The levels of certain organic and inorganic analytes were assessed using the following tests: VOA, SVOA, PCBs, dioxins and furans, cyanide and sulfide by IC, and TCLP. The HLW glass sub-samples were either analyzed directly (VOA, CN, and S [note: cyanide and sulfide typically would be analyzed from a distilled extract of the glass sample; the approach that was used for these analyses is being reviewed to confirm the method that was used.], or extracted prior to analysis (SVOA, PCB, dioxins and furans, and TCLP).

Discussion of Analytical Results: Analytes detected in the tank waste or glass product are summarized in Table B-10. One volatile compound (methylene chloride) was detected in the 241-C-104 glass sample at a concentration below the DL. Methylene chloride also was found in the blank sample and can probably be attributed to laboratory contamination. One semi-volatile compound (Bis [2-Ethylhexyl]phthalate) was detected at a concentration less than the DL (Sample 730J $\mu\text{g}/\text{kg}$, DL=1000 $\mu\text{g}/\text{kg}$). Although concentrations of Bis (2-Ethylhexyl) phthalate were undetected in both the process blank and hot cell blank, it is a common plasticizer, and its presence may be due to sample processing.

No PCBs, dioxins, or furans were detected in any of the glass samples.

Sulfide was not detected in 241-C-104 HLW glass samples. Cyanide was detected at a level approximately two times the DL. At this level, and with no cyanide detected in the 241-C-104 duplicate, the presence of cyanide in the 241-C-104 HLW glass is questionable.

241-C-104 glass samples were leached, and the TCLP leachate was analyzed for TC metals (As, Ba, Cd, Cr, Pb, Se, Ag). None of the TC metals exceeded TC limits.

Reference:

Goheen, S.C., et al. 2001. *Regulatory Analysis on Glass Product from C-104 and AZ-102 Pretreated HLW Sludge Mixed with Flowsheet Quantities of Secondary Wastes*, WTP-RPT-010, Rev. 0. Pacific Northwest National Laboratory, Richland, Washington.

2.4.2 Tank 241-AZ-102

2.4.2.1 Waste Characterization

Summary: 400 g of wet Hanford Tank sludge from 241-AZ-102 were evaluated to test pretreatment processes for Envelope D Hanford sludge, before vitrification of HLW. Pretreatment steps reduce the quantity of HLW generated by removing components such as Al, Cr, Na, and P that are soluble in either water or high temperature caustic; these constituents often limit the waste loading in the glass.

The report describes the test apparatus, the experimental approach, the results of the tests, and the chemical and radiochemical analysis of the sludge from Tank 241-AZ-102 and filtrates generated during the washing and caustic-leaching steps.

Purpose: The first objective of this work was to test crossflow filtration using actual Envelope D Hanford tank waste (241-AZ-102). The second objective was to evaluate washing and leaching characteristics of the 241-AZ-102 sludge.

Analyses: Chemical and radiochemical analyses were performed on the initial sludge composite and initial decanted supernatant as well as the final slurry. Chemical analyses consisted of metals, anions, TIC, TOC, TC, CN, and C₂O₄ (oxalate ion). Table B-11 summarizes the initial supernatant, initial slurry, and final slurry sample ("pretreated slurry") results.

Discussion of Analytical Test Results

ICP Metals: Arsenic and barium analyses resulted in low recovery (22 % and 5 %) for the matrix spiked sample. The reason is unclear, but may be related to the high sulfate concentration in the sample. Low matrix spike recovery for silver (13 %) was most likely due to hydrochloric acid used in sample preparation.

IC Anions: Interferences from suspected organic anions significantly affect the ability to accurately quantify the fluoride peak; therefore, the fluoride results should be considered qualitative. The blank spike produced high recoveries for chloride (197 %). The reported chloride may be higher than the actual chloride concentration in the sample.

Other Test Results: The initial de-watering steps, as well as dilute caustic washing, appear to have removed a majority of the sodium, potassium, and the anions. During the caustic leaching, aluminum, phosphorus, silicon, and chromium were removed, as well as additional potassium. During the course of washing and leaching, most of the soluble anions measured by IC were washed from the solids, with small amounts of chloride, phosphate, sulfate, and fluoride remaining.

Of the major radioactive isotopes, only Cs-137 was significantly removed during leaching and washing. As expected, Sr-90 and transuranic isotopes remained with the slurry.

An evaluation of removal efficiencies indicates that 80.2 % of the sodium was removed from the slurry during the water-washing steps. Nearly all of the soluble fluoride, nitrite, nitrate, sulfate, oxalate, and cyanide were removed during the first water washes. Chloride and phosphate were the only exceptions, with phosphate having only 8.5 % removal, and no measurable chloride was removed during the water washes. Other non-radioactive components with significant removal efficiencies during the water wash were boron, with 63 % removal, calcium, with 60 % removal, chromium, with 44 % removal, potassium,

with 81 % removal, and molybdenum, with 66 % removal. In terms of radioactive components, 61 % of the Cs-137 was removed during the initial water-wash steps. Only 1.9 % of the aluminum was removed during the dilute caustic washing, but 59.3 % of aluminum was removed during the caustic-leaching step.

Conclusions

The quantity of HLW glass produced from the as-received 241-AZ-102 waste would have been limited by the high aluminum oxide concentration. With a DOE limit of 21 % for the $Al_2O_3 + Fe_2O_3 + ZrO_2$, and a mass of 430 g of dried initial sample, 934 g of HLW glass would be produced with the initial sludge. Even with almost 64 % removal of aluminum from the sample after washing and leaching, $Al_2O_3 + Fe_2O_3 + ZrO_2$ are still the limiting constituents in the glass. However, with the aluminum reduction, 725 g of HLW glass would be produced with the final sludge, resulting in a reduction of 22 %.

Reference:

Brooks, K. P., et al. 2000. *Characterization, Washing, Leaching, and Filtration of AZ-102 Sludge*. PNWD-3045, BNFL-RPT-038, Rev. 0. Battelle, Pacific Northwest Division, Richland, Washington.

2.4.2.2 Glass Product Analysis

Summary: PNNL was retained to produce, test, and characterize vitrified IHLW waste forms from an Envelope D HLW sample from Tank 241-AZ-102. A pretreated tank sludge sample along with a HLW process simulant (identified as the HLW process blank) were prepared as melter feeds for vitrification. The pretreated sludge was converted to HLW glass.

Purpose: An objective of this work is to provide analytical data that can be used to support hazardous waste delisting petitions for immobilized HLW forms (IHLW) generated from processing of 241-AZ-102 wastes, as well as providing data that demonstrate compliance with applicable LDR. The testing and characterization is being conducted to aid in planning for treatment and eventual disposition of Hanford tank waste.

Analyses: The data assess the levels of certain organic and inorganic analytes using the following tests: VOA, SVOA, PCBs, dioxins and furans, cyanide and sulfide by IC, and TCLP. The HLW glass sub-samples were either analyzed directly (i.e., VOA, CN, and S) or extracted prior to analysis (i.e., SVOA, PCB, dioxins and furans, and TCLP).

Discussion of Analytical Results: Results are provided in Table B-11 for the analysis of a glass sample produced from pretreated sludge. One VOC, methylene chloride, was detected in the 241-AZ-102 sample. The concentration of methylene chloride, however, was below the DL and the constituent also was found in the sample blank. Its presence can probably be attributed to laboratory contamination. One semi-volatile compound, Bis (2-Ethylhexyl) phthalate, was detected at a concentration less than the DL (Sample 110J $\mu\text{g}/\text{kg}$; DL=1000 $\mu\text{g}/\text{kg}$). Although Bis (2-Ethylhexyl) phthalate was not present in detectable concentrations in the process blank or the hot cell blank, it is a common plasticizer and its presence may be due to sample handling.

No PCBs, cyanide, sulfide, dioxins, or furans were detected in any of the glass samples.

The 241-AZ-102 glass sample was leached and the TCLP leachate was analyzed for TC metals (As, Ba, Cd, Cr, Pb, Se, Ag). None of the TC metals exceeded TC limits.

Reference:

Goheen, S.C., et al. 2001. *Regulatory Analysis on Glass Product from C-104 and AZ-102 Pretreated HLW Sludge Mixed with Flowsheet Quantities of Secondary Wastes*, WTP-RPT-010, Rev. 0. Pacific Northwest National Laboratory, Richland, Washington.

2.4.3 Tank 241-AZ-102

2.4.3.1 Waste Characterization

Summary: The SRTC received and chemically characterized a sample from Hanford waste Tank 241-AZ-102. The sample contained supernate (designated Envelope B) and a small amount of sludge solids (designated Envelope D) and was analyzed as-received. The filtered supernatant liquid, the total dried solids of the sample, and the washed insoluble solids obtained from filtration of the sample were analyzed. The results of these analyses should be reviewed in conjunction with the information presented in the preceding discussion (Section 2.4.2).

Purpose: The SRTC was contracted to provide pretreatment development and testing services to support the vitrification of Hanford tank waste. The tank samples allow for testing of the pretreatment processes with actual waste samples. The characterization data provide a basis for developing pretreatment processes, determining reagent requirements, and developing physical design parameters for the pretreatment plant.

Analyses: Analyses conducted on tank sample 241-AZ-102 included anions by IC (also fluoride and chloride by ISE), total metals by ICP, potassium and mercury by CVAA, and radioisotopic analyses by GEA, ICP-MS, and alpha counting spectroscopy.

Analyses Results Discussion:

Data from selected analytes of interest are summarized in Table B-12.

ICP metals: The analytical results for the filtered supernatant indicate the sample is a relatively dilute salt solution with a sodium concentration of 2.77 M. The supernatant contains low levels of other metals such as aluminum and phosphorus, but a relatively high concentration of chromium. The supernatant also contains a relatively high concentration of sulfate. A high sodium content is also evident in the solids samples. Other metals with significant concentrations in the total dried solids include potassium, iron, aluminum, chromium, and silicon. In contrast, iron and aluminum dominate the composition of the dried insoluble sludge solids. The insoluble solids also consist of lesser amounts of cadmium, zirconium, nickel, sodium, and silicon.

The TOC value exceeds the organic carbon derived from the sum of the formate and oxalate by nearly an order of magnitude. The TOC results indicate the potential presence of a significant organic carbon source besides the formate and oxalate. The report contains no discussion of QC samples.

Reference:

Hay, M. S., and Bronikowski, M. G. 2000. *Chemical Characterization of an Envelope B/D Sample from Hanford Tank 241-AZ-102*, BNF-003-98-0249, Rev. 0. Savannah River Technology Center, Aiken, South Carolina.

3 Simulant Testing

Vitreous State Laboratory (VSL) has conducted a series of tests on glass formulations created to mimic the performance of tank wastes. The first series of these tests were performed to evaluate the destruction of organics in LAW and HLW wastes. An additional series of tests were performed to evaluate the overall performance of the glass and the leaching of metals from the glass form. These various test are summarized below. It must be noted that VSL did not perform all of the QA/QC procedures required by SW 846. The following QC was not performed by VSL on a routine basis:

- MDLs have not been established.
- Calibration checks are not analyzed every 10 samples.
- MS and MSDs are not analyzed. However, using the matrix matching logic accepted by EPA, MS and MSDs are not needed.
- No interference check standards are analyzed. If the emission profiles of the NIST and LCS were available, Method 6010B QC criteria would be met because the method allows for the use of emission profiles.
- No preparation blank is prepared and digested with the samples.
- Duplicates are analyzed but not reported.

3.1 Organics Evaluation

3.1.1 Summary

The VSL performed a small-scale melter-testing program to obtain data to demonstrate that the WTP treatment process will meet the *Resource Conservation and Recovery Act of 1976* (RCRA) criteria for disposal (Muller, Buechele, and Pegg, 2001). The tests were performed on a small-scale vitrification system (DM10, 1/300th scale HLW melter) with WTP waste simulants (LAW-A, LAW-C, and HLW-D) that were spiked with selected hazardous organic compounds. LAW-A simulant contains low sulfur and low organics, and is representative of Tanks AW-101, AN-103, AN-104, and AN-105. LAW-C simulant contains the highest organics levels and is representative of Tank AN-107. HLW-D simulant is representative of Tanks AZ-101, AZ-102, AY-102, and C-106. Organic spikes were selected from a list provided by BNFL Inc., developed during the tank characterization DQO process. The analytes selected were examined with respect to destruction difficulty based on thermal stability and heats of combustion. As a result, benzene, phenol, and 1, 1, 2-trichloroethene were selected as organic spikes in the feed simulant.

The testing process involved the manipulation of a series of controllable variables (feed type, added reductants, plenum gas residence time, plenum gas temperature, bubbling rate, and cold cap coverage) to create worst-case scenarios for organic destruction and metal emissions.

Three additional tests were included to separate the effects of gas bubbling, plenum temperature, plenum gas residence time, and reductants.

The extent to which organic by-products are generated from organic compounds in the feeds as well as the additive sucrose was evaluated with a test in which no hazardous organic spike was used for both the LAW-A and LAW-C waste compositions.

3.1.2 Purpose

WTP waste streams have been designated as containing a variety of hazardous organic compounds. The proposed WTP treatment processes must be demonstrated to meet the regulatory requirements for disposal before a petition for delisting or LDR compliance can be submitted. The testing was performed in order to generate data to determine the extent of hazardous organics removal in the melters.

The purpose of the tests was to determine the extent to which hazardous organic constituents are destroyed in the melter itself; no account was taken of destruction or removal in offgas components. The tests were to obtain the following types of performance data:

- DRE data under “worst-case” conditions with respect to destruction of organics
- Effects of key operating parameters (glass bubbling, plenum temperature, plenum gas residence time, addition of reductants)
- Hazardous constituents in the offgas stream and emission of particulates
- Material mass balance

Four types of samples taken:

- Impinger samples for air sampling
- Continuous Air Monitoring
- Ground glass samples
- Feed samples

Only the latter two types of samples have bearing on the discussion for this Data Quality Objectives. These samples are discussed separately in the following sections.

3.1.3 Feed Sampling and Analysis Procedures

Three waste simulants were used to evaluate the performance of the vitrification process:

- LAW-A - representative of tanks 241-AW-101, 241-AN-103, 241-AN-104, and 241-AN-105
- LAW-C - representative of tank 241-AN-107
- HLW-D - composite of tanks 241-AZ-101, 241-AZ-102, 241-AY-102, and 241-C-106

Actual chemical composition can be found in the final report - *Determination of the Fate of Hazardous Organics During Vitrification of RPP-WTP LAW and HLW Simulants*, (Matlack and Pegg, 1999). For each test a sample of the feed was analyzed to confirm the organic spike concentration, total inorganic

content, chloride, nitrate, nitrite, sulfate and fluoride concentration. Table B-13 and Table B-14 identify the feed envelopes and resulting glasses that specific samples were developed to represent.

3.1.4 Organic Spike Concentration for Waste Feed Samples

The analytes used to spike the feed samples were chosen because they are difficult to destroy and are compatible with SW-846 analytical methods. The following analytes were selected:

- Benzene
- Trichloroethylene
- Hexachlorobutadiene

Subsequent analysis showed that hexachlorobutadiene formed a separate organic layer in the spiking mixture; therefore, it was replaced with phenol. Because phenol was not compatible with the rapid GC analysis required to support the R&T program, it was replaced with the following constituents:

- Chlorobenzene
- Toluene

Destruction and Removal Efficiencies (DREs) in the glass were found to be greater than 99.9996 % for benzene and greater than 99.9999 % for total carbon (Table B-15).

The following quality assurance (QA) problems were found with the data:

- Matrix spike results for Bromofluorobenzene, Dibromofluoromethane, and Toluene- d_8 were below acceptable limits.
- One of the duplicates for 1, 1-dichloroethylene was outside of acceptable limits.
- Trichloroethylene spike was outside of acceptable limits.

3.1.5 Ground Glass Sampling and Analysis Procedures

Metals Analysis

Ground glass samples from the vitrified waste product were subjected to a microwave digestion and analyzed by direct coupled plasma atomic emission spectroscopy (DCP-AES) for all constituents except for sulfur, which was analyzed by IC. The analytical results for the metals analysis were not included in the report; consequently, they are not included here.

TCLP

General Engineering Laboratories of Charleston, South Carolina, was contracted by VSL to perform TCLP analysis and total organic analyses on all of the glass samples produced in this test, following SW-846 procedures. The ground glass samples were analyzed by EPA Methods 1311 and 1310A and then analyzed for metals by DCP-AES. All organics analyses were done per applicable SW-846 protocols, as described below. Results are provided in Table B-16 and Table B-17 for LAW and HLW glass, respectively.

The following QA problems were found:

- Most of the matrix spikes for the Extractable Organics were below acceptable limits.
- Laboratory control samples for Barium and Cadmium were above acceptable limits.
- The laboratory control sample for Silver was below acceptable limits.

VOA

The glass samples were extracted by EPA Method 5030B and analyzed for VOCs using EPA Method 8260. Results are provided in Table B-18.

The following QA problems were found with the data:

- The matrix spike results for Bromofluorobenzene, Dibromofluoromethane and Toluene-d8 were below acceptable limits.
- 2-Hexanone, Acetone and Methylene Chloride were found in the blanks.
- The laboratory control sample for Chlorobenzene fell outside of acceptable limits.

Semi-Volatile Analysis

The glass samples were extracted using EPA Method 3540 and analyzed for semi-volatile compounds using EPA Method 8270C. Results are provided in Table B-19.

3.1.6 Effects on DREs

Plenum temperature appears to have the greatest effect on organic DREs. Benzene DRE values were approximately 90 % at 550 °C, 99 % at 750 °C, and 99.9 % at 950 °C. Benzene DRE in the glass appears to approach levels of 99.9999 %. DRE values were generally unaffected by simulant composition. The presence of sugar as a feed additive did not have an effect on DRE values or on dioxin or furan production, but it increased the generation of other byproducts in the melter offgas at low plenum temperatures. Plenum gas residence time did not have an observed effect on DRE values, with the possible exception of phenol. Glass bubbling did not have a discernible effect on DRE values.

3.1.7 Organic Byproducts in the Melter Offgas

Plenum temperature was the primary variable affecting type and amount of organic byproducts that were formed in the melter offgas. Feed composition also had a discernable effect. Most tests conducted at plenum temperatures over 900 °C produced no significant byproducts in the melter offgas. In tests below 900 °C, acrylonitrile (vinyl cyanide) was the most abundant byproduct. Nitrophenol and dibenzofuran were also common byproducts in the melter offgas.

Very small but detectable amounts of dioxins and furans were produced in the melter. Concentrations of dioxins and furans in the melter offgas were significantly higher for HLW-D tests than LAW tests. This higher concentration may be related to the fact that certain heavy metals can catalyze the formation of these compounds and the HLW-D feed is richer in the amounts and types of these constituents.

3.1.8 Conclusions

Based on the results of the analyses, the following conclusions can be made:

- All glass samples contained TCLP organics at concentrations below the relevant UTS.
- It is unlikely that the discharged glass product would contain volatile organic compounds.
- None of the glass samples showed organics above the reporting levels for TCLP or total analysis.
- Plenum temperature had the greatest effect on the DREs.

All of the QC and MDL determinations requirements as cited in SW-846 must be performed, however, before any technically defensible conclusions can be drawn. The data, however, are appropriate for demonstrating the concept that vitrification is a viable immobilization process. Defensible environmental measures will be needed to better substantiate the conclusions that have been drawn from the research data. Note that to support the petition submittal, an evaluation of the data provided by commercial laboratories contracted by VSL will be done to determine if the data are appropriate for regulatory use, as opposed to research grade, demonstration of concept data.

3.2 Glass Formulation Testing

The VSL of the Catholic University of America performed additional testing on the LAW and HLW glass formulations (Muller, Buechele, and Pegg, 2001; Kot and Pegg, 2001). The formulations used in this testing were developed around specific tank wastes or blends of tank wastes with total waste oxide loadings ranging from 6 to 31 weight %. The selection of new glass formulations was guided by past experience of VSL, the glass-property models and the database developed and continuously updated by VSL. The development of viable glass formulations for each of the waste envelopes is an iterative process in that prospective glasses were formulated, melted in small crucible melts, and characterized to obtain the required property composition information. The results were analyzed and revised compositions were generated in order to optimize the properties of the glass.

3.2.1 TCLP for LAW & HLW

The EPA's TCLP, as defined in SW-846, Method 1311, was used to determine the leach resistance of crushed glass (<3/8-inch) in a sodium acetate buffer solution after 18 hours at 22 °C with constant end over end agitation. A mass of 100 g of glass was leached in 2 L of TCLP extract, using the non-volatiles extraction solution.

For each RCRA metal analyte, LAW glasses were spiked with 100 to 10,000 times the corresponding concentration listed in the UTS (40 CFR 268.48). Spike factors of 100 and 1000 were used for elements for which the UTS is above 0.5 mg/L, while factors of 1000 and 10,000 were used for elements for which the UTS limit is below 0.5 mg/L. Since the TCLP introduces a 20 fold dilution of the matrix tested (100 g of the sample is leached with 2 L of the leaching solution), this corresponds to TCLP factors of 5 times and 50 times for arsenic, barium, chromium, nickel, lead, selenium, antimony, and vanadium and for 50 to 500 times for silver, cadmium, mercury, and thallium (i.e., the factor by which the UTS TCLP limit would be exceeded if all the glass dissolved). The spike levels used on this basis are shown in Table B-20. In all cases, even the highest spike levels, the concentrations of the TCLP metals in the LAW glass leachate did not exceed the UTS limits.

VSL conducted additional HLW glass formulation work using a combination of “actively-designed” formulations and “statistically-designed” matrices of formulations (Kot and Pegg, 2001). The actively designed formulations focused on current best estimates of waste compositions for the candidate waste tanks and various LAW pretreatment products; these glass products are identified with a prefix HLW98. For the statistically-designed formulations, design criteria were converted to a set of composition constraints that were then used to generate a set of glass formulations that provided the “best” coverage of that composition space according to specified statistical criteria. Some of these glasses extended beyond contract specifications and process requirements in order to define the corresponding compositional boundaries. The statistically-based glass products were assigned a prefix of HLW99. Crucible melts were performed with simulated HLW waste that met these formulations to determine the characteristics of the resulting glass. Unlike the LAW samples discussed above, these formulations were not spiked.

The concentrations for the spiked LAW were determined using DCP-AES and the results are listed in Table B-21 through Table B-24. Thirty-three of the 45 glasses evaluated during this series of tests were subjected to the TCLP procedure, SW-846, Method 1311. The results from the analyses of HLW glasses are presented in Table B-25. All of the glasses that were evaluated performed satisfactorily with respect to the TCLP limits. When the results are compared against the more stringent UTS limits, however, the results indicate that cadmium often exceeds the criteria of 0.11 mg/L (ppm), particularly for glasses with much more than 0.5 wt % of CdO. It should be noted that the glass data presented in Table B-25 apply to a more broad glass composition region than the qualified glass composition region that will apply to glasses subject to this DQO.

3.2.2 Process Control Testing

VSL performed process control tests on both LAW and HLW glass formations as described below.

Compressive Strength

The compressive strength of the glass was measured on annealed coupons. Annealing was done at the transition temperature of the glass for 12 hours, followed by a slow cooling to 450 °C, and then cooling in ambient air to room temperature. The compressive strength measurements were made according to ASTM C39-94. VSL determined the mean compressive strength of the glass form by testing non-radioactive samples. The compressive strength of the glass had to be at least 3.45E6 Pa when tested according to ASTM C39-94 or equivalent.

When tested, the LAW glass form exceeded this requirement by several orders of magnitude. Although the compressive strength can vary greatly due to minor surface flaws, it was determined that the mean value exceeded 3.45E6 Pa, after being exposed to thermal, radiation, biodegradation, and immersion degradation. It must be noted, however, that there is considerable scatter in the individual data.

Compressive strength tests were not required for HLW glass.

Leachability Index

VSL determined the Leachability Index of the representative glass formulations to be greater than 6.0 when tested for 90 days in deionized water using the ANSI/ANS-16.1 procedure. The values actually ranged from 15 to 18 on the logarithmic scale.

Product Consistency Test (PCT)

The PCT was used to evaluate the relative chemical durability of the glass by measuring the concentration of the chemical species released from 100-200 mesh crushed glass to the test solution. VSL measured the mass loss of sodium, silicon, and boron using the seven-day PCT test run at 90 °C, as defined in ASTM C1285-98. The test was conducted with a glass to water ratio of 1g of glass (-100 + 200 mesh) per 10 mL of water. All tests were conducted in triplicate and in parallel with a standard glass. The leachates were sampled at predetermined times, the first of which is seven days. One milliliter of sample leachate is mixed with 20 mL of 1 M HNO₃ and then analyzed by DCP-EAS.

The PCT results for all the LAW glasses were below the maximum leach rate criterion of 2 g/m²/day. The PCT results for all the actively designed HLW glasses were below the maximum leach rate criterion of SRL-EA reference glass; however, normalized PCT leach rates of two of the three statistically designed HLW glasses were greater than the SRL-EA reference glass.

Vapor Hydration Test (VHT)

VSL measured the glass corrosion rate using the seven day VHT test run at 200 °C, as defined in the DOE concurred upon *Product and Secondary Waste Plan* (24590-WTP-PL-RT-02-001). The VHT tests were run in Parr series 4700 screw cap pressure bombs. Glass coupons were fashioned to about 10 mm square, about 2 mm thick, and with one cut and one fracture surface face. A hole about 1.6 mm was drilled near one corner so that the coupon could be suspended from a hanger made of stainless steel wire. The area of the coupon was calculated and it was weighed both before and after the VHT. The coupon was then suspended in the bomb and sufficient deionized water was added to the bomb to saturate the volume at the test temperature of 200 °C. The bomb was then flushed with argon, sealed, weighed, and placed in an oven at 200 °C. At the completion of the test, the coupon was removed and partially immersed in an ice bath to condense the water vapor near the bottom of the bomb. Once cooled, the bombs were weighed and opened. The coupons were then removed, weighed, and examined by low-level microscopy. They were then sectioned and the pieces mounted separately to allow for Scanning Electron Microscope (SEM) examination. The measured glass alteration rate had to be less than 50 g (m² -day). All waste tested met this requirement.

All of the LAW glasses gave alteration rates below the contract requirements. The VHT is not a testing requirement for IHLW.

Compositional Analysis

Glass samples were subjected to a microwave assisted total acid dissolution in Teflon vessels for compositional analysis. Twenty mL of a 1:5 mixture of concentrated HF:HNO₃ was diluted to 50 mL and used for the dissolution. The resulting solutions were analyzed by DCP-AES for all constituents except sulfur. Sulfur was analyzed by Dionex Ion Chromatography as well as x-ray fluorescence.

Viscosity

The melt viscosity was measured using the Brookfield Viscometer. Measurements were performed at 950-1250 °C using a National Institute of Standards and Technology reference standard for calibration.

The vast majority of the LAW glasses met the viscosity requirement of 10 to 150 Poise at 1100 °C. A number of the HLW samples had viscosities outside the desired limits.

Electrical Conductivity

The electrical conductivity of each glass was determined by measuring the resistance of the melt glass as a function of frequency, using a calibrated platinum/rhodium electrode probe attached to a Hewlett-Packard Model 4194A impedance analyzer. Measurements were made over similar temperature ranges to those employed for the melt viscosity measurements. The results were extrapolated to zero frequency to obtain the direct current conductivity. The data were then interpolated to standard temperatures.

The majority of the LAW glasses met the electrical conductivity requirement of 0.2-0.7 S/cm at 1100 - 1200 °C. A number of the HLW glasses had conductivities outside the desired limits.

Liquidus Temperature and Percent Crystallinity

The approximate liquidus temperature of the glass was obtained by heat treatments followed by analysis using an optical and/or an electron microscope. Samples of 500 mg were heated in a platinum/gold crucible at a pre-melt temperature of 1200 °C for one hour to destroy any pre-existing nuclei, followed by a 20-hour or longer heat treatment at 950 °C.

The heat treated glass was then quenched by submerging the outside of the crucible in cold water. This quenching freezes in the phase assemblage in equilibrium with the melt at the heat treatment temperature. If no crystals are observed in the cooled glass, then it is inferred that no crystals were observed at the heat treatment temperature and the liquidus temperature is below 950 °C. If no crystals are observed the glass is subjected to similar treatment at 850 °C.

The HLW glasses tested did not perform well against the liquidus temperature requirement (due primarily to Fe₂O₃) and further development of glass formulations is needed primarily as a result of the liquidus temperature requirement. Unlike HLW formulations, liquidus temperature is not particularly constraining for LAW glasses.

Time Temperature Transformation

The glass samples were heat treated according to a systematic matrix of time/temperature conditions. Each heat treated sample was then examined with a SEM and by x-ray spectroscopy to identify any crystalline phases and to estimate their volume fractions. Quantities of specific crystalline phases were determined by x-ray diffraction.

Only one of the LAW glasses (LAW B45) showed any crystallization during the heat treatments. The crystalline form that develops during heat treatment is spinel and more than half of the HLW showed up with more than 15 vol% spinel. The liquidus temperature requirement is below 950 °C. This is especially restrictive for 241-AZ-101 and 241-AZ-102 wastes.

Glass Density

Density measurements were made on 5 to 15 g of crushed glass using ASTM Method D 854-83, a pycnometric method. Analysis was performed in triplicate.

All of the density values for the LAW glasses fell between 2.6 to 2.7 g/cc. Two of the HLW glasses were very dense, HLW98005 (3.15 g/ml) and HLWMS-11 (3.37 g/ml), while all the remaining glasses fell generally within the range of 2.64-2.99 g/mL, which is within acceptable limits.

Glass Transition Measurement

The glass transition temperature was measured by differential thermal analysis with a reference material that has no transitions in the region of interest. Thirty mg of powdered glass was analyzed with a Perkin Elmer Differential Thermal analyzer. The sample was heated from 300 to 700 °C at a rate of 10 °C/minute. During the heating any exothermic or endothermic transitions of the sample were reflected as a simultaneous temperature difference between the sample and the reference. The glass transition temperature was determined as the extrapolated onset temperature established through a process similar to the procedure described in ASTM E1356-91.

The glass transition temperatures for the LAW varied between 484 to 516 °C. The results for the HLW fell between 434-517 °C, despite the wide range of compositions tested. These values are in general agreement with the glasses from West Valley and Savannah River HLW glasses.

4 Biological Testing of Vitrified Tank Waste Samples

In 1997, bioassay testing was performed on vitrified samples derived from three low-activity wastes representing envelopes A, B and C. It was concluded from these tests that ILAW is likely to not designate as either Toxic Dangerous Waste or as Extremely Hazardous Waste. A report on the testing was submitted to the State of Washington Department of Ecology on January 5, 1998 (Smith 1998). The letter report by the laboratory actually doing the work (Parametrix, Inc.) was attached to the letter. The table below summarizes the data on survival at 96 hours. The report also included data on survival at intermediate times. There were 10 rainbow trout (*O. mykiss*) in each group.

Bioassay Test - Survival of *O. Mykiss* (Rainbow Trout) at 96 Hours (Smith 1998)

Concentration		Samples		
		Envelope B LAWBF-20F	Envelope C LAWC-95D	Envelope A LAWA-17
Control	A	10	10	10
	B	10	10	10
	C	10	10	10
10 mg/L	A	10	10	10
	B	10	10	9
	C	10	10	10
100 mg/L	A	10	10	10
	B	10	10	10
	C	9	10	10

Concentration	Samples		
	Envelope B LAWBF-20F	Envelope C LAWC-95D	Envelope A LAWA-17
	Proportion Dead		
Control	0	0	0
10 mg/L	0	0	0.033
100 mg/L	0.033	0	0

According to these tests, the vitrified product does not qualify for even the lowest toxicity category, D, and therefore is not a dangerous waste according the State of Washington criteria for toxic dangerous wastes.

Similar tests were performed for the -WTP by Battelle's Pacific Northwest Divisions, and the results were similar (Antrim 1997).

Bioassay Test - Survival of *O. Mykiss* (Rainbow Trout) at 96 Hours (Antrim 1997)

Concentration	Replica	Samples		
		Envelope B VIT-131	Envelope C VIT-132	Envelope A VIT-130
Control	1	10	10	10
	2	10	10	10
	3	10	10	10
10 mg/L	1	10	10	10
	2	10	10	10
	3	6	10	10
100 mg/L	1	10	10	10
	2	10	10	10
	3	10	10	10
		Proportion Dead		
Control		0	0	0
10 mg/L		0.13	0	0
100 mg/L		0	0	0

No explanation for the mortality in the third Envelope B (VIT-131), 10 mg/L replicate was found during the test procedure, however, both the 1st and 2nd replicates had no mortalities.

Similar testing for IHLW has not been done to date. Different results for IHLW would not be expected given the insolubility of the waste form.

5 References

Project Documents

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Table B-1 Estimated Concentrations of TC Metals for AW-101 Feed

CAS #	Analyte	TC Limit µg/ml (equal to mg/L)	Estimated TCLP concentration µg/ml ¹
7440-22-4	Silver	5.0	0.9
7440-38-2	Arsenic	5.0	14.6
7440-39-3	Barium	100.0	0.3
7440-43-9	Cadmium	1.0	0.5
18540-29-9	Chromium	5.0	24.8
7439-97-6	Mercury	0.20	(see footnote 2)
7439-92-1	Lead	5.0	6.9
7782-49-2	Selenium	1.0	< 2.4

1 "Bolded" values indicate constituents that were detected at estimated concentrations above TC limits.

2 Mercury values were not available.

< Compound or analyte is less than the DL (the number following the "<" is the DL).

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-2 Summary Results for Tank AW-101. Target Analytes Detected LAW Envelope A

CAS #	Target Compound	Tank AW-101					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
VOA Compounds		DL($\mu\text{g/L}$)	$\mu\text{g/L}$	DL	$\mu\text{g/kg}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$
106-35-4	3-Heptanone	51	U	42	59	50	U
106-97-8	Butane	51	U	42	860	50	U
108-10-1	4-Methyl-2-pentanone	51	U	42	10 J	50	U
109-66-0	Pentane	51	U	42	150	50	U
109-99-9	Tetrahydrofuran	51	140	42	180	50	U
110-43-0	2-Heptanone	51	U	42	59	50	U
110-54-3	Hexane	51	U	42	200	50	U
111-65-9	Octane	51	U	42	200	50	U
111-84-2	Nonane	51	U	42	250	50	U
123-19-3	4-Heptanone	51	U	42	8 J	50	U
123-91-1	1, 4-Dioxane	51	180	42	97	50	U
142-82-5	Heptane	51	U	42	210	50	U
563-80-4	3-Methyl-2-butanone	51	U	42	34 J	50	U
591-78-6	2-Hexanone	51	U	42	40 J	50	U
67-64-1	Acetone	51	330	42	620 B	50	U
71-43-2	Benzene	51	U	42	10 J	50	U
75-05-8	Acetonitrile	51	U	42	41 J	50	U
78-93-3	2-Butanone	51	U	42	160	50	U
SVOA Compounds		DL($\mu\text{g/L}$)	$\mu\text{g/L}$	DL($\mu\text{g/L}$)	$\mu\text{g/kg}$	DL($\mu\text{g/kg}$)	($\mu\text{g/kg}$)
62-75-9	N-Nitro-sodimethylamine	300	160 J	4,000	12,000	1,000	U
10595-95-6	N-Nitro-somethylethylamine	300	160 J	4,000	1,300 J	1,000	U
134-32-7	1-Naphthylamine	300	U	4,000	1,400 J	1,000	U
Pesticides		DL($\mu\text{g/L}$)	$\mu\text{g/L}$	DL($\mu\text{g/L}$)	$\mu\text{g/kg}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$
319-84-6	Alpha-BHC	1.0	U	10	18.1	1000	U
76-44-8	Heptachlor	1.0	U	10	73.4	1000	U
PCBs		DL($\mu\text{g/L}$)	$\mu\text{g/L}$	DL($\mu\text{g/L}$)	$\mu\text{g/kg}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$
11097-69-1	Aroclor 1254	2.1	U	36	23 J	10	U

Table B-2 Summary Results for Tank AW-101. Target Analytes Detected LAW Envelope A

CAS #	Target Compound	Tank AW-101					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
		DL($\mu\text{g/L}$)	$\mu\text{g/L}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$
Dioxins/Furans		DL($\mu\text{g/L}$)	$\mu\text{g/L}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$	DL($\mu\text{g/kg}$)	$\mu\text{g/kg}$
Dioxin/Furans		0.07-0.14	U	1.0-2.1	U	0.02-0.08	U
Inorganics		DL($\mu\text{g/mL}$)	$\mu\text{g/mL}$	DL($\mu\text{g/g}$)	$\mu\text{g/g}$	DL($\mu\text{g/mL}$)	$\mu\text{g/mL}$ TCLP
7439-92-1	Lead	8.57	73 J*	660	38 J*	0.003	0.029 JB
7439-97-6	Mercury	No info	No info	No info	No info	0.001	U
7440-02-0	Nickel	2.57	6.1 J*	3.53	50.2	0.0005	0.013 B
7440-22-4	Silver	2.14	<2	2.94	16 J*	0.0003	0.0007 JB
7440-28-0	Thallium	42.9	<42	58.9	<63	0.010	U
7440-36-0	Antimony	42.9	<42	58.9	<63	0.0007	U
7440-38-2	Arsenic	21.4	140 J*	29.4	100 J*	0.006	U
7782-49-2	Selenium	21	U	29	U	0.013	U
7440-39-3	Barium	0.857	<1	1.18	5.0 J*	0.0008	0.043 B
7440-41-7	Beryllium	0.857	2.7 J*	1.18	<1	0.0005	U
7440-43-9	Cadmium	1.29	2.1 J*	29.4	6.7 J*	0.0003	U
18540-29-9	Chromium (total)	1.71	94	2.35	400	0.001	0.11 B
57-12-5	Cyanide	No info	No info	No info	No info	0.05	0.15 ($\mu\text{g/g}$) ¹
Organic Anions		DL($\mu\text{g/mL}$)	$\mu\text{g/mL}$	DL($\mu\text{g/g}$)	$\mu\text{g/g}$	DL($\mu\text{g/g}$)	$\mu\text{g/g}$
144-62-7	Oxalate	34	600 J	250	9,700	N/A	N/A
64-18-6	Formate	No info	2,200	No info	3,400	N/A	N/A
64-19-7	Acetate (2)	No info	1,200 J	No info	U	N/A	N/A
Headspace Analysis		DL($\mu\text{g/mL}$)	$\mu\text{g/mL}$	DL($\mu\text{g/g}$)	$\mu\text{g/g}$	DL($\mu\text{g/g}$)	$\mu\text{g/g}$
67-65-1	Methanol	30	1.1 J	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

U Compound or analyte is undetected (less than DL).

J Compound or analyte has been detected but the concentration is less than the DL.

J* Results are less than the estimated quantitation level (10 times the DL).

B Compound or analyte detected in the sample has also been detected in the blank.

< Compound or analyte is less than the value shown.

¹ Analysis was not performed on TCLP extract. Results are in $\mu\text{g/g}$.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-3 Summary Results for Tank 241-AP-101. Target Analytes Detected LAW Envelope A

CAS #	Target Compound	Tank 241-AP-101					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
		DL	µg/mL	DL	µg/kg	DL	µg/kg
VOA Compounds							
	Not Analyzed	N/A	N/A	N/A	N/A	N/A	N/A
SVOA Compounds		DL	µg/mL	DL	µg/kg	DL	µg/kg
	Not Analyzed	N/A	N/A	N/A	N/A	N/A	N/A
Pesticides		DL	µg/mL	DL	µg/kg	DL	µg/kg
	Not Analyzed	N/A	N/A	N/A	N/A	N/A	N/A
PCBs		DL	µg/L	DL	µg/kg	DL	µg/kg
	Total PCB	1.4	U	N/A	N/A	N/A	N/A
Dioxins/Furans		DL	µg/mL	DL	µg/kg	DL	µg/kg
	Not Analyzed	N/A	N/A	N/A	N/A	N/A	N/A
Inorganics		DL (µg/mL)	µg/mL	DL	µg/kg	DL	µg/kg
7439-92-1	Lead	2.5	15 J	N/A	N/A	N/A	N/A
7439-97-6	Mercury	0.025	<0.025	N/A	N/A	N/A	N/A
7440-02-0	Nickel	0.76	8.6	N/A	N/A	N/A	N/A
7440-22-4	Silver	0.63	<0.63	N/A	N/A	N/A	N/A
7440-28-0	Thallium	13	0.0192	N/A	N/A	N/A	N/A
7440-36-0	Antimony	0.014	1.045	N/A	N/A	N/A	N/A
7440-38-2	Arsenic	0.063	1.46	N/A	N/A	N/A	N/A
7440-39-3	Barium	0.25	0.32 J	N/A	N/A	N/A	N/A
7440-41-7	Beryllium	0.004	1.32	N/A	N/A	N/A	N/A
7440-43-9	Cadmium	0.38	2.0 J	N/A	N/A	N/A	N/A
18540-29-9	Chromium (and VI)	0.51	158	N/A	N/A	N/A	N/A
57-12-5	Cyanide	No info	5.81	N/A	N/A	N/A	N/A
Inorganic and Organic Anions		DL (µg/mL)	µg/mL	DL	µg/kg	DL	µg/kg
16984-48-8	Fluoride	130	2,880	N/A	N/A	N/A	N/A
16887-00-6	Chloride	130	2,000	N/A	N/A	N/A	N/A
14797-65-0	Nitrite	250	42,200	N/A	N/A	N/A	N/A
7697-37-2	Nitrate	250	133,000	N/A	N/A	N/A	N/A

Table B-3 Summary Results for Tank 241-AP-101. Target Analytes Detected LAW Envelope A

CAS #	Target Compound	Tank 241-AP-101					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
14265-44-2	Phosphate	250	1,040	N/A	N/A	N/A	N/A
14808-79-8	Sulfate	250	4,070	N/A	N/A	N/A	N/A
64-19-7	Acetate	550	1,540	N/A	N/A	N/A	N/A
64-18-6	Formate	450	1,130	N/A	N/A	N/A	N/A
144-62-7	Oxalate	890	1,800	N/A	N/A	N/A	N/A
Miscellaneous Analytes		DL (µg/mL)	µg/mL	DL	µg/kg	DL	µg/kg
	TIC	40	6,550	N/A	N/A	N/A	N/A
	TOC	80	1,860	N/A	N/A	N/A	N/A
	TC	80	8,410	N/A	N/A	N/A	N/A
	TC, method furnace	170	8,610	N/A	N/A	N/A	N/A
7664-41-7	Ammonia	0.20	1.83	N/A	N/A	N/A	N/A
14280-30-9	Total hydroxide	340	42,300	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

U Compound or analyte is undetected (less than DL)

J Compound or analyte has been detected but the concentration is less than the DL.

B Compound or analyte detected in the sample has also been detected in the blank.

< Compound or analyte is less than the value shown.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-4 Summary Results for Tank 241-AN-103. Target Analytes Detected

CAS #	Target Compound	Tank 241-AN-103									
		Tank Waste (Feed)								Glass Product	
		Filtered Supernatant (1 st half)		Filtered Supernatant (combined)		Total Dried Solids (1 st half)		Total Insoluble Solids (1 st half)			
DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg		
VOA Compounds		DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
75-65-0	tert-Butanol	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	5.0	5.6 J*
67-64-1	2-Propanone (Acetone)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	5.0	6.4 J*
108-88-3	Toluene	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	5.0	6.6 J*
556-67-2	Octamethyl cyclotetrasiloxane	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	5.0	3
SVOA Compounds		DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	500-1500	ND
Pesticides		DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	2-5-15	ND
PCBs		DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
		N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	49	ND
Dioxins/Furans		DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
35822-39-4	1,2,3,4,6,7,8-HpCDD	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No info	4.41 J*
39001-02-0	OCDF	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No info	4.90 J*

Table B-4 Summary Results for Tank 241-AN-103. Target Analytes Detected

CAS #	Target Compound	Tank 241-AN-103									
		Tank Waste (Feed)								Glass Product	
		Filtered Supernatant (1 st half)		Filtered Supernatant (combined)		Total Dried Solids (1 st half)		Total Insoluble Solids (1 st half)			
DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL	Average conc. in wt %	DL	Average conc. in wt %	DL (µg/L)	Metals TCLP µg/L		
Inorganics											
7439-92-1	Lead	No info	35.5	No info	36.8	No info	<0.064	No info	0.272	No info	<33.0**
7439-97-6	Mercury	No info	<0.127	No info	<0.149	No info	0.00101	No info	0.00099	No info	<0.50**
7440-02-0	Nickel	No info	0.767	No info	<1.93	No info	<0.017	No info	0.215	No info	9.44 J**
7440-22-4	Silver	No info	0.438	N/A	N/A	N/A	N/A	N/A	N/A	No info	<4.59 **
7440-28-0	Thallium	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No info	<67.6
7440-36-0	Antimony	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No info	<21.4
7440-38-2	Arsenic	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No info	<20
7440-39-3	Barium	No info	<0.255	No info	<0.297	No info	<0.0082	No info	0.0307	No info	2460**
7440-41-7	Beryllium	No info	N/A	No info	N/A	No info	N/A	N/A	N/A	No info	<0.889
7440-43-9	Cadmium	No info	0.573	No info	0.578	No info	<0.0031	No info	0.0859	No info	<1.33
18540-29-9	Chromium (and VI)	No info	73.3	No info	74.6	No info	0.0661	No info	6.02	No info	8.44 J*
57-12-5	Cyanide	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	No info	<0.102 ⁽¹⁾
Anions											
7697-37-2	Nitrate	No info	97,400	No info	61,900	N/A	N/A	N/A	N/A	N/A	N/A
14797-65-0	Nitrite	No info	47,700	No info	39,800	N/A	N/A	N/A	N/A	N/A	N/A
14265-44-2	Phosphate	No info	654	No info	559	N/A	N/A	N/A	N/A	N/A	N/A

Table B-4 Summary Results for Tank 241-AN-103. Target Analytes Detected

CAS #	Target Compound	Tank 241-AN-103									
		Tank Waste (Feed)								Glass Product	
		Filtered Supernatant (1 st half)		Filtered Supernatant (combined)		Total Dried Solids (1 st half)		Total Insoluble Solids (1 st half)			
14808-79-8	Sulfate	No info	743	No info	866	N/A	N/A	N/A	N/A	N/A	N/A
64-18-6	Oxalate (C ₂ O ₄)	No info	518	No info	604	N/A	N/A	N/A	N/A	N/A	N/A
144-62-7	Formate (CHO ₂)	No info	1,180	No info	1,250	N/A	N/A	N/A	N/A	N/A	N/A
16887-00-6	Chloride	No info	2,180	No info	300	N/A	N/A	N/A	N/A	N/A	N/A
14280-30-9	[OH ⁻] free	No info	42,700	No info	31,800	N/A	N/A	N/A	N/A	N/A	N/A
3812-32-6	[CO ₃ ²⁻]	15300	<15,300	No info	10,100	N/A	N/A	N/A	N/A	N/A	N/A
	[AlO ₂ ⁻]	No info	23,600	No info	48,100	N/A	N/A	N/A	N/A	N/A	N/A
16984-48-8	Fluoride	No info	161	No info	94	N/A	N/A	N/A	N/A	N/A	N/A
Miscellaneous Analytes		DL (mg/L)	mg/L	DL (mg/L)	mg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
	TIC	No info	2,520	No info	3,680	N/A	N/A	N/A	N/A	N/A	N/A
	TOC	No info	376	No info	568	N/A	N/A	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

ND Not Detected

< Compound or analyte is less than the value shown.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

J* Analyte was detected but at concentrations less than 10 times the method detection limit.

** Recoveries were not within the specified range on the matrix spike or the matrix spike duplicate for these analytes.

¹ Analysis was not performed on TCLP extract. Results are in mg/kg.

Table B-5 Summary Results for Tank 241-AZ-102. Target Analytes Detected Supernatant LAW B/Solids HLW Envelope D

CAS #	Target Compound	Tank 241-AZ-102					
		Tank Waste (Feed)					
		Supernatant (Env. B)		Total Dried Solids (Env. D)		Insoluble Dried Solids (Env. D)	
		DL (mg/L)	mg/L	DL	average conc. in wt %	DL	average conc. in wt %
Inorganics							
7439-92-1	Lead	0.100	<8.25	No info	0.0474	No info	0.298
7439-97-6	Mercury	0.25	<0.25	No info	<0.00098	No info	<0.000504
7440-02-0	Nickel	0.030	<1.75	No info	0.0659	No info	1.80
7440-22-4	Silver	N/A	N/A	N/A	N/A	N/A	N/A
7440-28-0	Thallium	N/A	N/A	N/A	N/A	N/A	N/A
7440-36-0	Antimony	N/A	N/A	N/A	N/A	N/A	N/A
7440-38-2	Arsenic	N/A	N/A	N/A	N/A	N/A	N/A
7440-39-3	Barium	0.5	<0.5	No info	0.00744	No info	0.119
7440-41-7	Beryllium	N/A	N/A	N/A	N/A	N/A	N/A
7440-43-9	Cadmium	0.015	<0.75	No info	0.0956	No info	3.30
18540-29-9	Chromium (and VI)	0.020	768	No info	0.392	No info	0.191
57-12-5	Cyanide	N/A	N/A	N/A	N/A	N/A	N/A
Anions		DL (mg/L)	mg/L	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
7697-37-2	Nitrate	No info	16,900	N/A	N/A	N/A	N/A
14797-65-0	Nitrite	No info	30,300	N/A	N/A	N/A	N/A
14265-44-2	Phosphate	No info	<250	N/A	N/A	N/A	N/A
14808-79-8	Sulfate	No info	16,500	N/A	N/A	N/A	N/A
144-62-7	Oxalate	No info	2,830	N/A	N/A	N/A	N/A
64-18-6	Formate	No info	<250	N/A	N/A	N/A	N/A
16887-00-6	Chloride	No info	<50	N/A	N/A	N/A	N/A
16984-48-8	Fluoride	No info	967	N/A	N/A	N/A	N/A

Table B-5 Summary Results for Tank 241-AZ-102. Target Analytes Detected Supernatant LAW B/Solids HLW Envelope D

CAS #	Target Compound	Tank 241-AZ-102					
		Tank Waste (Feed)					
		Supernatant (Env. B)		Total Dried Solids (Env. D)		Insoluble Dried Solids (Env. D)	
Miscellaneous Analytes		DL (mg/L)	mg/L	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
	TIC	No info	6,140	N/A	N/A	N/A	N/A
	TOC	No info	6,040	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

< Compound or analyte is less than the value shown.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-6 Summary Results for Tank 241-AN-102. Target Analytes Detected

CAS #	Target Compound	Tank 241-AN-102					
		Tank Waste (Feed)					
		"Small C" Supernatant		"Small C" Total Dried Solids		"Small C" Insoluble Dried Solids	
		DL (mg/L)	mg/L	DL	Avg. concentration wt %	DL	Avg. concentration wt %
Inorganics							
7439-92-1	Lead	No info	115	0.063	<0.063	0.02	<0.02
7439-97-6	Mercury	0.145	<0.145	0.001	<0.001	No info	0.00095
7440-02-0	Nickel	No info	257	No info	0.0542	0.028	<0.028
7440-22-4	Silver	0.304	<0.304	N/A	N/A	N/A	N/A
7440-28-0	Thallium	N/A	N/A	N/A	N/A	N/A	N/A
7440-36-0	Antimony	N/A	N/A	N/A	N/A	N/A	N/A
7440-38-2	Arsenic	N/A	N/A	N/A	N/A	N/A	N/A
7440-39-3	Barium	0.306	<0.306	0.008	<0.008	0.03	<0.03
7440-41-7	Beryllium	N/A	N/A	N/A	N/A	N/A	N/A
7440-43-9	Cadmium	No info	37.7	No info	0.00662	0.02	<0.02
18540-29-9	Chromium (and VI)	No info	159	No info	0.0397	N/A	2.10
57-12-5	Cyanide	N/A	N/A	N/A	N/A	N/A	N/A
Anions		DL (mg/L)	mg/L	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
7697-37-2	Nitrate	No info	120,000	N/A	N/A	N/A	N/A
14797-65-0	Nitrite	No info	52,000	N/A	N/A	N/A	N/A
14265-44-2	Phosphate	No info	3,140	N/A	N/A	N/A	N/A
14808-79-8	Sulfate	No info	8,150	N/A	N/A	N/A	N/A
144-62-7	Oxalate	No info	373	N/A	N/A	N/A	N/A
64-18-6	Formate	No info	6,790	N/A	N/A	N/A	N/A
16887-00-6	Chloride	No info	2,400	N/A	N/A	N/A	N/A
16984-48-8	Fluoride	No info	1,380	N/A	N/A	N/A	N/A
Miscellaneous Organic Analytes		DL (mg/L)	mg/L	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
	TIC	No info	9,213	N/A	N/A	N/A	N/A
	TOC	No info	17,049	N/A	N/A	N/A	N/A
77-92-9	Citrate	No info	3765	N/A	N/A	N/A	N/A

Table B-6 Summary Results for Tank 241-AN-102. Target Analytes Detected

CAS #	Target Compound	Tank 241-AN-102					
		Tank Waste (Feed)					
		"Small C" Supernatant		"Small C" Total Dried Solids		"Small C" Insoluble Dried Solids	
79-14-1	Glycolate	No info	8220	N/A	N/A	N/A	N/A
64-18-6	Formate	No info	8179	N/A	N/A	N/A	N/A
64-19-7	Acetate	No info	627	N/A	N/A	N/A	N/A
150-39-0	HEDTA	No info	4484	N/A	N/A	N/A	N/A
60-00-4	EDTA	No info	5820	N/A	N/A	N/A	N/A
23590-99-0	IDA	No info	2450	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

< Compound or analyte is less than the value shown.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-7 Estimated TCLP Concentrations for 241-AN-107

CAS #	Analyte	TC Limit µg/ml (equal to mg/L)	Estimated TCLP concentration µg/ml ¹
7440-22-4	Silver	5.0	<0.2
7440-38-2	Arsenic	5.0	8.8
7440-39-3	Barium	100.0	1.6
7440-43-9	Cadmium	1.0	3.8
18540-29-9	Chromium	5.0	41.1
7439-97-6	Mercury	0.20	(see footnote 2)
7439-92-1	Lead	5.0	29.1
7782-49-2	Selenium	1.0	< 2.1

< Compound or analyte is less than the value shown.

¹ "**Bolded**" values indicate constituents that were detected at estimated concentrations above TC limits.

² Mercury values were not available.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-8 Summary Results for Tank 241-AN-107. Target Analytes Detected LAW Envelope C

CAS #	Target Compound	Tank 241-AN-107					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
VOA Compounds		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
108-87-2	Methylcyclohexane	66	U	110	40 J	50	U
109-99-9	Tetrahydrofuran	66	31 J	110	43 J	50	U
67-64-1	Acetone	66	140 B	110	100 JB	50	U
75-05-8	Acetonitrile	66	94	110	U	50	U
75-45-6	Chlorodifluoromethane	66	37 JB	110	80 JB	50	U
78-93-3	2-Butanone	66	16 J	110	U	50	46 J
Semi-Volatile Compounds		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
62-75-9	N-Nitrosodimethylamine	300	170 J	4,300	U	1,000	U
134-32-7	1-Naphthylamine	300	U	4,300	5,400	1,000	U
84-66-2	Diethylphthalate	300	150 J	4,300	U	1,000	U
Pesticides		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
309-00-2	Aldrin	1.0	1.2	10	U	1,000	U
319-84-6	Alpha-BHC	1.0	U	10	11.8	1,000	U
PCBs		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
11097-69-1	Aroclor 1254	2.3	1.7 JB	33	U	10	U
Dioxins/Furans		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
	None detected	0.03-0.14	U	0.4-2.1	U	N/A	N/A
Inorganics		DL (µg/mL)	µg/mL	DL (µg/g)	µg/mL	DL (µg/mL)	µg/mL TCLP
7439-92-1	Lead	8.57	409	11.8	331	0.003	0.030 JB
7439-97-6	Mercury	No info	No info	No info	No info	0.001	U
7440-02-0	Nickel	2.57	569	3.53	283	0.0005	0.020 B
7440-22-4	Silver	2.14	<2	2.94	<3	0.0003	U
7440-28-0	Thallium	42.9	<45	58.9	<59	0.010	U
7440-36-0	Antimony	42.9	<45	58.9	<59	0.0007	U

Table B-8 Summary Results for Tank 241-AN-107. Target Analytes Detected LAW Envelope C

CAS #	Target Compound	Tank 241-AN-107					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
7440-38-2	Arsenic	21.4	112 J*	29.4	110 J*	0.006	0.006 JB
7440-39-3	Barium	0.857	6.4 J*	1.18	29	0.0008	0.024 B
7440-41-7	Beryllium	0.857	<1	1.18	<1	0.0005	U
7440-43-9	Cadmium	1.29	67	1.77	33	0.0003	0.013 B
18540-29-9	Chromium (III and VI)	1.71	173	2.35	743	0.001	0.13 B
57-12-5	Cyanide	No info	No info	No info	No info	0.04	U
7782-49-2	Selenium	23	U	30	U	0.013	U
Organic Anions		DL (µg/mL)	µg/mL	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
144-62-7	Oxalate	1300	200 J	900	22,000	N/A	N/A
64-18-6	Formate	1700	1700	1200	600 J	N/A	N/A
64-19-7	Acetate	4400	4,000 J	1000	U	N/A	N/A
Headspace Analysis		DL (µg/mL)	µg/mL	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
67-65-1	Methanol	30	4.6 J	N/A	N/A	N/A	N/A
121-44-8	Triethylamine	20	5.8 J	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

U Compound or analyte is undetected (less than DL).

J Compound or analyte has been detected but the concentration is less than the DL.

B Compound or analyte detected in the sample has also been detected in the blank.

< Compound or analyte is less than the value shown.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-9 Estimated Inorganic TC Concentrations for 241-C-104

CAS #	Analyte	TC Limit (µg/ml)	Estimated TCLP concentration (µg/ml) ¹
7440-22-4	Silver	5.0	2.5
7440-38-2	Arsenic	5.0	<3.7
7440-39-3	Barium	100.0	4.2
7440-43-9	Cadmium	1.0	20.7
18540-29-9	Chromium	5.0	35.7
7439-97-6	Mercury	0.20	2.02
7439-92-1	Lead	5.0	34.9
7782-49-2	Selenium	1.0	<3.7

< Compound or analyte is less than the value shown.

¹ "**Bolded**" values indicate constituents that were detected at estimated concentrations above TC limits.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-10 Summary Results for Tank 241-C-104. Target Analytes Detected HLW Envelope D

CAS #	Target Compound	Tank 241-C-104					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
VOA Compounds		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
106-35-4	3-Heptanone	1,000	74 J	400	420	50	U
106-97-8	Butane	1,000	U	400	2,100	50	U
109-66-0	Pentane	1,000	U	400	5,600	50	U
110-43-0	2-Heptanone	1,000	97 J	400	400 J	50	U
110-54-3	Hexane	1,000	5,000 B	400	7,000	50	U
111-65-9	Octane	1,000	3,800	400	3,400	50	U
111-84-2	Nonane	1,000	6,200	400	2,900	50	U
123-38-6	Propionaldehyde	1,000	U	400	880	50	U
142-82-5	Heptane	1,000	1,900	400	5,200	50	U
67-64-1	Acetone	1,000	1,000 B	400	190 JB	50	U
75-09-2	Methylene Chloride	1,000	8,000 B	400	880 B	50	23 JB
100-41-4	Ethyl benzene	1,000	U	400	26 J	50	U
107-87-9	2-Pentanone	1,000	U	400	40 J	50	U
123-19-3	4-Heptanone	1,000	U	400	52 J	50	U
591-78-6	2 Hexanone	1,000	24 J	400	130 J	50	U
627-13-4	Propyl Nitrate	1,000	U	400	30 J	50	U
71-43-2	Benzene	1,000	U	400	25 J	50	U
78-93-3	2-Butanone	1,000	290 J	400	52 J	50	U
SVOA Compounds		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
126-73-8	Tributyl phosphate	560	2,100 B	19,000	57,000 B	1,000	U
62-75-9	N-Nitrosodimethylamine	560	1,300	19,000	U	1,000	U
88-85-7	Dinoseb	560	2,200 B	19,000	6,400 BJ	1,000	U
100-02-7	4-Nitrophenol	560	290 J	19,000	U	1,000	U
109-06-8	2-Methylpyridine	560	350 J	19,000	U	1,000	U
534-52-1	4, 6-Dinitro-2-methylphenol	560	140 J	19,000	U	1,000	U

Table B-10 Summary Results for Tank 241-C-104. Target Analytes Detected HLW Envelope D

CAS #	Target Compound	Tank 241-C-104					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
117-81-7	Bis (2-Ethylhexyl) phthalate	560	480 J	19,000	5,900 J	1,000	730 J
Pesticides		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL	µg/kg
319-85-7	Beta-BHC	1.0	3.4	2.0	U	0.1-1	U
58-89-9	Gamma-BHC	1.0	U	2.0	8.2	0.1-1	U
1024-57-3	Heptachlor Epoxide	1.0	U	2.0	2.7	0.1-1	U
319-86-8	delta-BHC	1.0	U	2.0	6.4	0.1-1	U
72-55-9	4, 4'-DDE	2.0	U	4.0	5.6	0.1-1	U
7421-93-4	Endrin Aldehyde	2.0	U	4.0	4.3	0.1-1	N/A
PCBs		DL (µg/L)	µg/L	DL (µg/kg)	µg/kg	DL (µg/kg)	µg/kg
12674-11-2 53469-21-9	Aroclor 1016/1242	2.0	3.8	4.0	121	10	U
12672-29-6	Aroclor 1248	2.0	4.3	4.0	278	10	U
11097-69-1	Aroclor 1254	2.0	1.8	4.0	72.8	10	U
11096-82-5 37324-23-5	Aroclor 1260/1262	2.0	U	4.0	37.8	10	U
Total PCB^(a)		2.0	9.9	4.0	510	10	U
Dioxins/Furans		DL (µg/L)	µg/L	DL (µg/kg)	µg/Kg	DL (µg/kg)	µg/Kg
35822-37-4	Heptachloradibenzo-p-dioxin	0.04	0.002 J	0.08	U	0.04	U
39001-02-0	Octachlorodibenzo furan	0.08	0.005 J	0.16	U	0.08	U
Inorganics		DL (µg/mL)	µg/mL (acid digest)	DL (µg/g)	µg/g (acid digest)	DL (µg/mL)	µg/mL
7439-92-1	Lead	4.9	<4.9	29	709	0.003	0.071B
7439-97-6	Mercury	0.01	0.722	0.05	41.1	0.001	U
7440-02-0	Nickel	1.5	121	8.6	1,320	0.0005	0.048B
7440-22-4	Silver	1.2	1.4 J	7.1	54 J	0.0003	0.0096B

Table B-10 Summary Results for Tank 241-C-104. Target Analytes Detected HLW Envelope D

CAS #	Target Compound	Tank 241-C-104					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
7440-28-0	Thallium	25	<25	140	<143	0.010	U
7440-36-0	Antimony	25	<25	140	<143	0.0007	U
7440-38-2	Arsenic	12	<12	114	<71	0.006	U
7440-39-3	Barium	0.50	<0.5	2.9	85	0.0008	0.023B
7440-41-7	Beryllium	0.5	<0.5	2.9	19 J	0.0005	U
7440-43-9	Cadmium	0.74	9.0	4.3	411	0.0003	0.011B
18540-29-9	Chromium (III and IV)	1.0	55.4	5.7	709	0.001	0.14B
57-12-5	Cyanide (total)	0.025	7.4	0.20	11.4	0.09	0.21 µg/g ^(b)
Organic Anions		DL (µg/mL)	µg/mL	DL (µg/g)	µg/g	DL (µg/g)	µg/g
144-62-7	Oxalate	No info	1,090	No info	1,230	N/A	N/A
64-18-6	Formate	No info	2,670	No info	750	N/A	N/A
Inorganic Anions		DL (µg/mL)	µg/mL	DL (µg/g)	µg/g	DL (µg/g)	µg/g
16984-48-8	Fluoride	No info	9,710 ^(c)	25	46,200	N/A	N/A
16887-00-6	Chloride	No info	790	No info	250	N/A	N/A
14797-65-0	Nitrite	No info	34,200	50	10,500	N/A	N/A
24959-67-9	Bromide	No info	3,270	25	1,020	N/A	N/A
7697-37-2	Nitrate	No info	17,600	50	5,630	N/A	N/A
14265-44-2	Phosphate	No info	3,040	50	9,650	N/A	N/A
14808-79-8	Sulfate	No info	3,870	50	1,430	N/A	N/A
Headspace Analysis		DL (µg/mL)	µg/mL	DL (µg/g)	µg/g	DL (µg/g)	µg/g
67-56-1	Methanol	No info	16.0	N/A	N/A	N/A	N/A
64-17-5	Ethanol	No info	8.0 B	N/A	N/A	N/A	N/A
71-23-8	1-Propanol	No info	2.7	N/A	N/A	N/A	N/A
71-36-3	n-Butanol	No info	28	N/A	N/A	N/A	N/A
121-44-8	Triethylamine	No info	15 J	N/A	N/A	N/A	N/A

Table B-10 Summary Results for Tank 241-C-104. Target Analytes Detected HLW Envelope D

CAS #	Target Compound	Tank 241-C-104					
		Tank Waste (Feed)				Glass Product	
		Supernatant		Wet Solids			
Miscellaneous Analytes		DL (µg/mL)	µg/mL	DL (µg/g)	µg/g	DL (µg/g)	µg/g
	TIC (persulfate)	70	8,330	120	4,200	N/A	N/A
	TOC (persulfate)	200	6,500	350	10,300	N/A	N/A
	TC (sum of persulfate)	270	14,800	470	14,500	N/A	N/A
	TC (furnace)	No info	14,900	No info	24,800	N/A	N/A
7664-41-7	Ammonia	No info	17.4	No info	3.38	N/A	N/A

- U Compound or analyte is undetected (less than DL).
 - J Compound or analyte has been detected but the concentration is less than the DL.
 - B Compound or analyte detected in the sample has also been detected in the blank.
 - < Compound or analyte is less than the value shown.
 - N/A Not applicable, analyte not analyzed.
 - (a) If no Aroclors are detected, the total PCB concentration (DL for total PCBs) is considered the highest single Aroclor DL for the tank waste matrix. If one or more Aroclors are detected, the total PCBs in a sample is calculated by summing the detected Aroclors, but does not include Aroclor values below the DL.
 - (b) Analysis was not performed on TCLP extract. Results are in µg/g.
 - (c) IC system quantifies F based on retention time; however, fluoride, formate, and acetate can not be resolved. Reported value reflects contribution from formate and/or acetate.
- Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-11 Summary Results for Tank 241-AZ-102. Target Analytes Detected HLW Envelope D

CAS #	Target Compound	Tank 241-AZ-102							
		Tank Waste (Feed)						Glass Product	
		Initial Sludge Composite		Initial Supernate		Final Slurry			
		DL (µg/mL)	µg/mL	DL (µg/mL)	µg/mL	DL (µg/g)	µg/g	DL (µg/kg)	µg/kg
VOA Compounds									
75-09-2	Methylene Chloride	N/A	N/A	N/A	N/A	N/A	N/A	100	25 JB
SVOA Compounds									
117-81-7	Bis (2-ethylhexyl) phthalate	N/A	N/A	N/A	N/A	N/A	N/A	1,000	110 J
Pesticides									
Not Analyzed in Feed		N/A	N/A	N/A	N/A	N/A	N/A	1,000	No Detects
PCBs									
Not Analyzed in Feed		N/A	N/A	N/A	N/A	N/A	N/A	10	No Detects
Dioxins/Furans									
Not Analyzed in Feed		N/A	N/A	N/A	N/A	N/A	N/A	0.02-0.08	No Detects
Inorganics									
7439-92-1	Lead	0.100	1350	No Info	<2.0	0.1	2,250	0.003	0.033B
7439-97-6	Mercury	No info	19.1	No info	0.212	No info	26.6	0.001	U
7440-02-0	Nickel	0.030	9,310	No info	<0.73	No info	16,200	0.0005	0.084B
7440-22-4	Silver	0.025	352	No info	<0.61	No info	470	0.0003	0.0067B
7440-28-0	Thallium	0.500	<3,000	No info	<12	No info	<3,000	0.010	U
7440-36-0	Antimony	0.500	<3,000	No info	<12	No info	<3,000	0.0007	U
7440-38-2	Arsenic	0.250	<1000	No info	<6.1	No info	<1000	0.006	0.014 JB
7440-39-3	Barium	0.010	550	No info	0.260	No info	958	0.0008	0.016B
7440-41-7	Beryllium	0.010	13.5	No info	<0.24	No info	22.50	0.0005	U
7440-43-9	Cadmium	0.015	20,700	No info	<0.37	No info	33,000	0.0003	0.14B
18540-29-9	Chromium (III and VI)	0.020	2,140	No info	826.5	No info	1,640	0.001	0.14B

Table B-11 Summary Results for Tank 241-AZ-102. Target Analytes Detected HLW Envelope D

CAS #	Target Compound	Tank 241-AZ-102							
		Tank Waste (Feed)						Glass Product	
		Initial Sludge Composite		Initial Supernate		Final Slurry			
		DL (µg/mL)	µg/mL	DL (µg/mL)	µg/mL	DL (µg/g)	µg/g	DL (µg/g)	µg/g
57-12-5	Cyanide (total)	0.25	13.5	No info	9.6	No info	8.30	0.25 ^(a)	U
16984-48-8	Fluoride	25	1,700	10	750	10	300	N/A	N/A
16887-00-6	Chloride	100	<250	4.0	<100	4.0	1,350	N/A	N/A
14797-65-0	Nitrite	No info	66,100	20	41,700	20	<530	N/A	N/A
24959-67-9	Bromide	25	<250	10	<100	10	<260	N/A	N/A
7697-37-2	Nitrate	No info	21,400	20	13,800	20	<530	N/A	N/A
14265-44-2	Phosphate	20	569	20	435	20	885	N/A	N/A
14808-79-8	Sulfate	No info	29,300	20	21,100	20	690	N/A	N/A
144-62-7	C ₂ O ₄	50	3,900	20	3,290	20	<530	N/A	N/A
TOC/TIC/TC Analysis		DL (gC/mL)	µgC/mL	DL (gC/mL)	µgC/mL	DL (gC/g)	µgC/g	DL (µg/g)	µg/g
	TIC	No info	7,990	No info	8,620	No info	2,870	N/A	N/A
	TOC	No info	760	No info	1,070	No info	2,750	N/A	N/A
	TC	No info	8,750	No info	9,690	No info	5,620	N/A	N/A

- U Compound or analyte is undetected (less than DL).
- J Compound or analyte has been detected but the concentration is less than the DL.
- B Compound or analyte detected in the sample has also been detected in the blank.
- < Compound or analyte is less than the DL (the number following the "<" is the DL).
- N/A Not applicable, analyte not analyzed.
- (a) Not analyzed on the TCLP extract. Results are in µg/g.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-12 Summary Results for Tank 241-AZ-102. Target Analytes Detected Supernatant LAW B/Solids HLW Envelope D

CAS #	Target Compound	Tank 241-AZ-102					
		Tank Waste (Feed)					
		Filtered Supernatant (Env. B)		Total Dried Solids (Env. D)		Insoluble Dried Solids (Env. D)	
		DL (mg/L)	mg/L	DL	Average Conc. in Wt %	DL	Average Conc. in Wt %
Inorganics							
7439-92-1	Lead	0.100	<8.25	No info	0.0474	No info	0.298
7439-97-6	Mercury	25	<0.25	0.00098	<0.00098	0.000504	<0.000504
7440-02-0	Nickel	0.030	<1.75	No info	0.0659	No info	1.80
7440-22-4	Silver	N/A	N/A	N/A	N/A	N/A	N/A
7440-28-0	Thallium	N/A	N/A	N/A	N/A	N/A	N/A
7440-36-0	Antimony	N/A	N/A	N/A	N/A	N/A	N/A
7440-38-2	Arsenic	N/A	N/A	N/A	N/A	N/A	N/A
7440-39-3	Barium	0.010	<0.5	No info	0.00744	No info	0.119
7440-41-7	Beryllium	N/A	N/A	N/A	N/A	N/A	N/A
7440-43-9	Cadmium	0.015	<0.75	No info	0.0956	No info	3.30
18540-29-9	Chromium (and VI)	0.020	768	No info	0.392	No info	0.191
57-12-5	Cyanide	N/A	N/A	N/A	N/A	N/A	N/A
Anions		DL (mg/L)	mg/L	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
7697-37-2	Nitrate	No info	16,900	N/A	N/A	N/A	N/A
14797-65-0	Nitrite	No info	30,300	N/A	N/A	N/A	N/A
14265-44-2	Phosphate	No info	<250	N/A	N/A	N/A	N/A
14808-79-8	Sulfate	No info	16,500	N/A	N/A	N/A	N/A
144-62-7	Oxalate	No info	2,830	N/A	N/A	N/A	N/A
64-18-6	Formate	No info	<250	N/A	N/A	N/A	N/A
16887-00-6	Chloride	100	<50	N/A	N/A	N/A	N/A
16984-48-8	Fluoride	No info	967	N/A	N/A	N/A	N/A

Table B-12 Summary Results for Tank 241-AZ-102. Target Analytes Detected Supernatant LAW B/Solids HLW Envelope D

CAS #	Target Compound	Tank 241-AZ-102					
		Tank Waste (Feed)					
		Filtered Supernatant (Env. B)		Total Dried Solids (Env. D)		Insoluble Dried Solids (Env. D)	
Miscellaneous Analytes		DL (mg/L)	mg/L	DL (mg/kg)	mg/kg	DL (mg/kg)	mg/kg
	TIC	No info	6,140	N/A	N/A	N/A	N/A
	TOC	No info	6,040	N/A	N/A	N/A	N/A

N/A Not applicable, analyte not analyzed.

< Compound or analyte is less than the value shown.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-13 Feed Identification

Composition	Sample Number
LAWA	OD-CM45A
LAWA	OD-CM-63A
LAWA	OD-CM-103A
LAWC	OD2-CM-16A
LAWC	OD2-CM-26A
LAWC	OD2-CM-35A
LAWC	OD2-CM-48A
LAWC	OD2-CM-57A
LAWC	OD2-CM-89A
LAWC	OD2-CM-98A
LAWC	OD2-CM-109A
LAWC	OD2-CM-115A
HLWD	OD3-CM-32A
HLWD	OD3-CM-44A
HLWD	OD3-CM-53A
HLWD	OD3-CM-65A
LAWC	OD3-CM-76A
LAWC	OD3-CM-88A
LAWC	OD3-CM-114A
LAWA	OD3-CM-126A

Table B-14 Glass Identification

Composition	Sample Number
LAWA	OD-G-19A
LAWA	OD-G-25A
LAWA	OD-G-29A
LAWA	OD-G-45A, 46A
LAWA	OD-G-47A
LAWA	OD-G-49A
LAWA	OD-G-63A
LAWA	OD-G-64A
LAWA	OD-G-64B
LAWA	OD-G-78A, 79A
LAWA	OD-G-86A, 97A, 99A
LAWA	OD-G-103AB
LAWA	OD-G-109A
LAWA	OD-G-115A
LAWA	OD-G-122A
LAWA	OD-G-128A
LAWA	OD-G-131A, 136AB
LAWA	OD-G-136C, 137A
LAWC	OD2-G-13A, 16A
LAWC	OD2-G-17AB
LAWC	OD2-G-18A
LAWC	OD2-G-24AB
LAWC	OD2-G-25A, 26A
LAWC	OD2-G-34A, 35A
LAWC	OD2-G-37A
LAWC	OD2-G-47AB
LAWC	OD2-G-50A
LAWC	OD2-G-52B
LAWC	OD2-G-52C
LAWC	OD2-G-59A
LAWC	OD2-G-59B
LAWC	OD2-G-65A, 66AB
LAWC	OD2-G-72A
LAWC	OD2-G-74A

Table B-14 Glass Identification

Composition	Sample Number
LAWC	OD2-G-77A, 82A
LAWC	OD2-G-89AB
LAWC	OD2-G-89C
LAWC	OD2-G-98AB
LAWC	OD2-G-100AB
LAWC	OD2-G-104A, 109A
LAWC	OD-G-111A, 115A
HLWD	OD3-G-12A
HLWD	OD3-G-12B, 15A
HLWD	OD3-G-16A
HLWD	OD3-G-22AB
HLWD	OD3-G-27AB
HLWD	OD3-G-36AB
HLWD	OD3-G-44AB
HLWD	OD3-G-47A, 53AB
HLWD	OD3-G-65A
HLWD	OD3-G-67A, B
LAWA	OD3-G-68A
LAWA	OD3-G-68B
LAWA	OD3-G-68C
LAWA	OD3-G-76A, B,C
LAWA	OD3-G-85A, 88A
LAWA	OD3-G-98A, B
LAWA	OD3-G-110A, 113A
LAWA	OD3-G-114A, 121A
LAWC	OD3-G-121B
LAWC	OD3-G-121C
LAWC	OD3-G-121D
LAWC	OD3-G-121E
LAWC	OD3-G-122A, 126A, B
LAWC	OD3-G-127A, 131A
LAWC	OD3-G-131B
LAWC	OD3-G-131B
LAWC	OD3-G-140, 141A, 142A

Table B-15 % DRE Values from the Analysis of Glass Samples ¹

Test	Glass (µg/hr)				% DRE			
	Benzene	TCE	Phenol	TOC	Benzene	TCE	Phenol	TOC
2	<1.25	<0.75	<227.75	NA	>99.99993	>99.99996	>99.97559	NA
1	<0.65	<0.39	<118.43	18.77	>99.99994	>99.99997	>99.97868	99.99995
3	<0.75	<0.45	<136.65	NA	>99.99995	>99.99993	>99.98341	NA
9	<1.3	<0.78	<236.86	NA	>99.99989	>99.99994	>99.99041	NA
12	<0.75	<0.45	<136.65	NA	>99.99991	>99.99995	>99.99204	NA
5	<1	<0.6	<182.2	0.57	>99.99988	>99.99993	>99.98992	100.0000
11	<1.3	<0.78	<236.86	NA	NA	>99.99994	>99.99465	NA
10	<1.1	<0.66	<200.42	NA	>99.99992	NA	>99.99515	NA
4	<1.3	<0.78	<236.86	2.97	>99.99989	>99.99994	>99.99041	100.000
6	<1.05	<0.63	<191.31	NA	>99.99961	>99.99978	>99.96654	NA
8	<0.95	<0.57	<173.09	3.47	>99.99964	>99.99980	>99.96973	99.99999
7	<0.8	<0.48	<145.76	2.25	>99.99970	>99.99983	>99.97451	99.99999
15	<0.55	<0.33	<100.21	0.5	>99.99997	>99.99999	>99.99779	99.99999
14	<0.95	<0.57	<173.09	0.55	>99.99994	>99.99997	>99.99492	99.99999
13	<0.6	<0.36	<109.32	0.53	>99.99976	>99.99987	>99.98074	99.99999
OP4	<1.2	<0.72	<218.64	0.53	>99.99991	>99.99995	>99.99226	100.0000
OP1	<0.6	<0.36	<109.32	0.54	>99.99970	>99.99976	>99.97908	99.99990
16	<0.55	<0.33	<100.21	NA	>99.99972	>99.99978	>99.98082	NA

Table B-15 % DRE Values from the Analysis of Glass Samples ¹

Test	Glass (µg/hr)				% DRE			
	Benzene	TCE	Phenol	TOC	Benzene	TCE	Phenol	TOC
OP2	<0.5	<0.3	<91.1	1.67	NA	NA	NA	100.0000
OP3	<0.5	<0.3	<91.1	1.04	NA	NA	NA	100.0000

¹ Data reflect extent of analytical detection limits.

< Indicates compound or analyte is less than the value shown.

> Indicates data did not permit computation of greater quantity.

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-16 TCLP Results for LAW Glass (µg/L)

Glass ID	Ag	Ba	Cd	Cr	Pb	Hg
Detection Limit	1.51	1.93	1.12	2.99	1.55	0.00035
Reporting Limit ^(a)	1.51	1.93	2.00	15.00	1.55	0.02
Feed ^(b)	2.6	146	5.13	2700	1590	0.00063
Universal Treatment Standard	140	21000	110	600	750	25
OD-G-47	2.28	3.34	ND	54	2.93	ND
OD-G-64B	ND	4.12	ND	65.5	3.65	ND
OD-G-109A	3.63	3.68	ND	28.9	2.3	ND
OD2-G-18A	ND	2.76	ND	15.1	10.8	ND
OD2-G-26A	ND	2.66	ND	13.8	8.22	ND
OD2-G-37A	ND	2.87	ND	12.2	8.35	ND
OD2-G-50A	ND	2.52	ND	10.9	7.05	ND
OD2-G-52C	2.05	20.4	ND	5.12	32.2	0.00127
OD2-G-89C	ND	2.27	ND	19.2	7.8	ND
OD2-G-98B	ND	1.93	ND	23.2	7.81	ND
OD2-G-100B	ND	2.32	ND	28.1	9.13	ND
OD2-G-109B	ND	2.48	ND	31.6	7.83	ND
OD2-G-115A	ND	1.95	ND	35.2	7.67	ND
OD3-G-76B	4.53	17.9	11.89	54.2	7.92	ND
OD3-G-88A	3.21	7.12	3.37	62.6	3.88	ND
OD3-G-121A	ND	6.30	1.65	59.4	5.08	ND
OD3-G-126B	ND	3.12	ND	15.4	14.5	ND

(a) Reporting Limit is generally the same as the Estimated Quantitation (EQL) as defined by SW 846, with the exception that it is not always 5 to 10 times the Method Detection Limit (MDL). The reporting limit is greater than the MDL and is the lowest concentration which can be reliably quantified.

(b) Result of Toxicity Characteristic Leaching Procedure (TCLP) on raw melter feed sample

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-17 TCLP Results for HLW Glasses (mg/L)

Sample ID	Lab	Ag	As	Ba	Be	Cd	Cr	Hg	Ni	Pb	Sb	Se	Tl	V	Zn
OD3-G-36B	VSL	0.029	<0.05	0.130	<0.001	0.056	0.010	<0.05	0.066	0.057	0.123	<0.06	<0.05	<0.01	0.449
	GEL	0.031	0.005	0.097	NA	0.053	0.014	ND	NA	0.035	NA	ND	NA	NA	NA
OD3-G-44B	VSL	0.004	0.059	0.124	<0.001	0.077	0.010	<0.05	0.071	0.040	0.125	<0.06	<0.05	<0.1	0.513
	GEL	0.007	0.005	0.079	NA	0.058	0.013	ND	NA	0.040	NA	ND	NA	NA	NA
OD3-G-53B	VSL	0.013	<0.05	0.115	<0.001	0.077	0.010	<0.05	0.074	0.048	0.143	<0.06	<0.05	<0.01	0.471
	GEL	0.012	0.005	0.077	NA	0.060	0.014	ND	NA	0.039	NA	ND	NA	NA	NA
	GEL (duplicate)	0.012	0.005	0.077	NA	0.060	0.014	ND	NA	0.039	NA	ND	NA	NA	NA
OD3-G-67B	VSL	0.04	0.08	0.13	<0.001	0.07	0.01	<0.05	0.07	0.06	0.19	<0.06	<0.05	<0.01	0.42
	GEL	0.04	ND	0.085	NA	0.056	0.014	ND	NA	0.041	NA	ND	NA	NA	NA
GEL Detection limits		0.002	0.005	0.002	NA	0.001	0.003	4E-07	NA	0.002	NA	0.007	NA	NA	NA
GEL Reporting limits		0.002	0.010	0.002	NA	0.002	0.015	2E-05	NA	0.002	NA	0.010	NA	NA	NA
Universal Treatment Standard		0.14	5	21	1.22	0.11	0.60	0.025	11	0.75	1.15	5.7	0.20	NA	NA

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

< Compound or analyte is less than the value shown.

Table B-18 Results for TCLP Organics for LAW and HLW Glasses (µg/kg)

Glass ID	Benzene	Chlorobenzene	Chloroform	Trichloroethylene	1, 1-Dichloro ethylene	1, 2 Dichloro ethane	1, 4 Dichloro benzene	2 Butanone	Carbon Tetra chloride	Tetra chloro ethylene	Vinyl Chloride
TCLP Limit	500		6000	500	700	500		200,000	500		200
Detection Limit	3	3	7	6	7	2	3	59	2	7	4
Reporting Limit	50	1000	600	50	70	50	750	2000	20	70	20
BLANK		ND	1		ND	ND	ND	ND	ND	ND	ND
OD-G-47A	ND	ND	18.9	ND	ND	ND	ND	ND	ND	ND	ND
OD-G-64B	ND	ND	20.9	ND	ND	ND	ND	ND	ND	ND	ND
OD-G-109A	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-18AM1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-26A	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-37A	ND	ND	10.4	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-50A	ND	32.4	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-52C	ND	24.3	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-89C	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-98B	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-100B	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-109B	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD2-G-115A	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-36B	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table B-18 Results for TCLP Organics for LAW and HLW Glasses (µg/kg)

Glass ID	Benzene	Chlorobenzene	Chloroform	Trichloroethylene	1, 1-Dichloro ethylene	1, 2 Dichloro ethane	1, 4 Dichloro benzene	2 Butanone	Carbon Tetra chloride	Tetra chloro ethylene	Vinyl Chloride
OD3-G-44B	ND	7.40	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-53B	ND	ND	7.30	ND	ND	ND	ND	ND	ND	ND	ND
	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-67B	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-76C	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-88A	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-121A	ND	ND	13.3	ND	ND	ND	ND	ND	ND	ND	ND
OD3-G-126B	ND	ND	17.1	ND	ND	ND	ND	ND	ND	ND	ND
EA-101031-1	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-19 Volatile and Semi-volatile Analysis for Glass Samples (µg/kg)

Glass ID	Acetone	Chloroform	Methylene Chloride	Vinyl Acetate	Carbon Disulfide	Naphthalene
Detection Limit	10.3	0.1	1.4	2.1	0.3	0.6
Reporting Limit	10.3	2.0	5.0	10	10	2.0
Universal Treatment Standard	160000	6000	30000	NA	4800 (TCLP)	5600
Blank	ND	1	ND	ND	ND	ND
OD-G-47A	ND	ND	ND	ND	ND	ND
OD-G-64B	ND	ND	ND	ND	ND	ND
OD-G-109A	12.4	ND	6.37	ND	ND	ND
OD2-G-18A	ND	ND	ND	ND	ND	ND
OD2-G-26A	ND	ND	ND	ND	ND	ND
OD2-G-37A	ND	0.57	ND	ND	ND	ND
OD2-G-50A	ND	ND	ND	ND	ND	ND
OD2-G-52C	ND	ND	ND	ND	ND	ND
OD2-G-89C	ND	ND	2.97	ND	ND	ND
OD2-G-98B	ND	ND	2.81	2.24	ND	ND
OD2-G-100B	ND	1.33	6.67	ND	ND	ND
OD2-G-109B	ND	ND	3.47	ND	ND	ND
OD2-G-115A	ND	ND	2.25	ND	ND	ND
OD3-36B	ND	0.50	ND	ND	ND	ND
OD3-G-44B	ND	0.55	ND	ND	ND	ND
OD3-G-53B	ND	0.53	ND	ND	ND	ND
	ND	0.53	ND	ND	ND	ND
OD3-G-67B	ND	0.53	ND	ND	ND	ND
OD3-G-76C	ND	0.54	ND	ND	ND	ND
OD3-G-88A	ND	0.57	ND	ND	ND	ND
OD3-G-121A	ND	ND	ND	ND	0.79	0.88
OD3-G-126B	ND	ND	ND	ND	1.04	ND
EA-101031-2*	ND	ND	ND	ND	0.74	ND

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-20 Concentration of RCRA Spikes added to the LAW Glasses Formations for TCLP Testing

Glass Oxides	Medium Spike Concentration in wt% Oxide	Spike Factor	High Spike Concentration in wt% Oxide	Spike Factor
Silver	0.015	50	0.1504	500
Arsenic	0.066	5	0.066	50
Barium	0.2345	5	2.3447	50
Cadmium	0.0126	50	0.1257	500
Chromium	0.0135	5	0.1350	50
Mercury	0.0027	50	0.027	500
Nickel	0.1587	5	1.5873	50
Lead	0.0081	5	0.0808	50
Selenium	0.0801	5	0.8010	50
Antimony	0.0138	5	0.1377	50
Thallium	0.0223	50	0.2235	500
Zinc	3.00	Additive	3.00	Additive
Vanadium	0.0411	5	0.4113	50

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-21 TCLP Leachate Concentrations

Target Compound ^{1,2}	LAWA 44-8 TC		
	No Spike (ppm)	Medium Spike	High Spike
Silver	<0.0031	NA	NA
Arsenic	<0.049	NA	NA
Barium	0.005	NA	NA
Cadmium	<0.0027	NA	NA
Chromium	<0.0055	NA	NA
Nickel	<0.0079	NA	NA
Lead	<0.0243	NA	NA
Antimony	0.078	NA	NA
Selenium	<0.0532	NA	NA
Thallium	<0.0417	NA	NA
Vanadium	0.017	NA	NA
Zinc	1.211	NA	NA

< Compound or analyte is less than the value shown.

¹ No DL information available

² No EPA method number available

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-22 TCLP Leachate Concentrations

Target Compound ^{1,2}	LAWA 102				
	No Spike (ppm)	Medium Spike ³ (ppm)		High Spike ³ (ppm)	
		Value 1	Value 2	Value 1	Value 2
Silver	<0.0031	0.007	<0.0031	0.091	0.06
Arsenic	<0.049	<0.049	<0.049	0.064	0.207
Barium	0.003	0.814	1.199	1.88	2.211
Cadmium	<0.0027	<0.0027	<0.0027	0.074	0.082
Chromium	0.016	0.011	0.018	0.015	0.026
Nickel	0.017	0.069	0.079	0.691	0.698
Lead	<0.0243	<0.0243	<0.0243	0.035	<0.0243
Antimony	0.203	<0.0338	<0.090	<0.0338	0.055
Selenium	<0.0532	<0.0532	<0.0532	<0.0532	0.054
Thallium	<0.0417	<0.0417	<0.0417	<0.0417	<0.0417
Vanadium	0.012	0.013	<0.01	0.088	0.087
Zinc	1.327	2.032	1.703	2.028	1.721

< Compound or analyte is less than the value shown.

1 No DL information available

2 No EPA method number available

3 Analysis performed in duplicate

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-23 TCLP Leachate Concentrations

Target Compound ^{1,2}	LAWB45				
	No Spike (ppm)	Medium Spike ³ (ppm)		High Spike ³ (ppm)	
		Value 1	Value 2	Value 1	Value 2
Silver	<0.0031	0.006	<0.0031	0.093	0.058
Arsenic	0.051	<0.049	0.064	<0.049	0.179
Barium	0.004	0.768	1.237	2.248	2.525
Cadmium	<0.0027	<0.0027	0.006	0.093	0.11
Chromium	0.015	0.007	0.004	<0.0055	0.041
Nickel	0.016	0.106	0.091	0.991	0.995
Lead	<0.0243	<0.0243	<0.0243	0.047	0.054
Antimony	<0.0338	0.081	<0.0338	<0.0338	0.092
Selenium	<0.0532	<0.0532	<0.0532	<0.0532	0.114
Thallium	<0.0417	<0.0417	<0.0417	<0.0417	0.108
Vanadium	0.01	0.019	0.016	0.112	0.109
Zinc	1.014	2.275	1.697	2.58	2.38

< Compound or analyte is less than the value shown.

1 No DL information available

2 No EPA method number available

3 Analysis performed in duplicate

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-24 TCLP Leachate Concentrations

Target Compound ^{1,2}	LAWC21					
	No Spike (ppm)		Medium Spike ³ (ppm)		High Spike ³ (ppm)	
	Value 1	Value 2	Value 1	Value 2	Value 1	Value 2
Silver	<0.0031	<0.0031	<0.0031	<0.0031	0.072	0.054
Arsenic	<0.049	<0.049	<0.049	0.079	<0.049	0.206
Barium	0.921	0.972	0.726	0.923	1.856	2.02
Cadmium	0.005	<0.0027	0.005	0.01	0.086	0.054
Chromium	0.044	0.024	<0.0055	0.03	<0.0055	0.025
Nickel	0.042	0.022	0.039	0.052	0.652	0.527
Lead	<0.0243	<0.0243	<0.0243	<0.0243	<0.0243	0.033
Antimony	<0.0338	<0.0338	<0.0338	<0.0338	0.042	<0.0338
Selenium	<0.0532	<0.0532	<0.0532	0.092	<0.0532	0.076
Thallium	<0.0417	<0.0417	<0.0417	<0.0417	<0.0417	<0.0417
Vanadium	<0.01	<0.01	<0.01	0.011	0.087	0.07
Zinc	1.121	0.933	1.238	1.28	1.873	1.33

< Compound or analyte is less than the value shown.

1 No DL information available

2 No EPA method number available

3 Analysis performed in duplicate

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Table B-25 TCLP Value Ranges for HLW 98 and 99 Glasses^{1,2}

Element	Composite Waste		Tank 241-AZ 101		Tank 241-AZ 102		Tank 241-C-106/ 241-AY-102	
	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)
Silver	0.07	0.01	0.03	0.02	0.02	<0.01	0.07	0.02
Arsenic	<0.05	<0.05	0.06	0.01	0.12	0.05	NA	NA
Barium	0.32	0.09	0.16	0.02	0.47	0.04	0.30	0.12
Cadmium	0.37	0.06	0.18	0.06	0.48	0.16	0.08	0.01
Chromium	0.03	<0.01	0.03	<0.01	0.01	<0.01	0.02	<0.01
Lead	0.14	0.06	0.26	<0.03	0.64	<0.02	0.11	<0.06
Selenium	<0.05	<0.05	0.09	<0.05	0.06	<0.05	NA	NA
Element	HLW 99-01 to 08		HLW 99-09 to 16		HLW 99-17 to 24R		HLW 99-25 to 32	
Range Values	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)
Silver	0.36	0.03	0.58	0.02	0.74	0.03	0.33	0.03
Arsenic	0.41	0.05	2.77	0.05	0.63	0.05	0.10	0.05
Barium	35.74	0.01	99.56	0.10	28.94	0.05	41.82	0.11
Cadmium	33.35	0.01	53.87	0.03	43.54	0.01	30.94	0.08
Chromium	1.17	<0.01	0.09	<0.01	4.22	<0.01	0.58	<0.01
Lead	1.55	<0.02	4.87	<0.02	2.00	0.05	0.89	0.07
Selenium	0.71	0.05	0.81	0.05	1.33	0.06	0.42	0.05
Element	HLW 99-33 to 38		HLW 99-39 to 46		HLW 99-47 to 54		HLW 99-55 to 62	
Range Values	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)
Silver	0.68	0.05	0.49	0.03	0.22	0.05	0.23	0.05
Arsenic	2.43	0.05	0.43	0.05	2.36	0.05	0.29	0.05
Barium	8.05	0.03	58.93	0.01	76.90	0.01	78.00	0.03
Cadmium	6.41	0.01	56.47	<0.01	68.73	<0.01	67.01	<0.01
Chromium	0.10	<0.01	0.16	<0.01	5.36	<0.01	0.05	<0.01
Lead	1.19	0.09	0.40	<0.02	4.36	<0.02	3.92	<0.02
Selenium	1.92	0.05	0.56	0.05	1.85	0.06	0.96	0.05

Table B-25 TCLP Value Ranges for HLW 98 and 99 Glasses^{1,2}

Element	HLW 99-63 to 70		HLW 99-71 to 76		HLW 99-77 to 84		HLW 99-85 to 92	
	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)	High (ppm)	Low (ppm)
Silver	0.52	0.06	1.10	0.07	0.33	0.11	0.56	0.07
Arsenic	0.20	0.05	0.21	0.06	0.21	<0.05	0.24	<0.05
Barium	10.86	0.48	11.83	0.46	4.46	1.02	6.27	0.77
Cadmium	11.49	<0.01	10.33	<0.01	2.88	0.01	4.02	0.01
Chromium	0.32	<0.01	0.13	<0.01	0.03	<0.01	0.07	<0.01
Lead	0.83	<0.02	1.55	<0.02	0.69	0.04	1.02	<0.02
Selenium	0.34	0.05	0.25	0.05	0.17	<0.05	0.12	0.05
Element	HLW 99-93 to 100							
Range Values	High (ppm)	Low (ppm)						
Silver	0.80	0.16						
Arsenic	0.22	<0.05						
Barium	10.72	0.97						
Cadmium	8.64	<0.01						
Chromium	0.08	<0.01						
Lead	1.29	<0.02						
Selenium	0.13	<0.05						

< Compound or analyte is less than the value shown.

1 No DL information available

2 No EPA method numbers available

Note: The data presented are research data and are meant to provide general information on the overall viability of vitrification. SW-846 protocols were not strictly followed and MDLs were not determined in accordance with EPA procedures.

Appendix C

Glass Chemistry and Leachate Modeling

Appendix C

Glass Chemistry and Leachate Modeling

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1 Basic Glass Structure and Principles

Understanding glass structure and its resulting properties is fundamental to understanding the advantages of vitrification as a treatment technology. This section provides an elementary overview of glass properties and describes "how" glass is used to immobilize hazardous constituents.

Glass is a rigid, noncrystalline material of relatively low porosity, often composed primarily of silica, alumina, and oxides of alkali and alkaline earth elements. There are many glass-forming systems (such as silicates, borates, phosphates, and oxynitrides); only silicates and phosphates have been used for waste treatment. Most waste glasses used are borosilicates. Thermally formed glasses are produced by fusing (or melting) crystalline and/or amorphous materials (for example, previously formed glasses [frit]) at elevated temperatures to produce molten glass. The molten glass is subsequently cooled to a rigid condition without crystallization. Glass is amorphous; that is, there is no long-range molecular order, but it does exhibit short-range order (Doremus 1994). Most glasses contain a small portion of micro-crystalline phase; non-crystalline substances generally lack a definitive melting-point temperature.

Glasses are composed of three-dimensional networks consisting primarily of tetrahedrally coordinated orthosilicate monomers (SiO_4^{4-}), each silicon atom bonded to four oxygen atoms (see Figure 1-3). Some, or all four, of the oxygen atoms from the tetrahedron can be shared with other tetrahedra to form a three-dimensional network (see Figure C-1). Since the Si-O-Si bonds are random, the network remains irregular (amorphous) and non-crystalline. The shared oxygen atoms are called bridging oxygens. In pure silica glass, the ratio of silicon to oxygen is 1:2, and all oxygen atoms are bridging. Some atoms, such as sodium, are ionically bonded to oxygen when present in glass, and thus interrupt tetrahedral linking, and the continuity of the network. An oxygen atom that is not covalently bonded to another atom is called "non-bridging".

Most inorganic oxides can be incorporated into silicate glasses. Elements that can replace silicon are called network formers. Most monovalent and divalent cations do not enter the network, but form ionic bonds with non-bridging oxygen, and are termed network modifiers. However, as long as the number of A_2O or AO units ("A" being the alkali or alkaline earth ion) is in a less than 1:1 ratio to the number of SiO_2 units, the silicon-oxygen network is preserved because each silicon-oxygen tetrahedron is linked to at least three other tetrahedra, and the glass-forming tendency of the mixture is retained.

Chemical composition plays an important role in all glass properties, including glass durability. In general, network modifiers tend to decrease glass durability since they reduce the availability of bridging oxygen atoms. However, these elements do reduce melting temperature and viscosity and, thus, are used as fluxing agents to improve the ability to process (EPA 1992).

Alkalis included in the raw materials as carbonates or other salts react at elevated temperatures with silica to form a siliceous liquid. Alkalis, such as sodium, make fluxes in their oxide state, and provide network modifiers that will generate non-bridging oxygen atoms. The reaction of fluxes is complex, but they essentially lower the melting point of the glass formers and viscosity of the glass. However, alkalis generally decrease glass chemical resistance from that of silica glass. To decrease the aqueous solubility of alkali glasses, but to maintain lower melting points, alkaline earth fluxes, such as magnesium oxide and calcium oxide, are added. However, too much alkaline earth flux can result in crystallization (EPA 1992). Boron is another valuable additive that improves durability by moderating the rise of pH due to alkali release to the solution.

In general, the following reactions occur as inorganic compounds are incorporated into the glass structure.

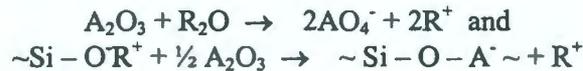
- Incorporation by monovalent network modifiers, R₂O (for example, Li₂O, Na₂O, K₂O, Cs₂O):



- Incorporation by divalent network modifiers, MO (for example, MgO, CaO, SrO, BaO, FeO, ZnO, PbO):



- Incorporation by trivalent network formers, A₂O₃ (for example, B₂O₃, Al₂O₃, Fe₂O₃), with charge compensation from R₂O and/or MO:



Many metals of environmental concern are incorporated into glass matrices and, in fact, are often used for coloration of glass in the commercial glass industry. Hazardous constituents can be immobilized in vitrification processes by two main interactions with the glass matrix: chemical bonding and encapsulation. In most waste glass, the waste constituents are chemically bonded.

Certain inorganic species can be immobilized by chemically bonding with the glass-forming materials, particularly silica. Bonding occurs within a vitrified material when the inorganic constituents bond covalently with oxygen, becoming part of the network. Inorganics that react this way are network formers since they essentially replace the silica in the glass network structure.

Other inorganic species become network modifiers by ionically bonding with oxygen or other elements in the glass network. This ionic bonding incorporates the inorganic constituent into the glass matrix, but disrupts the network's continuity by reducing the number of bridging oxygen atoms, thus changing the glass properties.

2 Glass Composition Region of Interest

In view of the large number of composition variables that are relevant for waste glasses, some level of simplification is often illuminating. Such simplification can be achieved by employing a reduced set of composition variables that are based on knowledge of the structural roles of the underlying components in the glass matrix. Data representations can provide insight into how the glass-melt properties vary with the structural indicators that are employed. It is also often the case that gross boundaries of glass stability or durability can be rationalized by using structural information on the microscopic scale.

Four parameters are used to represent the distribution of the glasses in a "reduced" compositional space: NBOT, M3T, BM3, and M1M12 (DOE/CH9601). These parameters are constructed in terms of the prevailing or characteristic short-range structures or configurations in the glasses, and are defined as follows:

- NBOT = Average number of non-bridging oxygens per network forming tetrahedral site. The number of total non-bridging oxygens is defined as being equal to the number of charges carried by the alkali, alkaline earth, and selected other metal cations (e.g., Zn^{2+}) that are not used to charge-balance tetrahedrally coordinated Al, B, and Fe^{3+} .
- M3T = M3T indicates the fraction, on average, of network tetrahedral sites occupied by trivalent cations. It is assumed that, with sufficient charge-balancing cations (if $M3T \leq 0.5$), all of the Al, B, and Fe^{3+} will reside as network formers (DOE/CH9601). Since the majority of the glasses have either sufficient or excess M^{1+} and M^{2+} to charge-balance the tetrahedrally coordinated M^{3+} species, the total number of non-bridging oxygens can often be simply calculated as the sum of the charges of M^{1+} and M^{2+} less the sum of M^{3+} cations.
- BM3 = Molar ratio of B^{3+} in network-forming tetrahedral sites to all trivalent cations in network-forming tetrahedral sites, or simply the fraction of trivalent cations that are B^{3+} .
- M1M12 = Ratio of charge contribution from alkali cations to the total charges from monovalent and divalent cations.

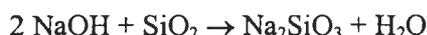
NBOT is an indicator of the degree of polymerization in silicate melts because the number of the non-bridging oxygens associated with a network-forming cation (such as Si^{4+} or Al^{3+}) controls, on average, the connectivity to other network forming cations surrounding it as next-nearest neighbors. The occupancy fraction of M^{3+} cations (M3T) in networking tetrahedra influences the intermediate range structure and the overall stability (for example, phase separation usually occurs when the ratio is too high). BM3 differentiates B from Al and Fe, which have significantly different effects on properties such as viscosity and leachability. Similarly, the proportion of charge compensation provided by alkalis versus alkaline earths (M1M12) has strong effects on the melt viscosity, conductivity, and glass leach resistance. In addition, from a structural point of view, M1M12 influences the bond strengths in the glass network and controls the Q^n species distribution at a given degree of polymerization (in this notation, Q refers to a tetrahedral site and (4-n) is the number of non-bridging oxygens associated with one SiO_4 tetrahedron).

All four parameters have reasonably well-defined structural significance for silicate melts and glasses. These parameters enable simplified visualization of the glass composition region of interest, and reasonable approximation of the essential characteristics of the prevailing glass structure. These four parameters have been used by the WTP for evaluating a database of possible glass formulations (such as glass composition region of interest). Figure C-2 shows a plot of the M3T (fraction of sites occupied by trivalent cations) versus the NBOT (average number of non-bridging oxygens per network of tetrahedral sites). The upper and lower dotted lines show the M3T of two naturally occurring crystalline minerals: Albite (Ab), with a formula of $NaAlSi_3O_8$, and Anorthite (An), with a formula of $CaAl_2Si_2O_8$. Since each tetrahedron can have a maximum of four bridging oxygens, Q^n is expressed as $n=4-NBOT$. Q^4 has the most bridged oxygens and is highly polymerized. Q^3 has three bridged oxygens per tetrahedron and is slightly less polymerized. As demonstrated, the majority of the various HLW glasses fall within the boundaries of the naturally occurring minerals and the highly bridged oxygens (Ab to An, Q^4 to Q^3). This shows the potential boundaries of the glasses with respect to stability and polymerization. This approach has been very successful in defining the compositional constraints that are appropriate for development of composition models and glass formulations.

3 Glass Reactivity

Vitreous materials are relatively inert due to their high resistance to corrosion; however, they are subject to some chemical breakdown under severe conditions. There are two major forms of chemical attack on vitrified material: matrix dissolution and interdiffusion.

Matrix dissolution is characterized by alkali attack (exposure to a high pH). It begins with the hydration of the silica network, and may proceed to dissolution of the vitreous material (EPA 1992). The following reaction illustrates this process.



The alkali silicate (Na_2SiO_3) is water soluble, so as the silica network is attacked, it is broken down and other constituents are released. Matrix dissolution occurs at the surface of the vitrified material. The presence of insoluble constituents in the material can retard the reaction rate.

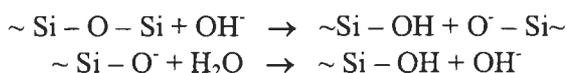
Interdiffusion involves the ionic exchange of hydronium ions in solution for ionically bonded network modifiers in the glass. Interdiffusion generally leaves the silica structure almost intact (EPA 1992). Although pH plays an important role in the interdiffusion rate, pH change has a stronger impact on matrix dissolution rates. Since the process is controlled predominantly by diffusion, the rate of leaching decreases as the thickness of the diffusion layer increases. However, this effect can be limited if the diffusion layer is dissolved, for example, by matrix dissolution.

Layer formation is favored in static or near-static conditions, and where silica is present, such as groundwater. Water can exhibit both acidic and alkaline reaction mechanisms because of readily formed hydronium and hydroxyl ions. The leaching of many glasses appears to be modified by the formation of surface layers. As matrix dissolution occurs, a surface layer composed of insoluble glass components forms. Initially, decomposition is dominated by interdiffusion (ionic exchange of alkali ions, such as sodium) as the network modifiers diffuse out of the glass and into solution, and the water diffuses into the surface of the glass. The concentration of alkali in the bulk of the glass is unaffected (Doremus 1994). During this process, the pH at the glass surface gradually increases (becomes more alkaline) due to the formation of alkali hydroxides in the solution. The result of the increase in pH is the onset of matrix dissolution and, eventually, the formation of a surface layer around the glass matrix. Within that surface layer, precipitation and adsorption of insoluble compounds occurs at the surface of the glass. These compounds are the more insoluble compounds, (such as iron and manganese oxides), that remain as the more soluble constituents dissolve and move into solution. The surface layer can exert a strong limiting effect on the leaching of the glass underneath. Under static or near-static conditions, leaching may be reduced further, as silica concentrations build up in the leachate and approach saturation, which reduces the tendency of more silica in the glass to move into solution (EPA 1992). The primary reactions are summarized below:

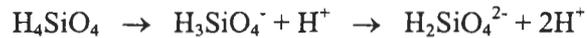
- Interdiffusion:



- Hydroxyl-Catalyzed Network Hydrolysis:



- Which, under higher pH, releases:



- Simultaneous with condensation:



Ultimately, solubility depends upon pH. Diffusion gives rise to an increase in pH until saturation occurs, eventually resulting in the formation of a secondary phase of crystalline and amorphous precipitants at the glass surface.

Glass leaching is controlled by the following conditions:

- Moderation of the rise in pH
- Incorporation of low-solubility species, such as aluminum and iron
- Controlling the secondary phase formations

In formulating waste glasses, there is generally a trade-off between leachability and processability. Addition of sodium and other modifiers decreases viscosity and alters other process variables, thus improving processability; however, this addition increases leachability.

4 Normalization of Data

In order to permit comparison of constituents on a common basis, data are typically normalized to glass composition. This enables data users to quickly assess glass performance with regards to the degree of constituent immobilization attained for any particular waste loading and glass formulation. It also enables data users to compare the constituent release rate for glass formers, as well as RCRA constituents. This approach to data reporting also makes sense as, generally, the release of element *i* depends on the amount of *i* in the glass. Normalized data are reported as a ratio of the concentration in the leachate versus that in the waste, or mass in leachate versus that in the waste. Data are presented in either a mass:mass or concentration:concentration ratio. Mass:mass is often presented as ppm in leachate versus the weight percent in the waste. If one desires the mass:mass ratio to be in ppm, the weight percent is converted to ppm, by multiplying the weight percent by 10,000.

5 Intrinsic Release Rates

From glass chemistry, it can be shown that immobilization of hazardous constituents is primarily through elemental bonding as network modifiers (ionic bonding with non-bridging oxygen) or as network formers (covalent bonding with bridging oxygen). The atomic structure of the glass makes no differentiation between regulated and non-regulated constituents. Additionally, glass theory has suggested a strong relationship between constituent-oxygen bond strength and coordination number, and resistance to leachability. Resistance of a glass to leaching can therefore be thought of as an intrinsic glass property with the leach rate of each constituent being primarily a function of the coordination number and amount (percent oxide) of the constituent in the glass. For simplicity, the release rate for each hazardous

constituent can be compared to that of boron, the most abundant and mobile of the glass formers used in WTP glass (release of sodium, the most prevalent network modifier, could not be measured). Under the 18-hour exposure time and pH conditions of the TCLP, the following categorization of metals can be deduced from the experimental data to date (Gan and Pegg 2002).

- Group 1: Advanced Elements [Release=1, relative to boron release]

This group includes alkalis (Li, K), alkaline earths (Mg, Ca, Sr, Ba), divalent transition metals (Ni, Cu, Mn, Co), cadmium, zinc, boron, silver, and uranium. The normalized release of each element in this group exhibits almost a one-to-one relationship (equality of normalized releases) with each other. This type of dissolution behavior is often referred to as “congruent”, and would be characteristic of a simple interface-controlled dissolution process in which the glass simply dissolves “layer-by-layer”.

- Group 2: Retarded Elements [Release ~ 1/4, relative to boron release]

This group includes several p-block elements (Si, Ti, Se, Sb, and Pb). Within this group, the normalized elemental releases were found to be approximately equal to each other; however, the normalized release of these elements is about one-fourth of that of the normalized release for the “advanced” group of elements.

- Group 3: Slow and Irregular Elements [Release ~ 1/10, relative to boron release]

Elements in this group include Al, Fe, and Zr, which have low solubilities at pH 5, as well as As and Cr. The normalized releases of these elements are much lower than those of the advanced or retarded elements, and generally show poor correlation to the advanced or retarded elements.

The relevance of this categorization is that it helps to simplify overall glass response (constituent leachability) to the TCLP. Glasses with a lower boron release are intrinsically more leach-resistant. Boron leachability can be used to assess glass performance early in the testing program to determine if additional development work is warranted. These characteristics are discussed in greater detail in later sections.

The formulations used in acceptable glasses can also be used for actively designing new formulations for new waste streams since constituent leaching is an intrinsic glass property. These simple element groupings can be used as a general guide to assess the relative “difficulty” of complying with each of the elemental concentration limits from a knowledge of those limits and the expected concentration of the elements in the glass. For example, while cadmium (advanced element) is likely to be a “difficult” element for some HLW tanks, chromium (slow/irregular element) is not. Furthermore, the TCLP behavior of elements that were not included in the present data set can be inferred based on their chemical characteristics. Thus, while beryllium was not included in the data set, it is very likely to behave as an advanced element, in that its normalized release from a given glass, and therefore its TCLP concentration, can be reliably estimated from the normalized boron release for that glass. In addition, a simple bounding model based on the advanced elements may be adequate for some purposes.

6 TCLP Response Models

The Vitreous State Laboratory of the Catholic University of America has conducted a series of experiments with glass formulation and TCLP leachate concentration in order to assess the performance of glass from a RCRA perspective (Gan and Pegg 2002). While only the concentrations of RCRA metals are routinely measured in the TCLP, the data used in the present work also included all of the major glass constituents. The inclusion of these elements provides valuable information on the way in which the glass dissolves under TCLP conditions. It should be noted that the use of sodium in the prescribed TCLP buffer solution precludes the determination of sodium release from the glass. After the TCLP, the leachate was analyzed by direct coupled plasma atomic emissions spectroscopy (DCP-AES). DCP-AES is a robust and proven analytical technique that often requires less dilution than its counterpart, inductively coupled plasma-atomic emissions spectroscopy (ICP-AES). Findings from this work have shown a correlation between glass formulae (sum of waste and contributions from glass-forming chemicals) and TCLP leachate concentration.

The previous grouping of constituents into “advanced”, “retarded”, and “slow/irregular” elements, based on their TCLP release rates, suggest a correlation that can be incorporated into models which can be used to predict glass TCLP performance, and assess the potential performance of a theoretical glass. The simple correlation observed between the normalized elemental TCLP releases for elements of advanced and retarded elements suggest that the TCLP leaching process for these glass elements is an apparent zero order kinetic process.

Disregarding solution saturation effects, the important factor for model development becomes the rate constant for the leaching reaction, and its dependence on the glass composition. It is reasonable to argue that the dissolution of the major glass constituents would have a significant impact on the release rate of the generally much-less-concentrated RCRA elements. For example, the dissolution of B^{3+} , a major component of the borosilicate network, is likely to be necessary for access to and continued release of minor elements. Conversely, higher concentrations of relatively insoluble components, such as Al and Fe, would likely tend to hinder that process. Furthermore, a more highly polymerized network (more bridging oxygen) is expected to dissolve more slowly than a less polymerized network (less bridging oxygen); the ratio of alkali to silica provides a simplistic measure of this effect. Finally, it is reasonable to say that the concentration of an element in solution would be proportional to its concentration in the glass, and to the amount of glass reacted, hence the relationships between the normalized releases.

Research to date has been used to define the “matrix partial dissolution” (MPS) parameter to quantify the inter-element relationships described in the discussion above. The MPS_i can be computed for each element i , and reflects the following:

- dependence on the dissolution of boron as a major structural component
- inhibiting effect of less-soluble components, specifically Al and Fe
- the dependence on the extent of polymerization of the glass matrix
- the observed consistency between the normalized releases

In contrast to boron, the other two major trivalent cations in the waste glasses, Al^{3+} and Fe^{3+} , in spite of their similar structural roles (they tend to reside in tetrahedral sites co-polymerized with silica as boron would), dissolve little, with no clear sign of correlation to B (boron) in the leachate. Therefore, the ratio of boron to the sum of the three trivalent cations (R_B) is one factor of MPS. The second factor is the ratio

of the total alkali to silica ($R_{M/Si}$), which is a measure of the extent of polymerization of the glass. The third factor of MPS_i is simply the concentration of element i in the glass (X_i). Thus, MPS is defined as (constituents are in weight percent):

$$MPS_i = R_B R_{M/Si} X_i$$

$$R_B = \left[\frac{B_2O_3 / 0.7}{B_2O_3 / 0.7 + Al_2O_3 + Fe_2O_3 / 1.6} \right]$$

$$R_{M/Si} = \left[\frac{0.67 \times K_2O + Na_2O + 2 \times Li_2O}{SiO_2} \right]$$

Such that,

$$MPS_i = R_B R_{M/Si} X_i = \left[\frac{(B_2O_3 / 0.7) \times (0.67 \times K_2O + Na_2O + 2 \times Li_2O)}{(B_2O_3 / 0.7 + Al_2O_3 + Fe_2O_3 / 1.6) \times SiO_2} \right] \times X_i$$

If, over the 18 hour duration of the TCLP, a simple zeroth-order rate equation with rate constant K is assumed for the reaction of glass with surface area A , with a large volume of solution V , then the rate of change of the concentration of element i in the solution is:

$$\frac{dC_i}{dt} = K \frac{A}{V}$$

Over the specified TCLP time interval (Δt), the logarithm of the change in the TCLP leachate concentration of element i is then given by:

$$\ln \Delta C_i = -\ln\left(\frac{V}{A\Delta t}\right) + \ln K = -\ln\left(\frac{V}{A\Delta t}\right) + \ln K_0 + \frac{E}{RT}$$

where the rate constant K is assumed, as is typically the case, to follow an Arrhenius dependence on the absolute temperature T , and is a function of the activation energy, E . Since it is often the case that energetic terms are roughly additive with respect to the contributions of the constituents of the glass, the activation energy term and the logarithm of the pre-exponential term, (which can be viewed as the limiting case of the energy term), can be approximated by a function of the glass composition $f(X_1, X_2, \dots, X_n)$:

$$\ln \Delta C_i = M + f(X_1, X_2, \dots, X_n),$$

where M is a combination of constants.

Researchers established a simple monotonic dependence of $\ln \Delta C_i$ on the MPS_i parameter. Because of the non-linear nature of that simple monotonic dependence, a second-order polynomial in MPS is used to describe the TCLP release. (It should be noted that the adoption of a second-order equation is not inconsistent with the assumption of a zeroth-order rate equation since the latter relates to the dependence

of the rate on the leachate concentration, whereas the former relates to the dependence of the rate constant on the glass composition.) Consequently, the function $f(X_1, X_2, \dots, X_n)$ is expressed as:

$$f(X_1, X_2, \dots, X_n) = B + d_1 \text{MPS} + d_2 \text{MPS}^2$$

and

$$B = \sum_i b_i X_i$$

where a linear composition dependence is assumed for variable B to account for the variation in the TCLP release/percent weight oxide correlation that is not accounted for by the MPS parameter. For each constituent, a coefficient (b) is determined by linear regression, and is multiplied by the percent oxide (by weight, X) of the corresponding constituent. The quantity $b_i X_i$ is summed for all constituents to determine B. Note that B is a variable in this equation, and is not the amount of boron. The final form of the model is then:

$$\ln \Delta C_i = M + \sum_i b_i X_i + d_1 \text{MPS} + d_2 \text{MPS}^2$$

where M, b_i , and d_i are parameters to be determined by multiple linear regression, since this equation is linear in its parameters. This model is described in full detail in *Proceedings of the International Symposium on Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries VII*, "Effect of Glass Composition on the Leaching Behavior of HLW Glasses Under TCLP Conditions," (Gan and Pegg 2002). The final WTP models may differ slightly in form from this model. Modeling efforts are still underway.

In order to meet delisting limits, the above can be summarized. Essentially, for each constituent, the estimated release, plus the allowance for uncertainties, must be less than the delisting limit. The uncertainties are discussed in sections 6 and 7 of this document. For evaluation of the TCLP leaching versus the delisting levels, the leaching can be summarized as the:

- Release = % in glass × Normalized release

while

- % in glass = % in waste × waste loading × retention.

Waste loading is the amount of waste versus the total glass formers and composition. The retention includes a factor for the likelihood of the material to be retained in the glass, versus moving into the gas phase. Volatile compounds or elements, such as mercury, that may be lost due to their volatility, will have less retention, and will result in the appearance of release; however, the release is not into the leachate, but into the air above the melter.

As previously discussed, the release rate can be assessed relative to the release of boron. Table 1-3 of this DQO shows the waste tank or envelope, glass formulation, and the normalized release rate based on boron.

The relative release rate can then be used to estimate the constituent of potential concern (COPC) oxide levels that would be allowed in the glass before the delisting level would be exceeded based on TCLP leaching. The following formula shows the calculation of the COPC oxide level.

$$\text{COPC Oxide Level} = \text{Delisting Level} / [(\text{Group Rate})(\text{Norm. B Rate})(\text{Oxide Factor})]$$

Figure C-3 shows the weight percent oxide that could be allowed in the glass before delisting levels using TCLP were exceeded. The data are presented based on three different release rates, 0.2 ppm/wt%, 2 ppm/wt%, and 20 ppm/wt%. It is evident that less beryllium, cadmium, and mercury can be allowed in the glass before the leachate concentration potential exceeds delisting levels.

Based on the rates in Figure C-3, the rate of 0.2ppm/wt% (light grey bar) represents the HLW glass, and the LAW glass is represented by rates between 2 and 20 ppm/wt% (dark grey and white bars).

7 References

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Figure C-1 Three Dimensional Network of Glass Modifiers and Formers

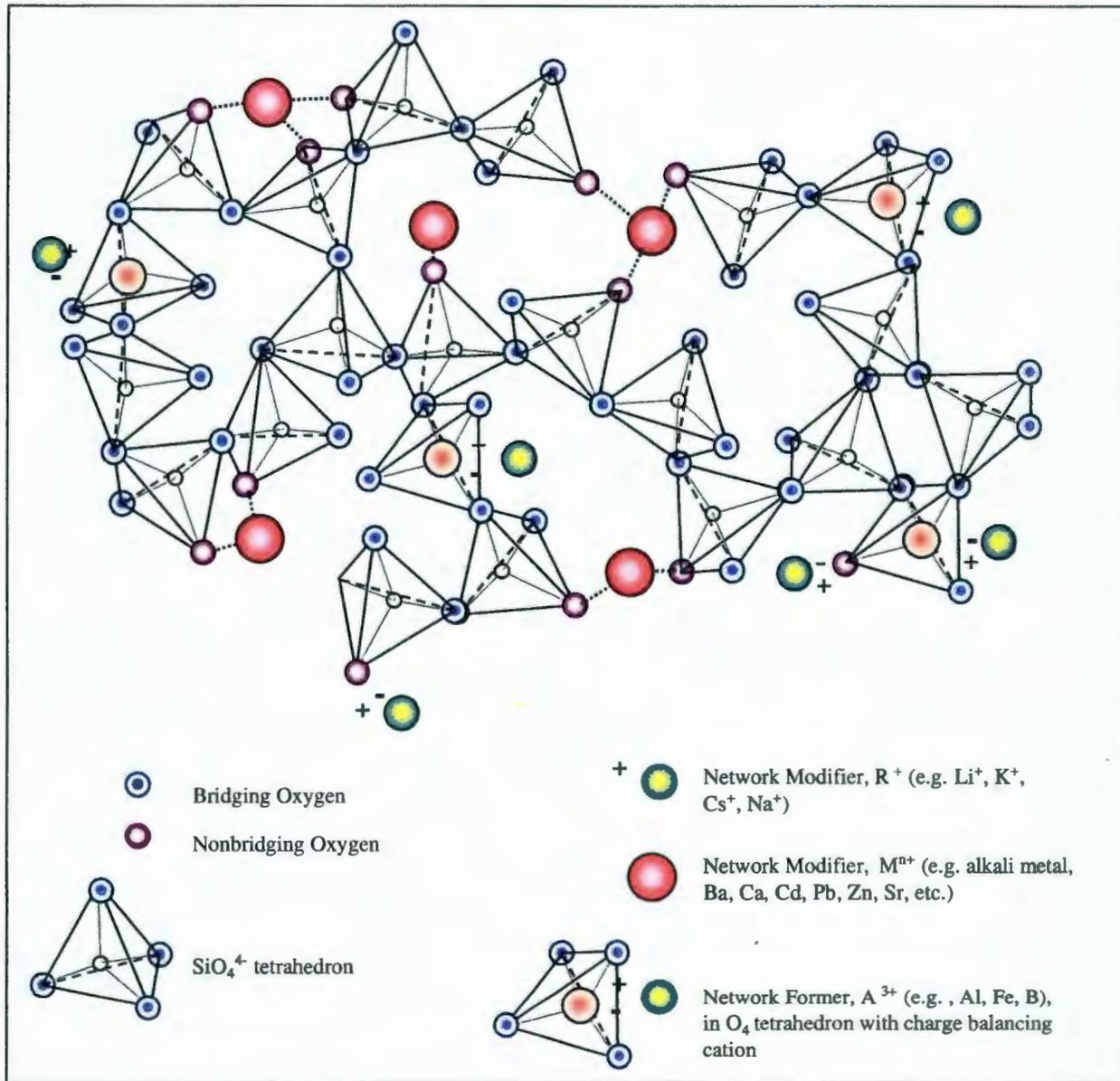
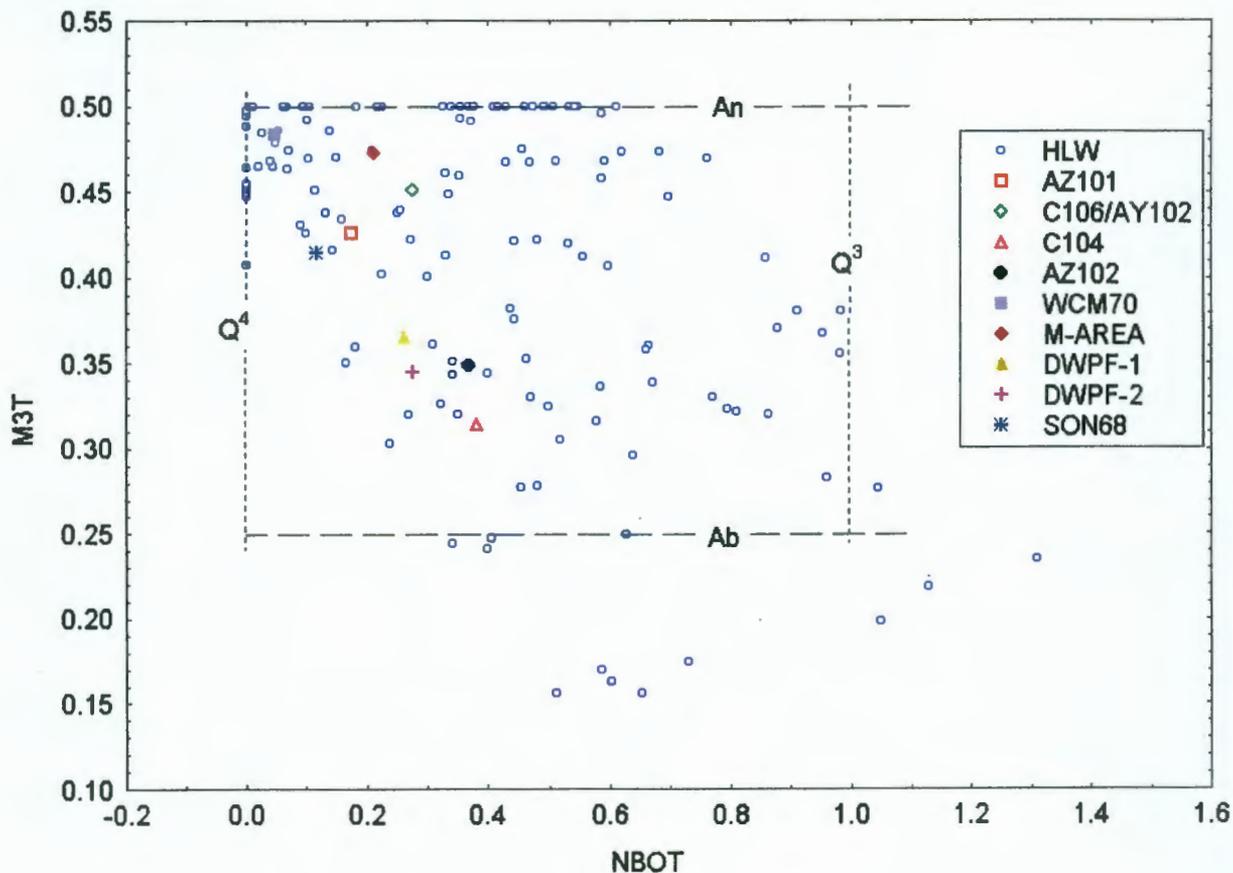


Figure C-2 HLW Glass Distribution



M3T = Fraction, on average, of network tetrahedral sites occupied by trivalent cations

NBOT = Average number of non-bridging oxygens per network forming tetrahedral site

HLW = Hypothetical glass (statistically developed composition)

AZ-101, AZ-102, Present reference formulations for the WTP
 C-106/AY-102,
 C-104 =

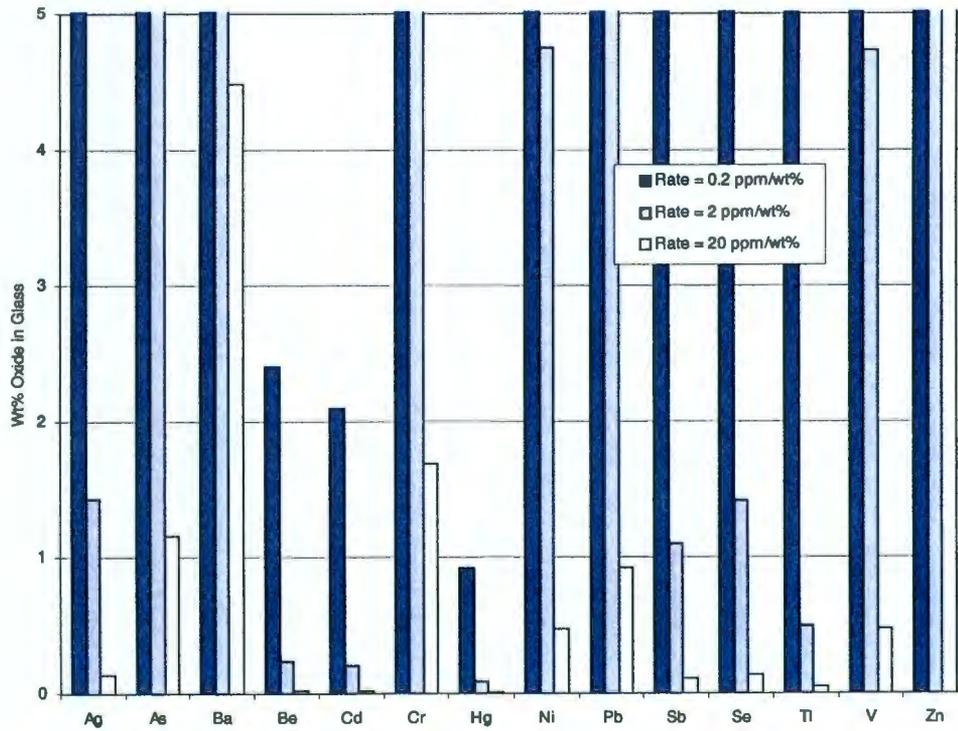
WCM70 = Glass formulation that was used at the West Valley Demonstration Project (WVDP) to produce about 500 metric tonnes of HLW glass

M-Area = Glass formulation for M-Area mixed waste vitrification facility at the Savannah River site, which produced about 1000 metric tonnes of glass

DWPF-1, DWPF-2 = The "Batch 1" and "Batch 2" formulations developed for vitrification of HLW at the Savannah River site

SON68 = glass formulation used for HLW vitrification in the French AVM/AVH process

Figure C-3 COPC Oxide Content in Glass to Exceed Delisting Level



Appendix D

LDR and Delisting COPC Selection

Appendix D

LDR and Delisting COPC Selection

This appendix contains the tables referenced in step 3 of the DQO that contain information regarding selection of organic and inorganic COPCs for delisting and LDR.

Tables

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Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
100-01-6	4-Nitroaniline					X	X			X
100-02-7	4-Nitrophenol					X	X			X
100-21-0	p-Phthalic acid						X			X
100-25-4	1, 4-Dinitrobenzene						X			X
100-41-4	Ethyl benzene						X	X	X	
100-42-5	Styrene							X		
100-44-7	Benzyl chloride					X				
10061-01-5	cis-1, 3-Dichloropropene						X			X
10061-02-6	trans-1, 3-Dichloropropene					X	X			X
100-75-4	N-Nitrosopiperidine					X	X			X
10102-43-9	Nitric oxide					X				
10102-44-0	Nitrogen dioxide					X				
10102-45-1	Thallium(I) nitrate					X				
101-14-4	4, 4'-Methylenebis (2-chloroaniline)						X			
101-27-9	Barban					X	X			X
101-55-3	4-Bromophenylphenyl ether					X	X			X
1024-57-3	Heptachlor Epoxide					X	X			X
1024-57-D	Heptachlor epoxide isomers	X	Heptaclor Epoxide	1024-57-3		X				
1031-07-8	Endosulfan Sulfate						X			X
103-85-5	Phenylthiourea					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
105-67-9	2, 4-Dimethylphenol					X	X			X
10595-95-6	N-Nitrosomethylethylamine					X	X			X
10605-21-7	Carbenzadim					X	X			X
106-44-5	4-Methylphenol (p-Cresol)	X	Cresols (total)	1319-77-3			X	X		X
106-46-7	1, 4-Dichlorobenzene					X	X	X		X
106-47-8	4-Chloroaniline					X	X			X
106-49-0	p-Toluidine					X				
106-51-4	p-Benzoquinone					X				
106-89-8	Epichlorohydrin					X				
106-93-4	Ethylene dibromide					X	X			X
107-02-8	Acrolein					X	X			X
107-05-1	3-Chloropropene						X			X
107-06-2	1, 2-Dichloroethane					X	X	X	X	X
107-10-8	n-Propylamine					X				
107-12-0	Propionitrile					X	X			X
107-13-1	Acrylonitrile					X	X			X
107-18-6	2-Propen-1-ol					X				
107-19-7	Propargyl alcohol					X				
107-20-0	Chloroacetaldehyde					X				
107-30-2	Chloromethyl methyl ether					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
107-49-3	Tetraethyl pyrophosphate					X				
108-10-1	4-Methyl-2-pentanone (MIBK)						X		X	X
108-31-6	Maleic anhydride (2, 5-Furandione)					X				
108-39-4	m-Cresol	X	Cresols (total)	1319-77-3			X	X		X
108-46-3	Resorcinol (1, 3-Benzenediol)					X				
108-60-1	Bis(2-Chloroisopropyl) ether					X				
108-88-3	Toluene					X	X		X	X
108-90-7	Chlorobenzene					X	X	X	X	X
108-94-1	Cyclohexanone						X		X	X
108-95-2	Phenol					X	X			X
108-98-5	Thiophenol					X				
109-06-8	2-Methylpyridine					X				
109-77-3	Malononitrile					X				
110-75-8	2-Chloroethyl vinyl ether					X	X			X
110-80-5	2-Ethoxyethanol					X			X	
110-86-1	Pyridine					X	X	X	X	X
111-44-4	Bis(2-chloroethyl) ether					X	X			X
1114-71-2	Pebulate					X	X			X
111-54-6	Ethylenebisdithiocarbamic acid					X				
1116-54-7	N-Nitrosodiethanolamine					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
111-91-1	Bis(2-Chloroethoxy)methane					X	X			X
1120-71-4	1, 3-Propane sultone					X				
1129-41-5	Metolcarb (3-methylcholanthrene)					X	X			X
1134-23-2	Cycloate					X				
114-26-1	Propoxur					X	X			X
115-02-6	Azaserine					X				
115-29-7	Endosulfan					X				
11-54-6D	Ethylenebisdithiocarbamic acid, salts and esters	X	Ethylenebisdithiocarbamic acid	111-54-6		X				
116-06-3	Aldicarb					X				
117-81-7	Bis(2-ethylhexyl) phthalate					X	X			X
117-84-0	Di-n-octylphthalate					X	X			X
118-74-1	Hexachlorobenzene					X	X	X		X
118-79-6	2, 4, 6-Tribromophenol					X	X			X
119-38-0	Isolan					X				
119-90-4	3, 3'-Dimethoxybenzidine					X				
119-93-7	3, 3'-Dimethylbenzidine.					X				
120-12-7	Anthracene						X			X
12039-52-0	Thallium selenite					X				
120-54-7	Bis(pentamethylene)-thiuram tetrasulfide					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
120-58-1	Isosafrole					X	X			X
120-82-1	1, 2, 4-Trichlorobenzene					X	X			X
120-83-2	2, 4-Dichlorophenol					X	X			X
121-14-2	2, 4-Dinitrotoluene					X	X	X	X	X
121-44-8	Triethylamine					X	X			X
122-09-8	alpha,alpha-Dimethylphenethylamine					X				
122-39-4	N, N-Diphenylamine					X	X			X
122-42-9	Propham					X	X			X
122-66-7	1, 2-Diphenylhydrazine					X	X			X
123-33-1	Maleic hydrazide					X				
123-63-7	Paraldehyde					X				
123-91-1	1, 4-Dioxane					X	X			X
124-48-1	Dibromochloromethane						X			X
126-68-1	O,O,O-Triethyl phosphorothioate					X				
126-72-7	Tris(2, 3-dibromopropyl) phosphate					X	X			X
126-85-2	Nitrogen mustard N-oxide					X				
126-85-D	Nitrogen mustard, N-oxide, HCL salt	X	Nitrogen mustard N-oxide	126-85-2		X				
126-98-7	2-Methyl-2-propenenitrile					X	X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
126-99-8	Chloroprene					X	X			X
127-18-4	1, 1, 2, 2-Tetrachloroethene					X	X	X	X	X
128-03-0	Potassium dimethyldithiocarbamate					X				
128-04-1	Sodium dimethyldithiocarbamate					X				
129-00-0	Pyrene						X			X
130-15-4	1, 4-Naphthoquinone					X				
1303-28-2	Arsenic pentoxide					X				
131-11-3	Dimethyl phthalate					X	X			X
1314-32-5	Thallic oxide					X				
1314-62-1	Vanadium pentoxide					X				
1314-84-7	Zinc phosphide					X				
131-52-2	Sodium pentachlorophenate					X				
131-89-5	2-Cyclohexyl-4, 6- dinitrophenol					X				
1319-77-3	Cresol polymers	X	Cresols (total)	1319-77-3		X		X	X	
13256-22-9	N-Nitrososarcosine					X				
1327-53-3	Arsenic trioxide					X				
1330-20-7	Xylene	X	Xylene (total)	1330-20-7			X		X	X
1335-32-6	Lead subacetate					X				
1336-36-3	Polychlorinated biphenyls (PCBs)						X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
1336-36-D	Polychlorinated biphenyls (total PCBs), N.O.S.	X	Polychlorinated biphenyls (PCBs)	1336-36-3	X	X				
1338-23-4	Methyl ethyl ketone peroxide					X				
134-32-7	alpha-Naphthylamine					X				
13463-39-3	Nickel carbonyl					X				
136-30-1	Sodium dibutyldithiocarbamate					X				
137-26-8	Thiram					X				
137-29-1	Copper dimethyldithiocarbamate					X				
137-30-4	Ziram					X				
137-41-7	Potassium n-methyldithiocarbamate					X				
137-42-8	Metam Sodium					X				
13765-19-0	Calcium chromate					X				
1402-68-2	Aflatoxins					X				
140-57-8	Aramite					X	X			X
141-78-6	Acetic acid ethyl ester						X		X	X
14324-55-1	Ethyl ziram					X				
143-33-9	Sodium cyanide					X				
143-50-0	Kepon					X	X			X
144-34-3	Selenium, tetrakis (dimethyl-dithiocarbamate)					X				
14484-64-1	Ferbam					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
145-73-3	Endothall					X				
1464-53-5	1, 2, 3, 4-Diepoxybutane					X				
148-18-5	Sodium diethyldithiocarbamate					X				
148-82-3	Melphalan (alanine nitrogen mustard)					X				
14901-08-7	Cycasin					X				
151-50-8	Potassium cyanide					X				
151-56-4	Ethyleneimine					X				
152-16-9	Octamethylpyrophosphoramidate					X				
15339-36-3	Manganese dimethyldithiocarbamate					X				
1563-38-8	Carbofuran phenol					X	X			X
1563-66-2	Carbofuran					X	X			X
156-60-5	1, 2-trans-Dichloroethene					X	X			X
1615-80-1	N, N'-Diethylhydrazine					X				
1634-02-2	Tetrabutylthiuram disulfide					X				
1646-88-4	Aldicarb sulfone					X	X			X
16543-55-8	N-Nitrosonomnicotine					X				
16752-77-5	Methomyl					X	X			X
16984-48-8	Fluoride						X			X
1746-01-6	TCDD	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
17702-57-7	Formparanate					X				
17804-35-2	Benomyl					X	X			X
18496-25-8	Sulfide						X	X		X
18883-66-4	Streptozotocin					X				
1888-71-7	Hexachloropropylene					X	X			X
189-55-9	Dibenzo[a,i]pyrene					X				
189-64-0	Dibenzo[a,h]pyrene					X				
191-24-2	Benzo(ghi)perylene						X			X
192-65-4	Dibenzo[a,e]pyrene					X	X			X
1929-77-7	Vernolate					X	X			X
193-39-5	Indeno(1, 2, 3-cd)pyrene					X	X			X
194-59-2	7H-Dibenzo[c, g]carbazole					X				
2008-41-5	Butylate					X	X			X
2032-65-7	Methiocarb					X	X			X
205-82-3	Benzo[j]fluoranthene					X				
205-99-2	Benzo(b)fluoranthene					X	X			X
206-44-0	Fluoranthene					X	X			X
207-08-9	Benzo(k)fluoranthene					X	X			X
20816-12-0	Osmium tetroxide					X				
20830-81-3	Daunomycin					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
20859-73-8	Aluminum phosphide					X				
208-96-8	Acenaphthylene						X			X
218-01-9	Chrysene					X	X			X
2212-67-1	Molinate					X	X			X
224-42-0	Dibenz[a,j]acridine					X				
225-51-4	Benz[c]acridine					X				
226-36-8	Dibenz[a,h]acridine					X				
22781-23-3	Bendiocarb					X	X			X
22961-82-6	Bendiocarb phenol					X				
2303-16-4	Diallate					X				
2303-17-5	Triallate					X	X			X
23135-22-0	Oxamyl					X	X			X
23422-53-9	Formetanate hydrochloride					X	X			X
23564-05-8	Thiophanate-methyl					X	X			X
23950-58-5	Pronamide					X	X			X
25154-54-5	Dinitrobenzene				X	X				
25265-76-3	Phenylenediamine					X				
25321-22-6	Dichlorobenzene				X	X				
25322-20-7	Tetrachloroethane				X	X				
25323-30-2	Dichloroethylene				X	X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
25376-45-8	Toluenediamine					X				
25567-55-9	2, 3, 4, 6-Tetrachlorophenol					X				
25735-29-9	Trichloropropane				X	X				
2631-37-0	Promecarb					X	X			X
26419-73-8	Tirpate					X				
26471-62-5	Toluene diisocyanate					X				
26545-73-3	Dichloropropanol				X	X				
26638-19-7	Dichloropropane				X	X				
26952-23-8	Dichloropropene				X	X				
2763-96-4	5-(Aminomethyl)-3-isoxazolol					X				
297-97-2	O,O-Diethyl O-pyrazinyl phosphoro- thioate					X				
298-00-0	Methyl parathion					X	X			X
298-02-2	Phorate					X	X			X
298-04-4	Disulfoton					X	X			X
301-04-2	Lead acetate					X				
302-01-2	Hydrazine					X				
303-34-4	Lasiocarpine					X				
30402-15-4D	Pentachlorodibenzofurans					X				
305-03-3	Chlorambucil					X				
30558-43-1	A2213					X				

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CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
309-00-2	Aldrin					X	X			X
311-45-5	Diethyl-p-nitrophenyl phosphate					X				
315-18-4	Mexacarbate					X	X			X
319-84-6	alpha-BHC						X			X
319-85-7	beta-BHC						X			X
319-86-8	delta-BHC						X			X
3288-58-2	o, o-Diethyl -S- methyl dithiophosphate					X				
33213-65-9	Endosulfan II						X			X
3424-82-6	o, p'-DDE (2, 4'-DDE)						X			X
34465-46-8D	Hexachlorodibenzo-p-dioxins					X				
353-50-4	Carbon oxyfluoride					X				
35576-91-1D	Nitrosamines				X	X				
357-57-3	Brucine					X				
36088-22-9D	Pentachlorodibenzo-p-dioxins	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X				
3689-24-5	Tetraethyldithiopyrophosphate (TEDP)					X				
37871-00-4D	Heptachlorodibenzo-p-dioxins	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X				
38998-75-3D	Heptachlorodibenzofurans	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
39196-18-4	Thiofanox					X				
39638-32-9	Bis(2-chloroisopropyl)ether						X			X
4170-30-3	2-Butenaldehyde					X				
41903-57-5	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)					X	X			
4549-40-0	N-Nitrosomethylvinylamine					X				
460-19-5	Cyanogen					X				
465-73-6	Isodrin					X	X			X
492-80-8	Auramine					X				
494-03-1	Chlomaphazin					X				
496-72-0	Toluene-3, 4-diamine					X				
50-00-0	Formaldehyde					X				
50-07-7	Mitomycin C					X				
50-18-0	Cyclophosphamide					X				
50-29-3	4, 4-DDT					X	X			X
50-32-8	Benzo(a)pyrene					X	X			X
504-24-5	4-Aminopyridine					X				
50-55-5	Reserpine					X				
505-60-2	Mustard gas					X				
506-61-6	Potassium silver cyanide					X				
506-64-9	Silver cyanide					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
506-68-3	Cyanogen bromide					X				
506-77-4	Cyanogen chloride					X				
509-14-8	Tetranitromethane					X				
510-15-6	Chlorobenzilate					X	X			X
51026-28-9	Potassium hydroxymethyl-n-methyl-dithiocarbamate					X				
51-28-5	2, 4-Dinitrophenol					X	X			X
51-43-4	Epinephrine					X				
51-52-5	Propylthiouracil					X				
51-75-2	Nitrogen mustard					X				
51-75-D	Nitrogen mustard, HCL salt	X	Nitrogen mustard	51-75-2		X				
51-79-6	Ethyl carbamate (urethane)					X				
52-24-4	Tris(1-aziridinyl)phosphine sulfide					X				
52-85-7	Famphur					X	X			X
52888-80-9	Prosulfocarb					X	X			X
53-19-0	o, p'-DDD (2, 4'-DDD)						X			X
533-74-4	Dazomet					X				
5344-82-1	1-(o-Chlorophenyl)thiourea					X				
534-52-1	4, 6-Dinitro-o-cresol					X	X			X
534-52-D	4, 6-Dinitro-o-cresol salts	X	4,6-Dinitro-o-cresol	534-52-1		X				

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CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
53535-27-6	2, 3, 4, 6-Tetrachlorophenol, potassium salt					X				
53-70-3	Dibenz[a,h]anthracene					X	X			X
53-96-3	2-Acetylaminofluorene					X	X			X
540-73-8	1, 2-Dimethylhydrazine					X				
54-11-5	Nicotine					X				
54-11-D	Nicotine salts	X	Nicotine	54-11-5		X				
541-53-7	Dithiobiuret, syb 2, 4-Dithiobiuret					X				
541-73-1	1, 3-Dichlorobenzene					X	X			X
542-62-1	Barium cyanide					X				
542-75-6	1, 3-Dichloropropene					X				
542-76-7	3-Chloropropionitrile					X				
542-88-1	Dichloromethyl ether					X				
544-92-3	Copper cyanide					X				
55-18-5	N-Nitrosodiethylamine					X	X			X
55285-14-8	Carbosulfan					X	X			X
55406-53-6	3-Iodo-2-propynyl n-butylcarbamate					X				
55-63-0	Nitroglycerin					X				
55684-94-1D	Hexachlorodibenzofurans	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
557-19-7	Nickel cyanide					X				
557-21-1	Zinc cyanide					X				
55-91-4	Diisopropylfluorophosphate (DFP)					X				
56-04-2	Methylthiouracil					X				
56-23-5	Carbon tetrachloride					X	X	X	X	X
563-68-8	Thallium(I) acetate					X				
56-38-2	Parathion					X	X			X
56-49-5	3-Methylcholanthrene					X	X			X
56-53-1	Diethylstilbesterol					X				
56-55-3	Benzo(a)anthracene					X	X			X
57-12-5	Cyanide						X			X
57-12-5a	Cyanide (amenable)	X	Cyanide	57-12-5			X			X
57-12-5D	Cyanides (soluble salts and complexes)	X	Cyanide	57-12-5	X	X				
57-14-7	1, 1-Dimethylhydrazine					X				
57-24-9	Strychnine					X				
57-24-D	Strychnine salts	X	Strychnine	57-24-9		X				
57-47-6	Physostigmine					X	X			X
57-64-7	Physostigmine salicylate					X	X			X
57-74-9	Chlordane (Alpha and Gamma)					X	X	X		X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
57-97-6	7, 12-Dimethylbenz[a]anthracene					X				
58-89-9	gamma-BHC (Lindane)					X	X		X	X
58-90-2	2, 3, 4, 6-Tetrachlorophenol					X	X			X
591-08-2	1-Acetyl-2-thiourea					X				
592-01-8	Calcium cyanide					X				
59-50-7	4-Chloro-3-methylphenol					X	X			X
5952-26-1	Diethylene glycol, dicarbamate					X				
59669-26-0	Thiodicarb					X	X			X
598-31-2	Bromoacetone					X				
59-89-2	N-Nitrosomorpholine					X	X			X
60-11-7	p-Dimethylaminoazobenzene					X	X			X
60-29-7	Ethyl ether						X		X	X
60-34-4	Methylhydrazine					X				
60-51-5	Dimethoate					X				
60-57-1	Dieldrin					X	X			X
606-20-2	2, 6-Dinitrotoluene					X	X			X
608-93-5	Pentachlorobenzene					X	X			X
615-53-2	N-Nitroso-N-methylurethane					X				
61-82-5	Amitrole					X				
621-64-7	N-Nitroso-di-n-propylamine					X	X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
62-38-4	Phenylmercury acetate					X				
62-44-2	Phenacetin					X	X			X
624-83-9	Methyl isocyanate					X				
62-50-0	Ethyl methanesulfonate					X				
62-53-3	Aniline					X	X			X
62-55-5	Thioacetamide (Ethanethioamide)					X				
62-56-6	Thiourea					X				
62-74-8	Fluoroacetic acid, sodium salt (Fratol)					X				
62-75-9	N-Nitroso-N, N-dimethylamine					X	X			X
628-86-4	Mercury fulminate					X				
630-10-4	Selenourea					X				
630-20-6	1, 1, 1, 2-Tetrachloroethane					X	X			X
63-25-2	Carbaryl					X	X			X
6358-53-8	Citrus red No. 2					X				
636-21-5	o-Toluidine hydrochloride					X				
64-00-6	m-Cumenyl methylcarbamate					X	X			X
640-19-7	Fluoroacetamide					X				
64-18-6	Formic acid					X				
644-64-4	Dimetilan					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
6533-73-9	Thallium(I) carbonate					X				
66-27-3	Methyl methanesulfonate					X	X			X
66-75-1	Uracil mustard					X				
67-56-1	Methyl alcohol						X		X	X
67-64-1	2-Propanone (Acetone)						X		X	X
67-66-3	Chloroform					X	X	X	X	X
67-72-1	Hexachloroethane					X	X	X	X	X
684-93-5	N-Nitroso-N-methylurea					X				
692-42-2	Diethylarsine					X				
696-28-6	Dichlorophenylarsine					X				
70-25-7	MNNG (N-Methyl-N'-nitro- N-nitrosoguanidine)					X				
70-30-4	Hexachlorophene					X				
71-36-3	n-Butanol						X		X	X
71-43-2	Benzene					X	X	X	X	X
71-55-6	1, 1, 1-Trichloroethane					X	X		X	X
72-20-8	Endrin					X	X	X		X
72-20-D	Endrin metabolites	X	Endrin	72-20-8		X				
72-43-5	Methoxychlor					X	X	X		X
72-54-8	4, 4-DDD					X	X			X
72-55-9	4, 4-DDE					X	X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
72-57-1	Trypan blue					X				
7421-93-4	Endrin aldehyde						X			X
7439-92-1	Lead					X	X	X	X	X
7439-92-1D	Lead compounds	X	Lead	7439-92-1	X	X				
7439-97-6	Mercury					X	X	X	X	X
7439-97-D	Mercury compounds	X	Mercury	7439-97-6	X	X				
7440-02-0	Nickel					X	X	X		X
7440-02-0C	Nickel compounds	X	Nickel	7440-02-0	X	X				
7440-22-4	Silver					X	X	X	X	X
7440-22-4Db	Silver compounds	X	Silver	7440-22-4	X	X				
7440-28-0	Thallium					X	X			X
7440-28-D	Thallium compounds	X	Thallium	7440-28-0	X	X				
7440-36-0	Antimony					X	X			X
7440-36-D	Antimony compounds	X	Antimony	7440-36-0	X	X				
7440-38-2	Arsenic					X	X	X	X	X
7440-38-D	Arsenic compounds	X	Arsenic	7440-38-2	X	X				
7440-39-3	Barium					X	X	X	X	X
7440-39-3Db	Barium compounds	X	Barium	7440-39-3	X	X				
7440-41-7	Beryllium					X	X			X
7440-41-D	Beryllium compounds, N.O.S.	X	Beryllium	7440-41-7	X	X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
7440-43-9	Cadmium					X	X	X	X	X
7440-43-D	Cadmium compounds	X	Cadmium	7440-43-9	X	X				
7440-47-3	Chromium					X	X	X	X	X
7440-47-3Dd	Chromium compounds	X	Chromium	7440-47-3	X	X				
7440-62-2	Vanadium						X			X
7440-66-6	Zinc						X			X
7446-18-6	Thallium(I) sulfate					X				
7446-27-7	Lead phosphate					X				
74-83-9	Bromomethane					X	X			X
74-87-3	Chloromethane					X	X			X
74-88-4	Iodomethane					X	X			X
7488-56-4	Selenium sulfide					X				
74-90-8	Hydrogen cyanide					X				
74-93-1	Thiomethanol					X				
74-95-3	Dibromomethane					X	X			X
75-00-3	Chloroethane						X			X
75-01-4	1-Chloroethene					X	X	X	X	X
75-05-8	Acetonitrile					X	X			X
75-09-2	Dichloromethane (Methylene Chloride)					X	X		X	X
75-15-0	Carbon disulfide					X	X		X	X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
75-21-8	Oxirane					X	X			X
75-25-2	Tribromomethane					X	X			X
75-27-4	Bromodichloromethane						X			X
75-34-3	1, 1-Dichloroethane					X	X			X
75-35-4	1, 1-Dichloroethene					X	X	X	X	X
75-36-5	Acetyl chloride					X				
75-44-5	Phosgene					X				
75-55-8	2-Methylaziridine					X				
75-60-5	Cacodylic acid					X				
75-69-4	Trichlorofluoromethane					X	X		X	X
75-70-7	Trichloromethanethiol					X				
75-71-8	Dichlorodifluoromethane					X	X			X
757-58-4	Hexaethyl tetraphosphate					X				
75-86-5	2-Methylacetonitrile					X				
75-87-6	Chloral					X				
759-73-9	N-Nitroso-N-ethylurea					X				
759-94-4	EPTC					X	X			X
76-01-7	Pentachloroethane					X	X			X
76-13-1	1, 2, 2-Trichlorotrifluoroethane (Freon 113)						X		X	X
764-41-0	1, 4-Dichloro-2-butene					X				

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
76-44-8	Heptachlor					X	X	X		X
765-34-4	Glycidylaldehyde					X				
7664-39-3	Hydrogen fluoride					X				
77-47-4	Hexachlorocyclopentadiene					X	X			X
77-78-1	Dimethyl sulfate					X				
7778-39-4	Arsenic acid					X				
7782-41-4	Fluorine					X				
7782-49-2	Selenium					X	X	X	X	X
7783-00-8	Selenium dioxide					X				
7783-06-4	Hydrogen sulfide					X				
7791-12-0	Thallium(1) chloride					X				
78-00-2	Tetraethyl lead					X				
7803-51-2	Phosphine					X				
7803-55-6	Ammonium vanadate					X				
78-59-1	Isophorone							X		
78-83-1	2-Methylpropyl alcohol					X	X		X	X
78-87-5	1, 2-Dichloropropane					X	X			X
789-02-6	o, p'-DDT (2,4'-DDT)						X			X
78-93-3	2-Butanone (Methyl ethyl ketone)					X	X	X	X	X
79-00-5	1, 1, 2-Trichloroethane					X	X		X	X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
79-01-6	1, 1, 2-Trichloroethylene					X	X	X	X	X
79-06-1	Acrylamide					X	X			X
79-19-6	Thiosemicarbazide					X				
79-22-1	Methyl chlorocarbonate					X				
79-34-5	1, 1, 2, 2-Tetrachloroethane					X	X			X
79-44-7	Dimethylcarbamoyl chloride					X				
79-46-9	2-Nitropropane					X			X	
7978-73-6	Potassium pentachlorophenate					X				
8001-35-2	Toxaphene					X	X	X		X
8001-58-9	Creosote	X	Cresols (total)	1319-77-3		X				
8007-45-2	Coal tar creosote	X	Cresols (total)	1319-77-3		X				
80-62-6	Methyl methacrylate					X	X			X
81-07-2	Saccharin					X				
81-07-D	Saccharin salts	X	Saccharin	81-07-2		X				
81-81-2	Warfarin (>0.3%)					X				
81-81-2a	Warfarin (<0.3 %)	X	Warfarin	81-81-2		X				
81-81-D	Warfarin Salt (<0.3 %)	X	Warfarin	81-81-2		X				
81-81-Da	Warfarin Salt (>0.3 %)	X	Warfarin	81-81-2		X				
823-40-5	Toluene-2, 6-diamine					X				
82-68-8	Pentachloronitrobenzene (PCNB)					X	X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
83-32-9	Acenaphthene						X			X
84-66-2	Diethyl phthalate					X	X			X
84-74-2	Di-n-butylphthalate					X	X			X
85-01-8	Phenanthrene						X			X
85-44-9	Phthalic anhydride					X	X			X
85-68-7	Butylbenzylphthalate					X	X			X
86-30-6	N-Nitrosodiphenylamine						X			X
86-73-7	Fluorene						X			X
86-88-4	alpha-Naphthylthiourea					X				
87-65-0	2, 6-Dichlorophenol					X	X			X
87-68-3	Hexachlorobutadiene					X	X	X	X	X
87-86-5	Pentachlorophenol					X	X	X		X
88-06-2	2, 4, 6-Trichlorophenol					X	X	X		X
88-74-4	2-Nitroaniline						X			X
88-75-5	2-Nitrophenol						X			X
88-85-7	2-sec-Butyl-4, 6-dinitrophenol; syn Dinoseb					X	X			X
91-20-3	Naphthalene					X	X			X
91-58-7	2-Chloronaphthalene					X	X			X
91-59-8	2-Naphthylamine					X	X			X
91-80-5	Methapyrilene					X	X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
91-94-1	3, 3 -Dichlorobenzidine					X				
924-16-3	N-Nitrosodi-n-butylamine					X	X			X
92-67-1	4-Aminobiphenyl					X	X			X
92-87-5	Benzidine					X				
930-55-2	N-Nitrosopyrrolidine					X	X			X
93-72-1	Silvex (2, 4, 5-TP)					X	X	X		X
93-76-5	2, 4, 5-T					X	X			X
94-58-6	Dihydrosafrole					X				
94-59-7	Safrole					X	X			X
94-75-7	2, 4-D					X	X	X		X
94-75-D	2, 4-D, salts and esters	X	2, 4-D	94-75-7		X				
95-06-7	Sulfallate					X				
95-48-7	o-Cresol	X	Cresols (total)	1319-77-3			X	X		X
95-50-1	1, 2-Dichlorobenzene					X	X		X	X
95-53-4	o-Toluidine (2-methylaniline)					X				
95-57-8	2-Chlorophenol					X	X			X
95-80-7	Toluene-2, 4-diamine					X				
95-94-3	1, 2, 4, 5-Tetrachlorobenzene					X	X			X
95-95-4	2, 4, 5-Trichlorophenol					X	X	X	X	X
959-98-8	Endosulfan I						X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
96-12-8	1, 2-Dibromo-3-chloropropane					X	X			X
96-18-4	1, 2, 3-Trichloropropane					X	X			X
96-45-7	Ethylenethiourea					X				
97-63-2	Ethyl methacrylate					X	X			X
97-74-5	Tetrabutylthiuram monosulfide					X				
97-77-8	Disulfiram					X				
98-05-5	Benzeneearsonic acid					X				
98-07-7	Benzotrichloride					X				
98-86-2	Acetophenone					X	X			X
98-87-3	Benzal chloride					X	X			X
98-95-3	Nitrobenzene					X	X	X	X	X
99-35-4	1, 3, 5-Trinitrobenzene					X				
99-55-8	5-Nitro-o-toluidine					X	X			X
HCFC	Chlorinated fluorocarbons	X	1,2,2-Trichlorotrifluoroethane (Freon 113)	76-13-1	X	X			X	
HxCDDs	HxCDDs (All Hexachlorodibenzo-p-dioxins)	X	Tetrachlorodibenzo-p-dioxin (2,3,7,8-)	41903-57-5			X			X
HxCDFs	HxCDFs (All Hexachlorodibenzofurans)	X	Tetrachlorodibenzo-p-dioxin (2,3,7,8-)	41903-57-5			X			X
I132	Selenium compounds	X	Selenium	7782-49-2	X	X				
I189	Dithiocarbamates (total)	X	Sodium dimethyldithiocarbamate	128-04-1			X			X

Table D-1 Starting List of Initial COPCs Considered for Delisting and LDR, and Substitutions for Isomer/NOS and Addition of PCBs

CAS#	Constituent	Substitution?	With What?	CAS# of What	NOS	Appendix VIII	UTS	EPA 530/R-93/007	DST Part A	UHC
NA10	Chlorinated benzenes	X	1,2,4-Trichlorobenzene	120-82-1	X	X				
NA15	Chlorinated phenol	X	4-Chloro-3-methylphenol	59-50-7	X	X				
NA36	Halomethanes	X	Chloromethane	74-87-3	X	X				
NA37	Chlorinated ethanes	X	1, 2-Dichloroethane	107-06-2	X	X				
NA5	Chloroalkyl ethers	X	Bis(2-chloroethyl) ether	111-44-4	X	X				
NA8	Chlorinated naphthalene	X	2-Chloronaphthalene	91-58-7	X	X				
O&G	Oil and Grease							X		
PeCDDs	PeCDDs (All Pentachlorodibenzo-p-dioxins)	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5			X			X
PeCDFs	PeCDFs (All Pentachlorodibenzofurans)	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5			X			X
TCDDs	TCDDs (All Tetrachlorodibenzo-p-dioxins)	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X	X			X
TCDFs	TCDFs (All Tetrachlorodibenzofurans)	X	Tetrachlorodibenzo-p-dioxin (2, 3, 7, 8-)	41903-57-5		X	X			X
UN16	Phthalic acid esters	X	Bis(2-ethylhexyl) phthalate	117-81-7	X	X				

Footnote 1

Headers in this table are directly listed in Sections 3.1.1 and 3.1.2, Figures 3-2 and 3-5.

Text describes substitutions for isomers, dioxins/furans, Not Otherwise Specified (NOS) compounds classes and addition of PCBs. The following headers denote the regulatory lists from which the starting list of compounds originated: Appendix VIII, Universal Treatment Standards (UTS), Delisting EPA Delisting Guidance (EPA 530/R-93/007), Double Shell Tanks RCRA Part A Permit (DST Part A) and the Underlying Hazardous Constituents (UHC).

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/Mixture	Polymer
100-01-6	4-Nitroaniline	X								
100-44-7	Benzyl chloride	X								
100-75-4	N- Nitrosopiperidine	X								
101-14-4	4, 4'-Methylenebis (2-chloroaniline)	X								
101-27-9	Barban	X	X							
10595-95-6	N- Nitrosomethylethylamine	X								
10605-21-7	Carbenzadim	X	X							
106-47-8	4-Chloroaniline	X								
106-49-0	p-Toluidine	X								
106-51-4	p-Benzoquinone	X								
106-89-8	Epichlorohydrin	X					X			
107-19-7	Propargyl alcohol	X								
107-20-0	Chloroacetaldehyde	X								
107-30-2	Chloromethyl methyl ether	X								
107-49-3	Tetraethyl pyrophosphate	X								
108-31-6	Maleic anhydride (2, 5-Furandione)	X								
108-46-3	Resorcinol (1, 3-Benzenediol)	X								
108-98-5	Thiophenol	X								
110-80-5	2-Ethoxyethanol	X								
1114-71-2	Pebulate	X	X							

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/ Mixture	Polymer
1120-71-4	1, 3-Propane sultone	X								
114-26-1	Propoxur	X	X							
115-29-7	Endosulfan	X	X							
119-90-4	3, 3'-Dimethoxybenzidine	X			X					
119-93-7	3, 3'-Dimethylbenzidine.	X			X					
120-58-1	Isosafrole	X						X		
121-14-2	2, 4-Dinitrotoluene	X								
122-42-9	Propham	X	X							
126-72-7	Tris (2, 3-dibromopropyl) phosphate	X						X		
126-85-2	Nitrogen mustard N-oxide	X		X						
126-99-8	Chloroprene	X								
137-26-8	Thiram	X				X				
137-30-4	Ziram	X	X							
140-57-8	Aramite	X	X							
143-50-0	Kepone	X	X							
14484-64-1	Ferbam	X	X							
151-56-4	Ethyleneimine	X								
1563-38-8	Carbofuran phenol	X	X							
1563-66-2	Carbofuran	X	X							
1615-80-1	N, N'-Diethylhydrazine	X								
1646-88-4	Aldicarb sulfone	X								

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/ Mixture	Polymer
16752-77-5	Methomyl	X	X							
17804-35-2	Benomyl	X	X							
1888-71-7	Hexachloropropylene	X								
1929-77-7	Vernolate	X	X							
2008-41-5	Butylate	X	X							
2032-65-7	Methiocarb	X	X							
2212-67-1	Molinate	X	X							
2303-17-5	Triallate	X	X							
23135-22-0	Oxamyl	X	X							
23564-05-8	Thiophanate-methyl	X	X							
23950-58-5	Pronamide	X	X							
2631-37-0	Promecarb	X	X							
298-00-0	Methyl parathion	X	X							
298-02-2	Phorate	X	X							
298-04-4	Disulfoton	X	X							
30558-43-1	A2213	X	X							
315-18-4	Mexacarbate	X	X							
3424-82-6	o, p'-DDE (2, 4'-DDE)	X	X							
3689-24-5	Tetraethyldithiopyrophosphate (TEDP)	X	X							
509-14-8	Tetranitromethane	X		X						
51-79-6	Ethyl carbamate (urethane)	X								
52-85-7	Famphur	X				X				

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/ Mixture	Polymer
53-19-0	o, p'-DDD (2, 4'-DDD)	X	X							
534-52-1	4, 6-Dinitro-o- cresol	X								
53-96-3	2- Acetylaminofluorene	X								
540-73-8	1, 2-Dimethylhydrazine	X								
54-11-5	Nicotine	X				X				
542-88-1	Dichloromethyl ether	X								
55-18-5	N-Nitrosodiethylamine	X								
55-63-0	Nitroglycerin	X		X						
56-38-2	Parathion	X	X							
57-24-9	Strychnine	X	X							
57-47-6	Physostigmine	X				X				
57-64-7	Physostigmine salicylate	X				X				
59669-26-0	Thiodicarb	X	X							
60-11-7	p- Dimethylaminoazobenze ne	X								
606-20-2	2,6-Dinitrotoluene	X			X					
608-93-5	Pentachlorobenzene	X								
615-53-2	N-Nitroso-N-methyluret hane	X								
61-82-5	Amitrole	X	X							
62-44-2	Phenacetin	X	X							
62-74-8	Fluoroacetic acid, sodium salt (Fratol)	X	X							
63-25-2	Carbaryl	X	X							

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/Mixture	Polymer
636-21-5	o-Toluidine hydrochloride	X			X					
66-27-3	Methyl methanesulfonate	X								
684-93-5	N-Nitroso-N-methylurea	X								
696-28-6	Dichlorophenylarsine	X								
74-88-4	Iodomethane	X								
74-93-1	Thiomethanol	X								
74-95-3	Dibromomethane	X								
759-73-9	N-Nitroso-N-ethylurea	X								
759-94-4	EPTC	X	X							
764-41-0	1,4-Dichloro-2-butene	X								
765-34-4	Glycidylaldehyde	X								
77-78-1	Dimethyl sulfate	X								
7782-41-4	Fluorine	X								
7803-51-2	Phosphine	X				X				
789-02-6	o,p'-DDT (2,4'-DDT)	X	X							
79-06-1	Acrylamide	X								
79-44-7	Dimethylcarbamoyl chloride	X								
79-46-9	2-Nitropropane	X								
80-62-6	Methyl methacrylate	X								
81-81-2	Warfarin	X	X							
85-44-9	Phthalic anhydride	X								
86-88-4	alpha-Naphthylthiourea	X								

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/ Mixture	Polymer
87-65-0	2, 6-Dichlorophenol	X								
91-80-5	Methapyrilene	X				X				
91-94-1	3, 3 -Dichlorobenzidine	X			X					
924-16-3	N-Nitrosodi-n-butylamine	X								
92-67-1	4-Aminobiphenyl	X								
92-87-5	Benzidine	X			X					
930-55-2	N-Nitrosopyrrolidine	X								
94-59-7	Safrole	X				X				
95-53-4	o-Toluidine (2-methylaniline)	X								
95-80-7	Toluene-2, 4-diamine	X								
95-94-3	1, 2, 4, 5-Tetrachlorobenzene	X								
96-18-4	1, 2, 3-Trichloropropane	X								
96-45-7	Ethylenethiourea	X								
97-63-2	Ethyl methacrylate	X								
97-77-8	Disulfiram					X				
98-07-7	Benzotrichloride	X								

Table D-2 Compounds Removed from Delisting Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent	Independent Review	Pesticide	Military	Dyestuff	Pharmaceutical	Solvent	Consumer	Group/Mixture	Polymer
98-87-3	Benzal chloride	X								
99-55-8	5-Nitro-o-toluidine	X								

Footnote 1

Compounds, headers in this table are from the Reg DQO, section 4.5.1 and Table B-15, Figure 4.3. A summary of the definition of the industrial use that resulted in removal of these compounds is listed below.

- Pesticide - Appendix II of the Reg. DQO provides detailed logic for the exclusion of these compounds. Examples of compounds potentially not used at Hanford are TEPP, (synonyms nifost; vapotone; tetron; killax)
- Military - This category includes compounds such as explosives and chemical war agents. Examples of compounds include nitrogen mustard N-oxide (CAS# 126-85-2) and nitroglycerin (CAS# 55-63-0).
- Dyestuff - This category includes compounds used in the fabrication of dyes or actual dyes used in all types of materials, food, textiles, etc. Examples of these compounds include xylydine (CAS# 1300-73-8) and o-Anisidine (CAS# 90-04-0).
- Pharmaceuticals - This category includes chemicals used in making pharmaceuticals. An example of a compound used in pharmaceuticals is safrole (CAS# 94-59-7).
- Solvent - This category includes solvents that were not used in Hanford processes. An example is epichlorohydrin (CAS# 106-89-8).
- Consumer - This category includes chemicals used in consumer products. An example is isosafrole (CAS# 120-58-1) used to manufacture Heliotropin; to modify oriental perfumes.
- Group/Mixtures - This category includes mixtures such as turpentine and asphalt.
- Polymers - This category includes chemicals used to make polymers such as neoprene and rubbers.

Table D-3 Compounds Removed from Delisting Based on Reg. DQO Stability Assessment

CAS#	Constituent
100-02-7	4-Nitrophenol
1024-57-3	Heptachlor Epoxide
1031-07-8	Endosulfan Sulfate
105-67-9	2, 4-Dimethylphenol
106-44-5	4-Methylphenol (p-Cresol)
108-60-1	Bis(2-Chloroisopropyl) ether
110-75-8	2-Chloroethyl vinyl ether
111-44-4	Bis(2-chloroethyl) ether
111-91-1	Bis(2-Chloroethoxy)methane
1129-41-5	Metolcarb (3-methylcholanthrene)
1134-23-2	Cycloate
119-38-0	Isolan
122-66-7	1, 2-Diphenylhydrazine
124-48-1	Dibromochloromethane
131-11-3	Dimethyl phthalate
1338-23-4	Methyl ethyl ketone peroxide
134-32-7	alpha-Naphthylamine
17702-57-7	Formparanate
22781-23-3	Bendiocarb
22961-82-6	Bendiocarb phenol
23422-53-9	Formetanate hydrochloride
26419-73-8	Tirpate
302-01-2	Hydrazine
33213-65-9	Endosulfan II
51-28-5	2, 4-Dinitrophenol
510-15-6	Chlorobenzilate
52888-80-9	Prosulfocarb
542-75-6	1, 3-Dichloropropene
55285-14-8	Carbosulfan
55406-53-6	3-Iodo-2-propynyl n-butylcarbamate
57-74-9	Chlordane (Alpha and Gamma)
5952-26-1	Diethylene glycol, dicarbamate

Table D-3 Compounds Removed from Delisting Based on Reg. DQO Stability Assessment

CAS#	Constituent
62-53-3	Aniline
64-00-6	m-Cumenyl methylcarbamate
644-64-4	Dimetilan
7421-93-4	Endrin aldehyde
75-25-2	Tribromomethane
76-01-7	Pentachloroethane
77-47-4	Hexachlorocyclopentadiene
78-59-1	Isophorone
86-30-6	N-Nitrosodiphenylamine
88-74-4	2-Nitroaniline
91-59-8	2-Naphthylamine
959-98-8	Endosulfan I
96-12-8	1, 2-Dibromo-3-chloropropane

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
100-25-4	1, 4-Dinitrobenzene	Reacts with hydroxyl radicals	http://ull.chemistry.uakron.edu/erd/chemicals/1001-1500/1325.html
103-85-5	Phenylthiourea	thiourea - reacts with oxidizers	Classic Organic Text
107-10-8	n-Propylamine	Amine - readily oxidizes	Classic Organic Text
107-18-6	2-Propen-1-ol	Alcohol - readily oxidizes	Classic Organic Text
108-94-1	Cyclohexanone	Ketone - reacts with hydroxide	Classic Organic Text
109-77-3	Malononitrile	Nitrile - reacts with hydroxide	Classic Organic Text
111-54-6	Ethylenebisdithiocarbamic acid	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
1116-54-7	N-Nitrosodiethanolamine	Alcohol - readily oxidizes	Classic Organic Text
115-02-6	Azaserine	Reacts with hydroxide	Classic Organic Text
116-06-3	Aldicarb	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian116-06-3.html
118-74-1	Hexachlorobenzene	Reacts with water, oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian118-74-1.html
118-79-6	2, 4, 6-Tribromophenol	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian118-79-6.html
120-54-7	Bis(pentamethylene)-thiuram tetrasulfide	Polysulfide - readily oxidizes	Classic Organic Text
121-44-8	Triethylamine	Amine - readily oxidizes	Classic Organic Text
123-33-1	Maleic hydrazide	Amine - readily oxidizes	Classic Organic Text
123-63-7	Paraldehyde	Aldehyde - readily oxidizes	Classic Organic Text
128-03-0	Potassium dimethyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
128-04-1	Sodium dimethyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
131-52-2	Sodium pentachlorophenate	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem8/Radian87-86-5.html
131-89-5	2-Cyclohexyl-4, 6-dinitrophenol	Reacts with hydroxyl radicals	http://www.speclab.com/compound/c131895.htm
136-30-1	Sodium dibutylthiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
137-29-1	Copper dimethyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
137-41-7	Potassium n-methyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
137-42-8	Metam Sodium	thiocarbamic acid - reacts with oxidizers	Classic Organic Text
1402-68-2	Aflatoxins	Oxidizes readily	Classic Organic Text
141-78-6	Acetic acid ethyl ester	Ester - reacts with hydroxide	Classic Organic Text
14324-55-1	Ethyl ziram	thiocarbamic acid -- reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian137-30-4.html
144-34-3	Selenium, tetrakis (dimethyl-dithiocarbamate)	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
145-73-3	Endothall	Decomposes in water	http://ace.ace.orst.edu/info/extoxnet/pips/endothal.htm
1464-53-5	1, 2, 3, 4-Diepoxybutane	Epoxide - Reacts with hydroxide	http://www.speclab.com/compound/c1464535.htm
148-18-5	Sodium diethyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
148-82-3	Melphalan (alanine nitrogen mustard)	Decomposes in water and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian148-82-3.html
14901-08-7	Cycasin	polyalcohol - reacts with oxidizers	Classic Organic Text
15339-36-3	Manganese dimethyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
1634-02-2 ^a	Tetrabutylthiuram disulfide	thiuram disulfide reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian137-26-8.html
16543-55-8	N-Nitrosomnicotine	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian16543-55-8.html
16984-48-5	Fluoride	No analysis	Logic presented in DQO for no analysis
18496-25-8	Sulfide	Oxidizes to sulfate in tanks	Classic Organic Text
18883-66-4	Streptozotocin	polyfunctional - alcohol, amide - reacts with oxidizers and hydroxide	Classic Organic Text
194-59-2	7H-Dibenzo[c,g]carbazole	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm1/Radian16543-55-8.html
20816-12-0	Osmium tetroxide	Not used at Hanford	Reg. DQO

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
20830-81-3	Daunomycin	alpha hydroxy ketone - reacts with oxidizers	Classic Organic Text
25154-54-5	Dinitrobenzene	Reacts with oxidizers and high alkaline environment	http://ull.chemistry.uakron.edu/erd/chemicals/1001-1500/1325.html , http://ull.chemistry.uakron.edu/erd/chemicals/501-1000/1000.html , http://ull.chemistry.uakron.edu/erd/chemicals/1001-1500/1324.html
25265-76-3	Phenylenediamine	Amine - readily oxidizes	Classic Organic Text
25321-22-6	Dichlorobenzene	Reacts with oxidizers	http://www.osha-slc.gov/SLTC/healthguidelines/p-dichlorobenzene/recognition.html
25322-20-7	Tetrachloroethane	Alkyl halide - reacts with hydroxide	Classic Organic Text
25323-30-2	Dichloroethylene	Reacts with oxidizers	http://www.osha-slc.gov/SLTC/healthguidelines/1_2-dichloroethylene/recognition.html#storage
25376-45-8	Toluenediamine	Amine - readily oxidizes	Classic Organic Text
25735-29-9	Trichloropropane	Alkyl halide - reacts with hydroxide	Classic Organic Text
26471-62-5	Toluene diisocyanate	isocyanate - reacts with hydroxide	Classic Organic Text
26545-73-3	Dichloropropanol	Alcohol - readily oxidizes	Classic Organic Text
26638-19-7	Dichloropropane	Alkyl halide - reacts with hydroxide	Classic Organic Text
2763-96-4	5-(Aminomethyl)-3-isoxazolol	Bifunctional - alcohol & amine - readily oxidizes	Classic Organic Text
303-34-4	Lasiocarpine	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem3/Radian303-34-4.html
305-03-3	Chlorambucil	Oxidizes readily	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem3/Radian305-03-3.html
309-00-2	Aldrin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm3/Radian309-00-2.html
311-45-5	Diethyl-p-nitrophenyl phosphate	phosphate ester - reacts with hydroxide	Classic Organic Text
3288-58-2	o, o-Diethyl -S- methyl dithiophosphate	phosphate ester - reacts with hydroxide	Classic Organic Text
353-50-4	Carbon oxyfluoride	inorganic compound, instantly hydrolyzes in	Merck Index 12th Ed.

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
		water	
35576-91-1D	Nitrosamines	Reacts with oxidizers	Classic Organic Text
357-57-3	Brucine	Reacts with oxidizers	http://ull.chemistry.uakron.edu/erd/chemicals/2001-2500/2066.html
39196-18-4	Thiofanox	polyfunctional - amine, amide, thioether -- reacts with oxidizers and hydroxide	Classic Organic Text
39638-32-9	Bis (2-chloroisopropyl)ether	Reacts with oxidizers	toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/BAAAAairD:l:cpp
4170-30-3	2-Butenaldehyde	Aldehyde - readily oxidizes	Classic Organic Text
4549-40-0	N-Nitrosomethylvinylamine	volatile - b. p. 47;	Classic Organic Text
460-19-5	Cyanogen	inorganic compound, reacts with oxidizers, degrades in melter	See Section 3.1.1 of DQO
494-03-1	Chlornaphazin	Oxidizes readily	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem9/Radian494-03-1.html
496-72-0	Toluene-3, 4-diamine	Amine -- readily oxidizes	Classic Organic Text
50-00-0	Formaldehyde	volatile; oxidizes	Classic Organic Text
50-07-7	Mitomycin C	Reacts readily with oxidizing agents and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem5/Radian50-07-7.html
50-18-0	Cyclophosphamide	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm5/Radian50-18-0.html
50-29-3	4, 4-DDT	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm5/Radian50-29-3.html
504-24-5	4-Aminopyridine	Amine -- readily oxidizes	Classic Organic Text
505-60-2	Mustard gas	oxidation under alkaline conditions	Classic Organic Text
506-68-3	Cyanogen bromide	inorganic compound, reacts with oxidizers, degrades in melter	See Section 3.1.1 of DQO
506-77-4	Cyanogen chloride	inorganic compound, reacts with oxidizers, degrades in melter	See Section 3.1.1 of DQO

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
51026-28-9	Potassium hydroxymethyl-n-methyl-dithiocarbamate	Thiocarbamate -- unstable with oxidizing agents	Classic Organic Text
51-43-4	Epinephrine	Reacts with oxidizers and hydroxide	Reacts with oxidizers and hydroxide
51-52-5	Propylthiouracil	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem5/Radian51-52-5.html
51-75-2	Nitrogen mustard	tertiary amine reacts with nucleophiles and/or including hydroxides	Classic Organic Text - nucleophilic substitution reaction
52-24-4	Tris(1-aziridinyl)phosphine sulfide	Decomposes in water	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem5/Radian52-24-4.html
533-74-4	Dazomet	Decomposes in water	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem5/Radian533-74-4.html
5344-82-1	1-(o-Chlorophenyl)thiourea	Reacts with hydroxyl radicals	http://www.speclab.com/compound/c5344821.htm
541-53-7	Dithiobiuret, syb 2,4-Dithiobiuret	thioamide -- reacts with hydroxide	Classic Organic Text
542-76-7	3-Chloropropionitrile	Nitrile -- reacts with hydroxide	Classic Organic Text
55-91-4	Diisopropylfluorophosphate (DFP)	phosphate ester - reacts with hydroxide	Classic Organic Text
56-04-2	Methylthiouracil	Reacts with oxidizing agents	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem5/Radian56-04-2.html
56-53-1	Diethylstilbesterol	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem5/Radian56-53-1.html
57-14-7	1, 1-Dimethylhydrazine	Reacts with oxidizers	http://ull.chemistry.uakron.edu/erd/chemicals/1-500/0153.html
591-08-2	1-Acetyl-2-thiourea	Reacts with hydroxide	http://www.speclab.com/compound/c591082.htm
598-31-2	Bromoacetone	Ketone -- reacts with hydroxide	Classic Organic Text
60-29-7	Ethyl ether	volatile	Classic Organic Text
60-34-4	Methylhydrazine	Amine -- readily oxidizes	Classic Organic Text
60-57-1	Dieldrin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm6/Radian60-57-1.html

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
62-38-4	Phenylmercury acetate	Organomercury compound - hydrolyzes with hydroxide	
62-50-0	Ethyl methanesulfonate	thiocarbamic - reacts with oxidizers	www.physchem.ox.ac.uk/MSDS/ET/ethyl_methanesulfonate.html
62-55-5	Thioacetamide (Ethanethioamide)	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem6/Radian62-55-5.html
62-56-6	Thiourea	thiourea -- reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm6/Radian62-56-6.html
630-10-4	Selenourea	Reacts with water & oxidizers	Classic Organic Text
640-19-7	Fluoroacetamide	Amide -- reacts with hydroxide	Classic Organic Text
66-75-1	Uracil mustard	Amide -- Reacts with hydroxide	Classic Organic Text
67-56-1	Methyl alcohol	Volatile; Alcohol - readily oxidizes	Classic Organic Text
692-42-2	Diethylarsine	Arsine -- reacts with base	Classic Organic Text
70-25-7	MNNG (N-Methyl-N'-nitro-N-nitrosoguanidine)	Reacts with hydroxides and with oxidizing agents	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem7/Radian70-25-7.html
71-36-3	n-Butanol	Alcohol - readily oxidizes	Classic Organic Text
72-20-8	Endrin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian72-20-8.html
72-43-5	Methoxychlor	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian72-43-5.html
72-54-8	4,4-DDD	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem7/Radian72-54-8.html
72-55-9	4,4-DDE	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem7/Radian72-55-9.html
72-57-1	Trypan blue	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem7/Radian72-57-1.html
75-21-8	Oxirane	reacts with hydroxides and water	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem7/Radian75-21-8.html

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
75-36-5	Acetyl chloride	Acid chloride -- Decomposes in water and hydroxide	Classic Organic Text
75-44-5	Phosgene	Reacts with water	Classic Organic Text
75-55-8	2-Methylaziridine	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian75-55-8.html
75-60-5	Cacodylic acid	Arsine oxide -- readily oxidized at high pH	Classic Organic Text
75-70-7	Trichloromethanethiol	Thiol -- readily oxidized	Classic Organic Text
757-58-4	Hexaethyl tetraphosphate	phosphate ester - reacts with hydroxide	Classic Organic Text
75-86-5	2-Methylactonitrile	Reacts with oxidizers	http://www.state.nj.us/health/eoh/rtkweb/0007.pdf
75-87-6	Chloral	Aldehyde - readily oxidizes	Classic Organic Text
76-13-1	1,2,2-Trichlorotrifluoroethane (Freon 113)	Volatile, b.p. 48 °C	Classic Organic Text
76-44-8	Heptachlor	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian76-44-8.html
7664-39-3	Hydrogen fluoride	no analysis	Logic presented in DQO for no analyses
7783-06-4	Hydrogen sulfide	Oxidizes to sulfate in tanks	Classic Organic Text
78-00-2	Tetraethyl lead	reacts with hydroxide	Classic Organic Text
79-19-6	Thiosemicarbazide	amine -- reacts with oxidizers	Classic Organic Text
79-22-1	Methyl chlorocarbonate	Acid chloride -- Decomposes in water and hydroxide	Classic Organic Text
7978-73-6	Potassium pentachlorophenate	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem8/Radian87-86-5.html
8001-35-2	Toxaphene	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem8/Radian8001-35-2.html
81-07-2	Saccharin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem8/Radian81-07-2.html
81-81-D	Warfarin Salt (<0.3%)	Reacts with oxidizers and hydroxide	http://www.state.nj.us/health/eoh/rtkweb/2012.pdf

Table D-4 Compounds From Delisting Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
823-40-5	Toluene-2,6-diamine	Amine -- readily oxidizes	Classic Organic Text
87-86-5	Pentachlorophenol	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem8/Radian87-86-5.html
93-76-5	2,4,5-T	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem9/Radian93-76-5.html
94-58-6	Dihydrosafrole	Parent compound (safrole) reacts with oxidizers	http://www.state.nj.us/health/eoh/rtkweb/1642.pdf
94-75-7	2,4-D	Decomposes in water; oxidizes readily	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem9/Radian94-75-7.html
95-06-7	Sulfallate	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem9/Radian95-06-7.html
97-74-5 ^b	Tetramethylthiuram monosulfide	thiuram monosulfide reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NTP_Chem1/Radian137-26-8.html
O&G	Oil and Grease	Petroleum analysis does not apply	

a - Appendix VIII lists the common name and chemical abstract name. The CAS# in the regulation does not match either name. The CAS# 137-26-8 matches the chemical abstract name and is used here.

b - This compound is excluded due to properties similar to tetramethylthiuram monosulfide.

Table D-5 Compounds Removed from LDR Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent
100-01-6	4-Nitroaniline
100-75-4	N-Nitrosopiperidine
101-14-4	4, 4'-Methylenebis(2-chloroaniline)
101-27-9	Barban
10595-95-6	N-Nitrosomethylethylamine
106-47-8	4-Chloroaniline
10605-21-7	Carbendazim
110-80-5	2-Ethoxyethanol
1114-71-2	Pebulate
114-26-1	Propoxur
120-58-1	Isosafrole
121-14-2	2, 4-Dinitrotoluene
122-42-9	Propham
126-72-7	Tris(2, 3-dibromopropyl) phosphate
126-99-8	Chloroprene
140-57-8	Aramite
143-50-0	Kepone
1563-38-8	Carbofuran phenol
1563-66-2	Carbofuran
1646-88-4	Aldicarb sulfone
16752-77-5	Methomyl
17804-35-2	Benomyl
1888-71-7	Hexachloropropylene
1929-77-7	Vernolate
2008-41-5	Butylate
2032-65-7	Methiocarb
2212-67-1	Molinate
2303-17-5	Triallate
23135-22-0	Oxamy
23564-05-8	Thiophanate-methyl
23950-58-5	Pronamide

Table D-5 Compounds Removed from LDR Based on Reg. DQO Determination of Use Unrelated to Hanford

CAS#	Constituent
2631-37-0	Promecarb
298-00-0	Methyl parathion
298-02-2	Phorate
298-04-4	Disulfoton
315-18-4	Mexacarbate
3424-82-6	o, p'-DDE (2, 4'-DDE)
52-85-7	Famphur
53-19-0	o, p'-DDD (2, 4'-DDD)
53-96-3	2-Acetylaminofluorene
534-52-1	4, 6-Dinitro-o-cresol
55-18-5	N-Nitrosodiethylamine
56-38-2	Parathion
57-47-6	Physostigmine
57-64-7	Physostigmine salicylate
59669-26-0	Thiodicarb
60-11-7	p-Dimethylaminoazobenzene
606-20-2	2, 6-Dinitrotoluene
608-93-5	Pentachlorobenzene
62-44-2	Phenacetin
63-25-2	Carbaryl
66-27-3	Methyl methanesulfonate
74-88-4	Iodomethane
74-95-3	Dibromomethane
759-94-4	EPTC
789-02-6	o, p'-DDT (2, 4'-DDT)
79-06-1	Acrylamide
79-46-9	2-Nitropropane
80-62-6	Methyl methacrylate
85-44-9	Phthalic anhydride
87-65-0	2, 6-Dichlorophenol
91-80-5	Methapyrilene

**Table D-5 Compounds Removed from LDR Based on Reg. DQO Determination of Use
Unrelated to Hanford**

CAS#	Constituent
92-67-1	4-Aminobiphenyl
924-16-3	N-Nitrosodi-n-butylamine
930-55-2	N-Nitrosopyrrolidine
94-59-7	Safrole
95-94-3	1, 2, 4, 5-Tetrachlorobenzene
96-18-4	1, 2, 3-Trichloropropane
97-63-2	Ethyl methacrylate
98-87-3	Benzal chloride
99-55-8	5-Nitro-o-toluidine

Table D-6 Compounds Removed from LDR Based on Reg. DQO Stability Assessment

CAS#	Constituent
100-02-7	4-Nitrophenol
1024-57-3	Heptachlor Epoxide
1031-07-8	Endosulfan Sulfate
105-67-9	2, 4-Dimethylphenol
106-44-5	4-Methylphenol
110-75-8	2-Chloroethyl vinyl ether
111-44-4	Bis (2-chloroethyl) ether
111-91-1	Bis (2-Chloroethoxy)methane
1129-41-5	Metolcarb (3-methylcholanthrene)
122-66-7	1, 2-Diphenylhydrazine
124-48-1	Dibromochloromethane
131-11-3	Dimethyl phthalate
22781-23-3	Bendiocarb
23422-53-9	Formetanate hydrochloride
33213-65-9	Endosulfan II
510-15-6	Chlorobenzilate
51-28-5	2, 4-Dinitrophenol
52888-80-9	Prosulfocarb
55285-14-8	Carbosulfan
57-74-9	Chlordane (Alpha and Gamma)
62-53-3	Aniline
64-00-6	m-Cumenyl methylcarbamate
7421-93-4	Endrin aldehyde
75-25-2	Tribromomethane
76-01-7	Pentachloroethane
77-47-4	Hexachlorocyclopentadiene
86-30-6	N-Nitrosodiphenylamine
88-74-4	2-Nitroaniline
91-59-8	2-Naphthylamine
959-98-8	Endosulfan I
96-12-8	1, 2-Dibromo-3-chloropropane

Table D-7 Organic Compounds and Sulfide From LDR Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
100-25-4	1, 4-Dinitrobenzene	Reacts with hydroxyl radicals	http://ull.chemistry.uakron.edu/erd/chemicals/1001-15--/1325.html
108-94-1	Cyclohexanone	Ketone - reacts with hydroxide	Classic Organic Text
118-74-1	Hexachlorobenzene	Reacts with water, oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT_P_Chem1/Radian118-74-1.html
118-79-6	2, 4, 6-Tribromophenol	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT_P_Chem1/Radian118-79-6.html
121-44-8	Triethylamine	Amine - readily oxidizes	Classic Organic Text
128-04-1	Sodium dimethyldithiocarbamate	Thiocarbamate - unstable with oxidizing agents	Classic Organic Text
141-78-6	Acetic acid ethyl ester	Ester - reacts with hydroxide	Classic Organic Text
18496-25-8	Sulfide	Oxidizes to sulfate in tanks	Classic Organic Text
309-00-2	Aldrin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm3/Radian309-00-2.html
39638-32-9	Bis (2-chloroisopropyl)ether	Reacts with oxidizers	toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/BAAAAa.irD:1:cpp
50-29-3	4, 4-DDT	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm5/Radian50-29-3.html
60-29-7	Ethyl ether	volatile	Classic Organic Text
60-57-1	Dieldrin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm6/Radian60-57-1.html
67-56-1	Methyl alcohol	Volatile; Alcohol - readily oxidizes	Classic Organic Text
71-36-3	n-Butanol	Alcohol - readily oxidizes	Classic Organic Text
72-20-8	Endrin	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian72-20-8.html

Table D-7 Organic Compounds and Sulfide From LDR Not Assessed in Reg. DQO and Unstable in Tank Waste

CAS#	Constituent	Logic for Removal or Indication Compound is Stable	Basis for Instability Assessment
72-43-5	Methoxychlor	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian72-43-5.html
72-54-8	4, 4-DDD	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem7/Radian72-54-8.html
72-55-9	4, 4-DDE	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem7/Radian72-55-9.html
75-21-8	Oxirane	reacts with hydroxides and water	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem7/Radian75-21-8.html
76-13-1	1, 2, 2-Trichlorotrifluoroethane (Freon 113)	Volatile, b.p. 48 °C	Classic Organic Text
76-44-8	Heptachlor	Reacts with hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/Cehm7/Radian76-44-8.html
8001-35-2	Toxaphene	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem8/Radian8001-35-2.html
87-86-5	Pentachlorophenol	Reacts with oxidizers and hydroxide	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem8/Radian87-86-5.html
93-76-5	2, 4, 5-T	Reacts with oxidizers	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem9/Radian93-76-5.html
94-75-7	2, 4-D	Decomposes in water; oxidizes readily	http://ntp-server.niehs.nih.gov/htdocs/CHEM_H&S/NT P_Chem9/Radian94-75-7.html

Appendix E

General Statistical Model for Sample Size Computations

Appendix E

General Statistical Model for Sample Size Computations

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1 Data Analysis Cases

The following three data analysis cases were defined in DQO Step 7.

- Case 1: Experimental TCLP leachate results are analyzed for each glass composition individually and for a single COPC spiking level.
- Case 2: Experimental TCLP leachate results are analyzed for each glass composition individually with multiple COPC spiking levels.
- Case 3: Experimental TCLP leachate results are analyzed for multiple glass compositions simultaneously at multiple COPC spiking levels.

The purpose of Appendix E is to discuss the general statistical model that underlies all three cases, to demonstrate how the three cases are related, and to explain how upper confidence limit (UCL) estimates of the mean are generated for each case. In addition, the process for generating sample sizes for Cases 2 and 3 are discussed. (The generation of sample sizes for Case 1 is presented in Section 7.3.1.)

The common statistical model from which each of the three cases is derived is called the general linear model. The goal of the general linear model is to express an observed random variable, Y , in terms of the sum of a set of weighted predictors, X , plus the random error in Y . The form of the general linear model that is probably most familiar is Case 2, where there is only one predictor. This model is often referred to as simple linear regression. The theoretical equation for predicting Y_i from one predictor is:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

This is just the equation for a line where:

- Y_i = the i th observed value of the random variable Y
- β_0 = the true but unknown intercept of the line
- β_1 = the true but unknown slope of the line
- X_i = the i th value of the random variable X
- ε_i = the random error in Y_i

This equation expresses values of Y in terms of their linear relationship to values of one predictor, X . Case 3 is more complex because values of Y are expressed in terms of their linear relationship to many predictors. Case 1 is simpler because values of Y are not expressed in terms of their linear relationship to any predictor. They are simply expressed in terms of the arithmetic mean of the Y s.

2 General Linear Model - Theoretical Equation

Below is a brief discussion of the general linear model, from which all three cases are derived, and an explanation of how each case is a special version of the general linear model. Because of its complexity, the equation for the general linear model is best expressed in terms of matrix algebra. (This discussion

does not attempt to educate the reader in matrix algebra, but rather assumes a working knowledge of the topic.)

The same underlying statistical model can represent all the three cases. Case 3 is represented by the full general linear model, while Cases 1 and 2 are just simplified versions that result from the related experimental designs. For this DQO, consider the following model where:

- Y_i = the observable TCLP leachate values
- N = the number of observable TCLP leachate values
- X_i = the values of the glass predictor parameters (e.g. glass composition or spiked COPC concentration)
- $p-1$ = the number of glass predictor parameters

Expressed in terms of matrix algebra, the equation for the full general linear model (Case 3) is:

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\mathcal{E}}$$

where

$\underline{Y} = [y_1, y_2, \dots, y_N]$ is a column vector of length N of observable TCLP leachate values for a particular COPC.

\underline{X} is an $N \times p$ matrix of glass predictor parameters. For $i = 1, 2, \dots, N$, the i^{th} row of matrix \underline{X} is $[1, x_{i,1}, \dots, x_{i,p-1}]$ representing the levels of the $p-1$ constituents in the i^{th} glass sample.

$\underline{\beta} = [\beta_0, \beta_2, \dots, \beta_{p-1}]$ is a column vector of length p of regression coefficients or weights for the $p-1$ glass constituents.

$\underline{\mathcal{E}} = [\varepsilon_1, \varepsilon_2, \dots, \varepsilon_N]$ is a column vector of length N of errors associated with the TCLP leachate values. These errors are due to sources such as measurement error, inherent glass variability, or poor model fit.

(Note that throughout this appendix, the “ β ” used has no relation to the Type II error discussed in step 6 of the DQO.) A pictorial representation of this matrix equation looks like the following:

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$$

$$\begin{matrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \\ \dots \\ y_N \end{pmatrix} \\ N \times 1 \end{matrix} = \begin{matrix} \begin{pmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,p-1} \\ 1 & x_{2,1} & x_{2,2} & \dots & x_{2,p-1} \\ 1 & x_{3,1} & x_{3,2} & \dots & x_{3,p-1} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 1 & x_{N,1} & x_{N,2} & \dots & x_{N,p-1} \end{pmatrix} \\ N \times p \end{matrix} \times \begin{matrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \dots \\ \beta_{p-1} \end{pmatrix} \\ p \times 1 \end{matrix} + \begin{matrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \dots \\ \dots \\ \varepsilon_N \end{pmatrix} \\ N \times 1 \end{matrix}$$

3 General Linear Model - Upper Confidence Limit

Given such a linear model, the least squares is method used to derive estimates for the β_i parameters and the ε_i error terms. Then given a new, fixed glass composition $X_0 = [x_{0,1}, x_{0,2}, \dots, x_{0,p-1}]$ = a new row in the X matrix, a predicted value \hat{P}_0 is computed using the estimated β_i s.

Since this prediction has uncertainty associated with it, a UCL for the true underlying TCLP leachate mean for this glass composition X_0 is then given by:

$$\hat{P}_0 + t_{\alpha, N-p} s [X_0(X'X)^{-1}X_0']^{1/2} \tag{E1}$$

where s is the Root Mean Square Error (RMSE) and $t_{\alpha, N-p}$ is the $1-\alpha$ percentile of a Student-t distribution with $N-p$ degrees of freedom. \hat{P}_0 is the predicted value obtained from the functional form of the model using the values in X_0 and the estimated β_i s. It is of the form $\hat{P}_0 = \sum x_{0j} \hat{\beta}_{0j}$ where the sum is over $j = 1$ to p . How the three respective cases fit into this model is described in the following sections.

4 Case 1 - Theoretical Equation

Case 1: Experimental TCLP leachate results are analyzed for each glass composition individually and for a single COPC spiking level.

In Case 1 there are no predictors, so p is set to 1 (recall the number of predictors is $p-1$). So $p=1$ indicates that only the “intercept” - and not any predictors - are included in the model. The matrix X reduces to an $N \times 1$ matrix equal to $[1, 1, \dots, 1]$ and can be thought of as a “place holder” column for intercept. The weight of the “intercept” β_0 is μ (the mean of the Y s) since there is no information about a linear relationship between Y and any predictor variable. This means the prediction of Y values cannot be enhanced or refined by knowing that Y has a relationship to some other variable X . So each $y_i = \mu + \varepsilon_i$. In other words, when there is no other information available (such as the linear relationship between two variables), the best estimate or prediction of a random variable is the mean of the random variable. Under these conditions, the general linear model equation reduces to:

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \\ \dots \\ y_N \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \times (\mu) + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \dots \\ \dots \\ \varepsilon_N \end{pmatrix}$$

$N \times 1 \quad N \times 1 \quad 1 \times 1 \quad N \times 1$

4.1 Case 1 - Upper Confidence Limit

When estimating the population mean of the TCLP leachate values from sample data in Case 1 with no predictors, $N = n$ (the actual sample size), $p = 1$ with $\underline{\beta} = \mu$ (the mean of the Y s), and $\underline{X} = [1, 1, \dots, 1]$. Then $(\underline{X}'\underline{X})^{-1}$ in Expression E1 is equal to $1/n$, and the estimate of μ is the sample mean \bar{y} . Then for $X_0 = 1$, Expression E1 reduces to the usual $(1-\alpha)\%$ UCL for the mean where S , the RMSE, is the usual sample standard deviation:

$$\bar{y} + t_{\alpha, n-1} s/n^{1/2} \tag{E2}$$

Given the presentation of the general linear model above, it may seem unusual that the predicted TCLP leachate mean in Case 1 is expressed as \bar{y} , and is not expressed in terms of independent or predictor variables X . Recall that in Case 1, no predictor variables were used. In other words, TCLP leachate scores are not predicted on the basis of knowing anything about glass composition parameters. Reviewing the matrix form of the equation for Case 1, it can be seen that there are no values of X (glass parameter values) in this equation. The X matrix is simply a column of 1's. The 1's in the X matrix are weighted by μ , which is the mean of the Y scores. And the error scores are independent of the predictors. So, there are no values of the random variable X in this form of the equation. Given this consideration, the decision was made to write the expression for the UCL for Case 1 using \bar{y} . In Cases 2 and 3, however, the predicted TCLP leachate mean is expressed in terms of independent or predictor X values. The reason for this is that the TCLP leachate scores *are* being predicted on the basis of knowing the values for glass composition parameters in these two cases. Therefore, for instance, the predicted TCLP leachate mean in Case 2 is expressed as $(\hat{\beta}_0 + \hat{\beta}_1 x_0)$.

Note that increasing the number of samples tested can reduce the uncertainty associated with sample mean.

4.2 Case 1 - Definition Of α

Recall that α is the probability of rejecting the null hypothesis when it is in fact true. For this DQO, the null hypothesis is that the population mean is equal to or greater than the AL. In other words, the null

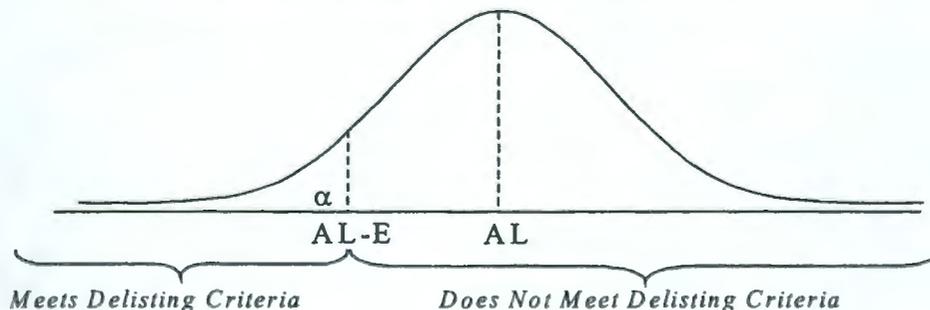
hypothesis states that the glass does not meet the delisting criteria. So making an α error means rejecting this initial assumption and mistakenly deciding that the glass does meet delisting criteria or that the population mean is less than the AL. Using upper confidence limits is a way to control or manage the probability of making this type of error.

The figure below is presented to illustrate how α is defined and requires a little explanation. The figure depicts a distribution of sample means. A sample mean is itself a random variable because different samples will yield different means. Therefore, it is theoretically possible to construct a distribution of all possible sample means (calculated from all possible samples) of some given size n . The figure represents such a distribution of sample means. In addition, the assumption is made here that the population mean is equal to the AL, which corresponds with the null hypothesis. Informally stated, the idea here is to see where the actual glass sample mean falls with respect to all possible sample means. Ideally, the mean would fall so far below the AL that there is convincing evidence to reject the null hypothesis that the population mean is above the AL.

To illustrate this graphically, let E represent the uncertainty around \bar{y} in Expression E2; that is, let $E = t_{\alpha, n-1} s/n^{1/2}$. In order to meet the criterion for delisting, the actual glass sample mean plus the uncertainty around it ($t_{\alpha, n-1} s/n^{1/2}$) must be less than the AL. This idea is illustrated in the figure below, which is the distribution of all possible means when the population mean is equal to the AL. Thinking graphically, if the true mean of the population is at the AL, then the sample mean must be at or below the AL by a distance of *at least* E in order for the delisting criteria to be met. This distance is marked as $AL-E$ on the figure below. The probability that a sample mean will fall below the $AL-E$ mark when the true mean of the population is at the AL is called α (in figure below, this is represented by the area in the left tail of curve, to the left of the $AL-E$ mark).

Whenever $\bar{y} < AL - E = AL - t_{\alpha, n-1} s/n^{1/2}$, the $UCL = \bar{y} + t_{\alpha, n-1} s/n^{1/2}$ will be less than AL, and the delisting criteria have been met as indicated on the figure. Whenever $\bar{y} > AL - E$, then $UCL > AL$, the delisting criteria will not be met.

**Distribution of Sample Mean when
 Population Mean is equal to the Action Level**



As illustrated on the curve, the probability $P[\bar{y} < AL - E] = P[\bar{y} < AL - t_{\alpha, n-1} s/n^{1/2}] = \alpha$. This explains why, when the underlying mean is in fact equal to the AL, and the confidence limit criterion is used, there is an α probability of mistakenly concluding the underlying glass qualifies for delisting ($\mu < AL$). For

true underlying mean value to the right of AL (that is, greater than the AL), there is an even smaller probability of incorrectly deciding the underlying glass qualifies for delisting. This was the motivation for selecting the UCL criteria for deciding whether glass qualifies for delisting. By so doing, the error of deciding a glass qualifies for delisting, when in fact it does not, is controlled to be less than α .

5 Case 2 - Theoretical Equation

Case 2: Experimental TCLP leachate results are analyzed for each glass composition individually with multiple COPC spiking levels.

Here $\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$, and, since there is only one predictor in this case, $p = 2$ with $\underline{\beta} = [\beta_0 \ \beta_1]$ with one weight for the intercept, β_0 , and another for the predictor, β_1 . The i_{th} row of the matrix \underline{X} is $[1, x_{i,1}]$. Assume there are “m” COPC spiking levels and “n” replicate glass samples tested per spiking level. This gives a total of $N = m \times n$ rows in the matrix \underline{X} . This equation is illustrated below.

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$$

$$\begin{matrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \dots \\ y_N \end{pmatrix} \\ N \times 1 \end{matrix} = \begin{matrix} \begin{pmatrix} 1 & x_{1,1} \\ 1 & x_{2,1} \\ 1 & x_{3,1} \\ \dots & \dots \\ 1 & x_{N,1} \end{pmatrix} \\ N \times 2 \end{matrix} \times \begin{matrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} \\ 2 \times 1 \end{matrix} + \begin{matrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \dots \\ \varepsilon_N \end{pmatrix} \\ N \times 1 \end{matrix}$$

This is the usual simple linear regression model with independent variable X and dependent variable Y. The least squares method generates a best-fit line to explain the relationship between X and Y. X represents the COPC spiking level in the glass and Y the TCLP leachate results.

5.1 Case 2 - Upper Confidence Limit

For a proposed COPC spiking level of interest, x_0 , the TCLP leachate upper confidence bound from Expression E1, reduces to:

$$(\hat{\beta}_0 + \hat{\beta}_1 x_0) + t_{\alpha, n-2} s/n^{1/2} [1/m + (x_0 - \bar{x})^2 / \sum (X_i - \bar{x})^2]^{1/2} \quad (E3)$$

Note that the uncertainty portion of this expression is minimized when $x_0 = \bar{x}$, in which case the uncertainty component, for a single spike level ($m=1$), is the same as in Expression E2 except for the decreased degrees of freedom for the t-distribution.

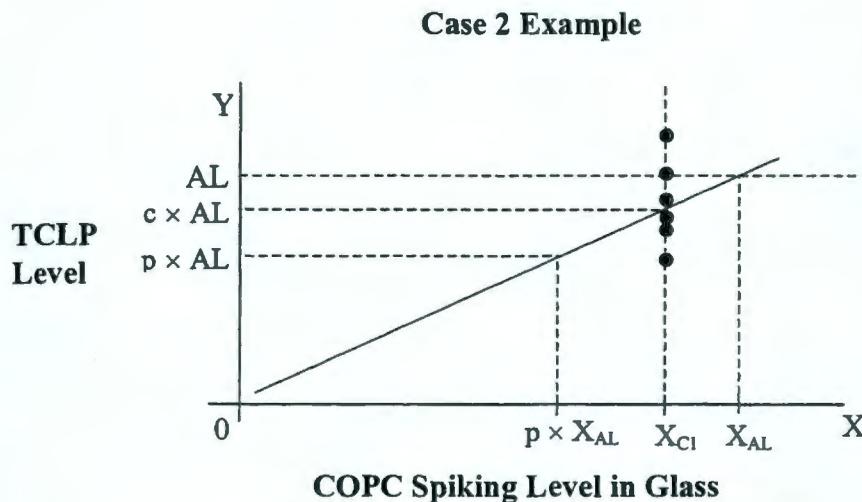
As in the first case, the uncertainty can be reduced, and the UCL decreased, by increasing the number of samples tested. In this case the number of COPC spiking levels (m) can be increased, or the number of

replications (n) at the spiking levels can be increased. Increasing the number of spiking levels (m) can reduce uncertainty by allowing a better model to be estimated as well as by reducing the replication uncertainty. If the range of spiking levels is sufficiently broad, it helps ensure a reasonable fit with the regression model. Increasing the number of replications (n) would reduce the impact of only the replication uncertainty.

5.2 Case 2 - Experimental Design And Sample Size

In order to illustrate how a Case 2 experimental design will be developed, consider the figure below. Recall that a Case 2 experimental design will be developed for COPCs that “fail” the Case 1 test. (See Section 7.3)

Assume that in Case 1, the TCLP leachate data obtained for a high spiking level X_{C1} (with a glass at the boundary conditions of the Glass Composition Region of Interest) is represented by the points in the following figure. Note that the indicated points are the resulting TCLP values that lead to a UCL value above or uncomfortably close to the AL.



The next step in developing a Case 2 experimental design is to decide where additional spiking levels should be set. One way to do this is to construct a line that connects the mean response for the data at X_{C1} to the origin. This line could be thought of as the potential regression line that might be generated if additional COPC spiking levels were used. Note that $c \times AL$, as indicated on the vertical axis, is the estimated TCLP leachate mean obtained when the COPC is spiked at level X_{C1} (the diagonal line then has slope $c \times AL / X_{C1}$ and $X_{AL} = X_{C1} / c$). Using the assumed diagonal line, X_{AL} is the spiking level that would generate TCLP leachate results with a mean approximately equal to the AL. (Note that for the particular example illustrated in the figure, c is less than 1.0. It could be the case that c is actually greater than 1.0, which would indicate the mean response at X_{C1} , is in fact larger than the AL. On the figure, X_{C1} would then be to the right of X_{AL} . The same discussion will still apply.)

Given such Case 1 results, an optimal experimental design consisting of “m” spiking levels and “n” samples per spiking level would then be sought to obtain the results illustrated in Figure 7-1 of Section 7. Note that data would already be available at the spiking level X_{C1} from Case 1. Therefore, $m - 1$ spiking levels need to be added. If $X_{C1} \geq X_{AL}$, it would be sufficient to consider X_{C1} as the largest spiking level.

If instead $X_{C1} < X_{AL}$, having one additional spiking level greater than X_{C1} could be considered, but it probably would still suffice to make X_{C1} the largest spiking level.

On the vertical axis, the point $p \times AL$ is the TCLP leachate level that represents the lower bound of the gray region (LBGR). This is the TCLP leachate where the β error probability is established. This would be the TCLP leachate mean located at the LBGR as described in Case 1. (If the 0.6 level proposed in Case 1 were still applied, p would equal 0.6). Given the assumed diagonal line, this mean TCLP leachate level would be achieved at the COPC level $p \times X_{AL}$ as indicated on the figure.

An experimental design for the additional spiking levels is now needed. Assume that the spiking levels will be equally spaced with the largest being X_{C1} and the smallest being some value X_{MIN} , a value that might depend on the particular COPC, its expected levels in glass, the observed and standard deviation of the Case 1 results, or other factors. Taking X_{MIN} to be one-third to one-half of the original spiking level X_{C1} might prove reasonable, but it will depend on the observed Case 1 results. Then given X_{MIN} and X_{C1} , $m - 2$ equally spaced spiking levels need to be added in between with n samples at each new spiking level to complete the design. The n samples would not be needed at the highest spiking level since the Case 1 results are already in hand. They would prove sufficient since n in Case 2 would certainly prove to be less than the value n used in Case 1.

Then for Case 2 sample size determinations, given...

- 1 $\alpha = 0.1, \beta = 0.2, LBGR = 0.6 \times AL$ (or $p = 0.6$);
- 2 The assumption of a zero regression intercept;
- 3 The observed Case 1 relative standard deviation;
- 4 The observed Case 1 mean, which generates the value c and the assumed diagonal line;
- 5 The particular spiking level selections in the experimental design strategy, such as that just proposed;

...optimum values for m and n could be derived.

Advance Case 2 sample size computations as part of this DQO report are not considered practical since so many more assumptions are needed than in Case 1. While the Case 1 sample size computations depend only on the specified parameters in item 1 above, and an assumed estimate of variability, in Case 2, items 2, 3, and 4 above are needed as well.

Recall that only marginal Case 1 failures would be considered in such a Case 2 scenario. Case 1 results that have average TCLP levels grossly larger than the AL , or those with extremely large variability, would more likely be addressed through Case 3 analyses. Given the marginal nature of the Case 1 failures, experience suggests that adding about 9 Case 2 samples to those already tested in Case 1 should be more than sufficient. This would give a total of 12-15 samples for Case 2. However, it should be understood that depending on the actual Case 1 results, an optimum sample size could be less than or slightly more than 12-15. However, if this computed sample size gets much larger than 12-15, then consideration needs to be given to moving to a Case 3 analysis.

6 Case 3 - Theoretical Equation and Upper Confidence Limit

Case 3: Experimental TCLP leachate results are analyzed for multiple glass compositions simultaneously at multiple COPC spiking levels.

Case 3 is represented by the full general linear model and can be thought of as just a more complex version of Case 2. There are now “k” glasses, “m” spiking levels, and “n” glass samples per glass/spiking level combination for a total of $N = k \times m \times n$. Since many more factors are considered influential, that is, spiking levels as well as other glass constituents, a many-dimensional space is involved. Thus a pictorial representation and closed form expression that does not rely on the given matrix notation are not possible. However, results are completely analogous with the UCL as previously given:

$$\hat{P}_0 + t_{\alpha, mk-p} s/n^{1/2} [X_0(X'X)^{-1}X_0']^{1/2} \quad (E4)$$

As in Case 2 where $X_0 = \bar{x}$ gives the minimum width confidence interval, the uncertainties here are again smaller for glasses and spiking levels within the region defined by the rows of the matrix X . Again uncertainties can be reduced by increasing the number of different glass compositions, the number spiking levels, or the number of replications at given glass composition/spiking level combinations. Increasing spiking levels (m) and glass composition (k) can again result in reduced uncertainties by improving the fit of the estimated model. Increasing the number of replications (n) would only reduce the impact of replication uncertainty.

6.1 Case 3 - Sample Size

Advance Case 3 sample size computations to meet required DQO optimization specifications would be even more complex and less practical than in Case 2. It would be necessary to make extremely limiting assumptions about Case 1, and possibly Case 2, analysis results and to make similarly limiting assumptions about the complex experimental designs that would then be needed. Instead, the DQO sample size optimization of k glasses, m spiking levels, with n samples each, will take place after Case 1 and/or Case 2 analyses are completed and initial experimental design considerations are made. Again, experience suggests that most decisions will be adequately supported by experimental designs involving about 40 to 60 glass samples. Typically larger numbers of glasses with minimal numbers of spiking levels and replications will be the optimal result.

Appendix F

Simulant Verification for Testing in Support of LDR/Delisting

Appendix F

Simulant Verification for Testing in Support of LDR/Delisting

Contents

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1 Simulant Requirements

As previously discussed, in order to minimize costs, as well as exposure of lab personnel to hazards, simulants will be used extensively for conducting experimental melts. Simulants are material designed to emulate specific types of chemical or physical behavior of real radioactive wastes. Simulated waste can be developed to exhibit only a limited set of important properties, or may be tailored to exhibit a broad range of properties.

Simulants used will likely have to represent both bounding conditions and nominal operating conditions. The simulants used will be based on the CRV contents as determined by the WTP process flowsheet model, with confirmation by comparison to pretreated samples. This is necessary because the actual pretreatment plant will not be online until after the petitioning process. Simulants used to test a process must expose the process limits. As such, it is important that each phenomenon in the process be understood, and how that phenomenon may become limiting under certain conditions. For compliance testing, it will be important for bounding conditions to be explored; that is, high spike levels must be used in conjunction with high sodium levels to ascertain the outer boundary of the QGCR.

Simulants will be required for both LAW and HLW for each of the sub-envelopes previously identified. Spikes will be added as necessary to create "bounding simulants" that represent wastes with uncharacteristically high levels of regulated constituents. Likewise, a range of simulants will be required to fully define the QGCR for some of the COPCs that potentially leach from the glass at or near the action limits. Simulants do not necessarily need to represent actual expected waste composition in so much as they support the identification of the QGCR and modeling (e.g., statistically formulated).

Simulant validation will be required for those simulants not already validated in accordance with *Simulant Definition and Verification Methodology* (Peterson et al., 2001). Should simulant validation be required (e.g., the simulant is not validated by the WTP in accordance with approved methodology), then the following approach shall apply prior to simulant use, to facilitate simulant validation:

- Samples shall be taken in triplicate (minimum) to provide the data needed to assess variability in the simulant formulation.
- Simulant results will be compared to 1) formulation requirements, 2) WTP process flowsheet model predictions for CRV content, and/or 3) results of actual pretreated waste material. Results will be reported as relative percent differences, as well as reporting the characterization results for the simulant and comparative data/substance (formulation requirements, flowsheet model predictions, and/or pretreated waste results) along side one another.

Differentiation of statistically designed simulants and simulants designed to mimic nominal or bounding case waste characteristics will be made so that the proper criteria are applied during simulant validation. Validated simulants will be added to the listing presented in *Simulant Definition and Verification Methodology*, in accordance with WTP configuration control procedures.

Additionally, all the simulants used will be constrained by the following requirements:

- Simulants used will be characterized prior to use, using the sum of their individual components (traceable to simulant batch sheets) or by the appropriate analytical method identified in this DQO. The analytical QA/QC will be that required by the method. Concentration levels will be reported in mg/L or mg/kg where necessary, in addition to wt% or wt% oxide.
- Simulant documentation will include simulant formulation and justification (or intended simulant use) along with a description of what the simulant is intended to represent. Spike levels will be identified.

2 References

Peterson, R. A. and P. S. Townson. 2001. *Simulant Definition and Verification Methodology*, 24590-WTP-RPT-TE-01-003, Rev. 0. Bechtel National Inc., Richland, Washington.

Appendix G

Analysis of the Applicability of the Multiple Extraction Procedure (MEP) for Evaluating Vitrified High Level Waste



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Acronyms

EPA	Environmental Protection Agency
IHLW	immobilized high-level waste
MEP	Multiple Extraction Procedure

1 Introduction

The River Protection Program-Waste Treatment Plant (WTP) is in the process of evaluating the ability of a vitrified¹ high-level mixed waste product to meet the environmental criteria to qualify for delisting under 40 CFR 260.22. The question has been raised as to the need for the project to evaluate the glass product using the Multiple Extraction Procedure (MEP), described in SW-846, Method 1320. The "Scope and Application" discussion of Method 1320 states that the MEP is designed to "simulate leaching that a waste will undergo from repetitive precipitation of acid rain on an improperly designed sanitary landfill." (EPA 1997). WTP's position is that MEP is not an appropriate analysis to be used for evaluating the glass product. This position is based on two facts: 1) the physical and chemical properties of immobilized high-level waste (IHLW) are not compatible with the intent and design of the MEP and 2) the Environmental Protection Agency (EPA) regulations and guidance apply the MEP only to chemically stabilized wastes.

2 Physical and Chemical Properties of IHLW

WTP does not consider the MEP to be an appropriate procedure to test the performance of vitrified waste forms for two reasons; 1) vitrified wastes have no significant pore structure to allow the leachant to penetrate the glass, and 2) the metallic species are covalently bound in the vitrified waste and are not encapsulated within a buffering cementitious matrix.

The MEP was designed to test the possibility that chemically stabilized (cementitious)² waste forms could be degraded by sequential acid rain events and release unacceptable levels of potentially hazardous metals in ionic form. The test leaches the waste form with ten batches of an acidic aqueous solution designed to simulate acid rain (pH = 3.0). Each leaching step uses a fresh portion of leachant applied to the solid separated from the previous step. EPA's expectation is that successfully stabilized waste forms will release successively smaller amounts of potential hazardous constituents, such as trace metals.

The vitrified high level waste form is a glass with no porosity available for penetration of water into the waste form. The glass is a supercooled liquid (polymer) with no interstitial pore space. Conversely, chemically stabilized waste forms have on the order of 16 – 24% pore space ranging in size from nanometers to millimeters (Glasser 1997). Many of these pores are interconnected. This high degree of porosity, together with the interconnectivity of the pores, makes cement waste forms vulnerable to intrusion by water and dilute acid that simulate the acid rain condition (MEP, EPA Method 1320). The sequential leaching of MEP is designed to test the buffering capacity of a cementitious waste. The porosity of cementitious waste forms creates a highly effective surface area for chemical reactions between the acidic leachant and the cement matrix resulting in dissolution reactions and release of metallic constituents from the matrix. This means that short term tests, such as the MEP which utilizes a dilute acid leachant and an 18 hour contact period, can attack a cement waste form effectively but will

¹ Vitrification is the process of converting materials into a glass or glass substance, typically through a thermal process (EPA 1992)

² 40 CFR 268.42 provides a description of stabilization in the context of LDR technology-based standards that reads as follows: "Stabilization with the following reagents (or waste reagents) or combinations of reagents: (1) Portland cement; or (2) lime/pozzolans (e.g., fly ash and cement kiln dust) – this does not preclude the addition of reagents (e.g., iron salts, silicates, and clays) designed to enhance the set/cure time and/or compressive strength, or to overall reduce the leachability of the metal or inorganic." The terms "chemically stabilized" waste forms and "cementitious" waste forms are used interchangeably in the context of this position paper.

have a lesser impact on vitrified waste forms because of the lack of an effective surface area upon which to act. As noted in the following paragraphs, the vitrified waste form is chemically resistant to dilute acids as well.

Vitrified waste forms are created through high temperature thermal processes with glass forming materials such as silica and glass frit. The majority of the metals of concern are immobilized by forming very strong, covalent bonds with the oxygen atoms in the glass matrix (EPA 1992). The remaining trace amounts (if any) of metallic cations are encapsulated in the glass. The glass is chemically very resistant to attack by acids; therefore, the metal cations are not readily released from the matrix through reaction (dissolution) with the aqueous acid. Moreover, vitrification does not rely upon chemical buffering as a mechanism for inhibiting dissolution kinetics, as do chemically stabilized waste forms. The physical structure of the glass remains intact and the small amount of metals (in the form of oxides) within the glass are generally not accessible to the aqueous acid solution of the MEP. Because glass is non-porous, any reactions are limited to the surface of the waste form and only a very small fraction of contaminants are susceptible to leaching. Under MEP test conditions, the sequential application of leaching would be of no value because the vitrified waste form would simply behave the same as in an initial extraction.

This is not true of chemically stabilized (cementitious) wastes which are alkaline in nature and use encapsulation as the primary mechanism for contaminant immobilization. The stabilization process mixes lime, Portland cement, and/or some other pozzolan³ such as fly ash with the waste in the presence of an excess of water. The trace metals immediately react to form precipitates (oxides, hydroxides, carbonates, etc.) which are stable in the alkaline media. The chemical additives react to form a rigid calcium-silica matrix that encapsulates the waste over time. The alkaline matrix and insoluble precipitates prevent solubilization and release of the metals. Only a very small amount of the trace metal cations are incorporated into the calcium-silica matrix, and this is primarily by weak ionic bonds. Because of the high porosity and alkaline nature of stabilized waste forms, the acidic leachant used in the MEP attacks the calcium-silica matrix but is neutralized as alkaline components are released from the waste form. Successive extractions with fresh leach solution deplete the buffering capacity of the waste form and expose the precipitated forms of the metals to dissolution in the aqueous acid solution. Therefore, the porosity, chemical reactivity, and successive leaching of a stabilized waste form with the dilute acid leachant of the MEP makes the MEP a reasonable test of the chemically stabilized waste's tendency to release metals under acid rain conditions.

3 Consideration of Potentially Applicable Regulations and Guidance

The MEP was designed for chemically stabilized wastes, not vitrified wastes. The EPA published guidance for developing a strategy and documentation to support delisting petitions (EPA 2000). The guidance includes sections that identify the analyses recommended for typical petitions, as well as those that are suggested by EPA for waste that requires special analyses. If waste is generated from a stabilization process, the guidance suggests the use of the MEP to provide additional information in

³ Pozzolan is defined in the Academic Press Dictionary of Science and Technology as a finely ground, burnt clay, shale, or siliceous tuff or ash used in making cement because of its ability to harden underwater when mixed with lime. The American Concrete Cement Association describes pozzolan as a siliceous or siliceous and aluminous material, which in itself possesses little or no cementitious value but will, in finely divided form and in the presence of moisture, chemically react with calcium hydroxide at ordinary temperatures to form compounds possessing cementitious properties.

support of delisting (EPA 2000, Exhibit 1). As noted in Section 6.2.2 of the Guidance, the MEP is recommended to help quantify the long-term stability of the leachable metals in a waste that has been chemically stabilized.

As described in the land disposal restrictions program (40 CFR 268.42), stabilization as a treatment technology (STABL) involves the use of specific reagents – Portland cement or lime/pozzolans (e.g. many fly ashes). This technology is called out separately from the vitrification treatment (HLVIT) that is specified for high-level vitrified waste, showing clearly that they are considered different processes by the EPA. A careful review of the EPA guidance in this area reveals no instance where the MEP is recommended as a meaningful test of vitrified waste forms.

4 Conclusion

The MEP was developed to evaluate the long-term durability of chemically stabilized (cementitious) waste forms in an acidic environment. Both the chemical and physical properties of chemically stabilized waste forms are amenable to short term testing for stability and leachability using sequential exposure to dilute acid solutions that simulate acid rain. Because of direct incorporation (chemical bonding) of contaminants into vitrified waste, vitreous waste forms are chemically resistant to weak solutions of aqueous acids and are impervious to penetration by aqueous solutions in short term tests. The different mechanisms for contaminant immobilization in vitrification (e.g., chemical bonding) versus cementation (e.g., encapsulation) must be considered in the application of acidic leach testing.

The MEP is applied to chemically stabilized waste forms based on guidance from the EPA. Vitrified glass forms are not products of the chemical stabilization process; therefore, the MEP does not apply to IHLW.

5 References

40 CFR 260.22. *Petitions to Amend Part 261 to Exclude a Waste Produced at a Particular Facility*, Code of Federal Regulations, as amended.

40 CFR 268.42. *Treatment Standards Expressed as Specified Technologies*, Code of Federal Regulations, as amended.

EPA. 1992. *Handbook. Vitrification Technologies for Treatment of Hazardous and Radioactive Waste*, EPA/625/R-92/002, USEPA, May 1992.

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Appendix H

Organic Compound Destruction as a Byproduct of Vitrification



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List of Acronyms

CRV	Concentrate Receipt Vessel
DOE	United States Department of Energy
DWPF	Defense Waste Processing Facility
EA	Environmental Assessment
EPA	United States Environmental Protection Agency
HLW	High-Level Waste
HpCDD	Heptachlorodibenzo-p-dioxin
HpCDF	Heptachlorodibenzofuran
HxCDD	Hexachlorodibenzo-p-dioxin
HxCDF	Hexachlorodibenzofuran
IHLW	Immobilized High-Level Waste
ILAW	Immobilized Low-Activity Waste
LAW	Low-Activity Waste
LCS	Laboratory Control Sample
LDR	Land Disposal Restrictions
MDL	Method Detection Limit
MFV	Melter Feed Vessel
MS	Matrix Spike
MSD	Matrix Spike Duplicate
MT	Metric Tons
NELAC	National Environmental Laboratory Accreditation Conference
OCDD	Octachlorodibenzodioxin
OCDF	Octachlorodibenzofuran
QC	Quality Control
RCRA	Resource Conservation and Recovery Act of 1976
RL	Reporting Limit
RPD	Relative Percent Difference
SRS	Savannah River Site
SRTC	Savannah River Technology Center
TCLP	Toxicity Characteristic Leaching Procedure
UDRI	University of Dayton Research Institute

VSL Vitreous State Laboratory
WTP Hanford Tank Waste Treatment and Immobilization Plant
WVDP West Valley Demonstration Project

1 Introduction

The United States Department of Energy (DOE) has contracted the Hanford Tank Waste Treatment and Immobilization Plant (WTP) to design and build facilities to treat a portion of the 54 million gallons of highly radioactive and mixed hazardous waste stored at the Hanford site. The process being implemented to treat these wastes involves separating the waste into Low-Activity Waste (LAW) and High-Level Waste (HLW) fractions, vitrifying the LAW for on-site disposal, and vitrifying the HLW for eventual disposition in a federal high-level waste repository.

Hanford tank wastes have regulatory status as hazardous waste under federal Resource Conservation and Recovery Act (RCRA) regulations, and as dangerous waste under State of Washington regulations. The hazardous and dangerous waste status is based on the hazardous and dangerous waste characteristics exhibited by the tank wastes that contain, or may contain, certain listed hazardous waste constituents. The immobilized (vitrified) wastes treated by WTP must comply with the requirements of the land disposal restrictions (LDR) found in 40 Code of Federal Regulations (CFR) 268 and Washington Administrative Code (WAC) 173-303-140. Treated, immobilized low-activity waste (ILAW) and immobilized high-level waste (IHLW) must either meet the performance-based treatment standards for the LDR-regulated constituents, or be treated according to specified LDR treatment technologies. WTP has elected to pursue a petition for a LDR treatability variance from the existing performance-based standards as the preferred method for demonstrating compliance with LDR requirements. In addition to LDR requirements, the IHLW must also meet health-based performance standards that will allow it to be excluded (delisted) from regulation under RCRA, in turn facilitating eventual disposal in a federal high-level waste repository. WTP is pursuing a petition to delist IHLW in accordance with the requirements from 40 CFR 260.20, 40 CFR 260.22 and WAC 173-303-072, concurrent with the LDR treatability variance. WTP will show that vitrification is an appropriate treatment technology for the reduction of toxicity and mobility of Hanford tanks wastes. One part of this process includes providing the technical basis for the assertion that organic compounds in the HLW and LAW wastes will be sufficiently volatilized or destroyed such that the final waste form may be delisted and disposed of in a land disposal unit. This document provides the information to substantiate that organic compounds are volatilized and destroyed as a byproduct of vitrification and will not persist in the final waste forms.

This report describes the processes that destroy organic compounds in the glass melt during vitrification, and presents data that is supplemental to data already presented in the *Data Quality Objectives Process in Support of LDR/Delisting at the WTP* (24590-WTP-RPT-ENV-01-012, revision 0). The following sections provide the technical background, justifications, and results of testing that demonstrate how organic compounds will be degraded by pyrolysis and oxidation during the vitrification process. The organization of the topics presented in this paper are meant to provide the reader with a basic understanding of the vitrification process, operations, precedence, and supplemental research data, all of which support the conclusion that organic compounds are volatilized or destroyed during vitrification. The following topics are presented.

- WTP Process Overview:

This section is meant to provide a description of the vitrification process and conditions which contribute to the pyrolysis of organic constituents. WTP melter specifications are also presented to support subsequent computations of theoretical melter residence times.

- **Theoretical Residence Time:**
This section presents the theoretical melter residence times (and supporting computations).
- **Precedents for Organics Destruction:**
This section summarizes the findings of organics decomposition studies by other vitrification operations currently operating at DOE's Savannah River Site, and the West Valley Demonstration Project, and addresses the recent Savannah River Site delisting.
- **WTP Glass Testing Results:**
This section summarizes the relevant test data from WTP research efforts, including recent data not discussed in previous documents.

2 WTP Process Overview

The WTP waste treatment process consists of three major process areas: pretreatment, HLW vitrification, and LAW vitrification. The Hanford tank waste slurry will be received at the WTP Pretreatment Facility via pipeline from the Hanford tank farm. The pretreatment facility consists of filtration and ion exchange processes used to separate the waste into LAW and HLW fractions. The LAW fraction is transported to the LAW vitrification facility and the HLW fraction to the HLW vitrification facility. The primary function of the Pretreatment Facility is to remove excess water from the waste, separate LAW from HLW, and remove selected radionuclides and transuranics from the LAW. The removed radionuclides are blended with the HLW feed for processing at the HLW Vitrification Facility.

At the vitrification facilities, feed concentrate (LAW or HLW solids with pretreatment intermediate waste products added) will be transferred from the pretreatment building to a concentrate receipt vessel (CRV). Batches of feed concentrate from the CRVs will then be transferred to the melter feed preparation vessel (MFPV) to be blended with glass formers and sucrose (as a reductant) to ensure a uniform mixture. The melter feed slurry will then be transferred to the melter feed vessel (MFV), from which it will be fed to the melter.

The LAW and HLW melters are functionally similar but vary in geometry, melter pool volume, and surface area. These differences are based on differing production rate requirements and waste compositions that affect melt rate. Both melters have a nominal operating temperature of 1150 °C, include a refractory-lined melt chamber, and an air-lift riser and pour spout.

The pretreated tank waste is mixed with glass forming chemicals and sucrose (if necessary) in the MFV and pumped at a specified feed rate to the melter. Because the hazardous organics constituents of Hanford tank waste are in minor quantities relative to the inorganic waste components, the sucrose addition during melter feed preparation is the primary source of organics in the melter feed. As the feed slurry is fed to the melter, a cold cap forms, which gradually dissolves into the molten glass pool.

The tank waste and glass formers first undergo partial denitration as the first major chemical reaction to occur in the melter. The sucrose reduces nitrates under boiling conditions yielding several gaseous species. Loss of chemically bound water is the second reaction. This water loss is initiated endothermically, but as the dried salts are heated above their melting points, exothermic reactions dominate, which include oxidation of sucrose by nitrates. Such redox reactions are common and rapidly occur at temperatures above the melting point of the organics and the nitrate salts, which are typically below 350 °C. Fused nitrate that reacts with carbohydrates rarely reduce the nitrate past nitrite, accounting for excess pyrolytic graphite after the elimination of nitrates (Bickford and others 1990b). As the temperature of the reacting material increases further, other salts, such as carbonates and hydroxides, are decomposed to the corresponding oxides and are incorporated into the fused mixture that forms the molten glass, which becomes part of the underlying glass pool.

The glass pool contains about 18.7 MT (41,150 lbs) of glass for the LAW melter and about 10 MT (22,100 lbs) of glass for the HLW melter. As a result of these large inventories, on average, the fresh glass formed in the cold cap is resident in the melt pool for many hours before exiting the melter, as is discussed below. The cold cap aids in melter operation by trapping heat within the melt pool. As the cold-cap heats and dissolves away, more feed is added to maintain cold-cap balance. During operation, feed rate, cold-cap coverage, and discharge rate are balanced to achieve the desired throughput.

Molten glass is discharged via an airlift riser and discharge trough located in a heated discharge chamber mounted adjacent to the melt chamber (see Figure 2-1). The melter is designed such that the glass enters the vertical airlift riser through the slightly angled riser throat near the bottom of the glass melter pool. The glass discharges from the melter by injecting air through a platinum tube located in the airlift riser. The molten glass is lifted by the air bubbles into the pour trough which is attached at the top of the riser. The pour trough is angled downward approximately 30 degrees where the glass travels prior to exiting the melter pour spout into a glass storage canister. The entire pour spout section is operated under a vacuum at temperatures greater than 950 °C to maintain a glass viscosity of less than 10 Pa·s. This viscosity is necessary to ensure the glass flows and exits the melter pour spout.

2.1 Melter Technical Parameters

This section highlights relevant melter specifications and operating conditions. The information presented was compiled from a variety of source documents, including *Basis of Design* (24590-WTP-DB-ENG-01-001), *Systems 211, 212, 213: LAW Melter System Description* (CHG 2000a), *System Description for System 211 HLW Melter, Pour Spout, and Canister Level Detection* (CHG 2000b) and various project drawings [see References, Section 6 and footnotes below]:

• General Melter Specifications (applies to both LAW and HLW Melter):		
- Nominal Operating Temperature ¹ :	1150 °C	2100 °F
- Plenum Temperature ¹ :	400 - 600 °C	750 - 1100 °F
- Pour Trough Temperature ¹ :	950°C	1750 °F
• HLW Melter Specifications:		
- Nominal Production Rate ¹ :	1.5 MT/d	3307 lb/d
- Maximum Production Rate ¹ :	3 MT/d	6614 lb/d
- Melter Feed Rate ² :	150 - 200 L/h	5.3 - 7 ft ³ /h
- Melter Holdup Time ³ :	6.7 d	
- Glass Density	2.43 MT/m ³	152 lb/ft ³
(glass pool weight + volume):		
- Melter Pool Weight ² :	10 MT	11 tons (22,046 lb)
- Melter Pool Volume:	4.10 m ³	145 ft ³
- Melter Pool Surface Dimensions ² :	3.72 m ² (2.44 m by 1.52 m)	40 ft ² (8 ft by 5 ft)
- Melter Pool Depth:	1.10 m	3.62 ft
- Pour Throat/Riser Diameter ⁴ :	0.0762 m	3.00 inch
- Pour Throat Length ⁴ :	0.4106 m	16.17 inch
- Airlift Riser Length ⁴ :	0.6513 m	25.64 inch
- Pour Trough Length ⁵ :	0.9163 m	36.07 inch

¹ 24590-WTP-DB-ENG-01-001, Rev. 0, *Basis of Design*, January 25, 2002

² CHG. 2000b. *System Description for System 211 HLW Melter, Pour Spout, and Canister Level Detection*, SD-W375HV-G00001, Rev. B, CH2M Hill Hanford Group, October 9, 2000.

³ Melter holdup is the projected average time period for which a melt pool is likely to be held in the melter (melt pool weight divided by the nominal production).

⁴ 24590-101-TSA-W000-0010-398-05, *RPP-WTP High Level Waste Melter 60% Design Drawings*, Volume IV, "Refractory Details Monofrax E", Drawing No. WTP-M-21106, Rev 1, Sheets 1 & 2.

- Pour Rate (30 minute pour event over 4 hrs)²: 0.25 – 0.50 MT/h 9.2 – 18.4 lb/min

• LAW Melter Specifications:

- Nominal Production Rate ¹ :	15 MT/d	33,070 lb/d
- Maximum Production Rate ¹ :	30 MT/d	66,140 lb/d
- Melter Feed Rate ⁶ :	500 L/h	17.7 ft ³ /h
- Melter Holdup Time ⁶ :	1.5 d	
- Glass Density (glass pool weight ÷ volume):	3.0 MT/m ³	185 lb/ft ³
- Melter Pool Weight ⁶ :	22.7 MT	25 tons (50,000 lb)
- Melter Pool Volume:	7.65 m ³	270 ft ³
- Melter Pool Surface Dimensions ⁶ :	10.0 m ² (4.93 m by 2.03 m)	108 ft ² (16' 2" by 6' 8")
- Melter Pool Depth ⁶ :	0.76 m	2.5 ft (30 inch)
- Pour Throat/Riser Diameter ⁷ :	0.102 m	4.00 inch
- Pour Throat Length ⁷ :	0.4602 m	18.12 inch
- Airlift Riser Length ^{7,8} :	0.6429 m	25.31 inch
- Pour Trough Length ⁹ :	1.429 m	56.26 inch
- Pour Rate:	2.1 – 3.0 MT/h	77 - 110 lb/min

The high temperatures and residence times ensure that the glass can be poured into canisters, and that volatiles will evaporate or decompose and be drawn off through the offgas system. Non-volatile metals will generally react to form oxides and become part of the molten glass. The organic waste constituents (underlying hazardous constituents) in the melt pool will be volatilized or destroyed.

⁵ 24590-101-TSA-W000-0010-407-149, *RPP-WTP High Level Waste Melter 90% Design*, Volume 13, "Discharge Chamber Trough", Drawing No. WTP-M-21562, Rev 0, Sheet 3.

⁶ CHG. 2000a. *Systems 211, 212, 213: LAW Melter System Description*, SD-W375LV-G00001, Rev. C, CH2M Hill Hanford Group, November 20, 2000.

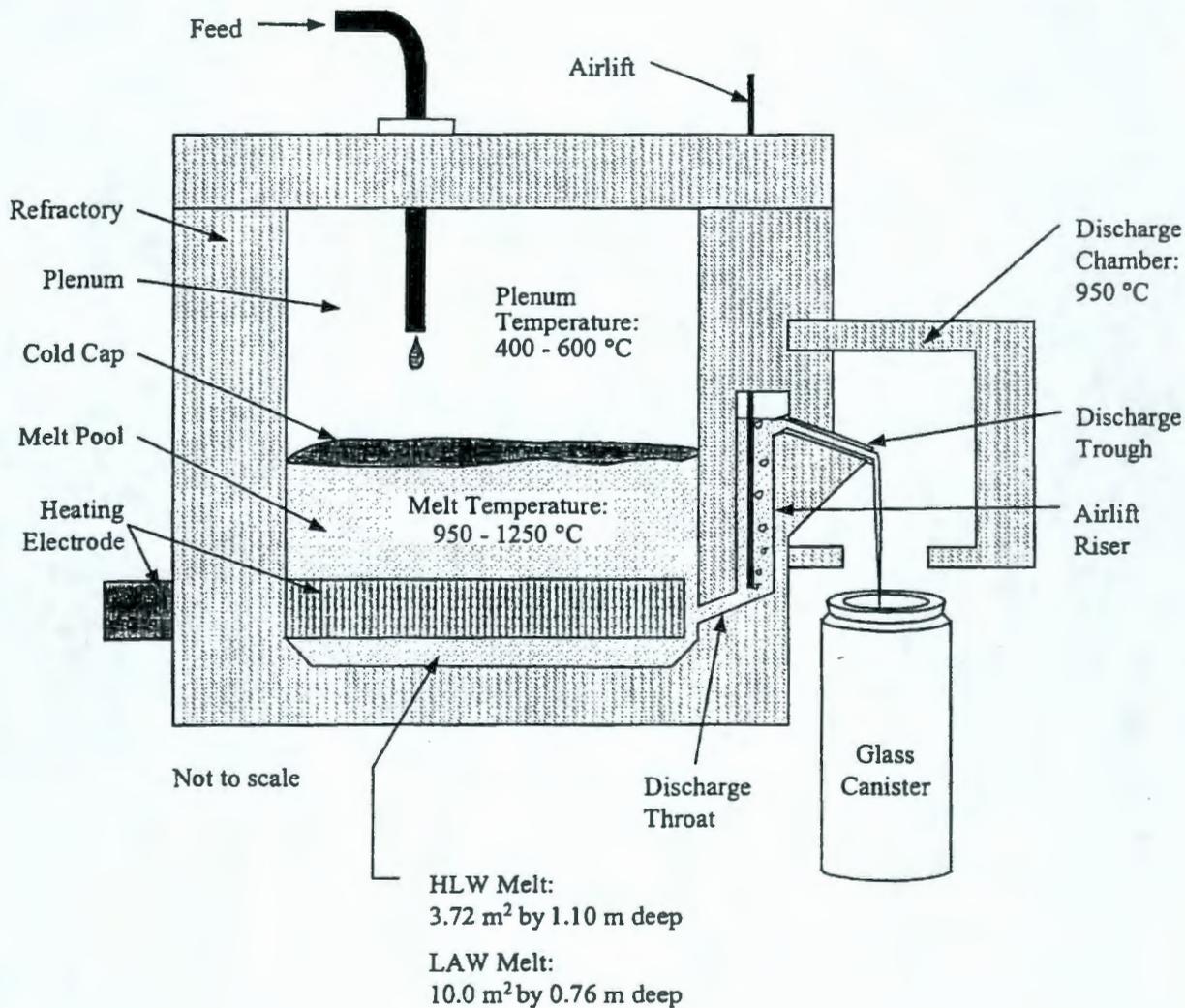
⁷ 24590-101-TSA-W000-0010-401-14, *RPP-WTP Low Active Waste Melter 60% Design Drawings*, Volume 13, "Glass Pool Contact Refractory (E) Details", Drawing No. WTP-M-11102, Rev 0, Sheet 1

⁸ 24590-101-TSA-W000-0010-401-14, *RPP-WTP Low Active Waste Melter 60% Design Drawings*, Volume 13, "Refractory Assembly", Drawing No. WTP-M-11050, Rev 0, Sheet 6.

⁹ 24590-101-TSA-W000-0010-401-14, *RPP-WTP Low Active Waste Melter 60% Design Drawings*, Volume 13, "Trough Assembly", Drawing No. WTP-M-11551, Rev A, Sheets 2 & 3.

Figure 2-1 General Layout of HLW/LAW Melter

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3 Theoretical Residence Time

Melter residence time can be approximated by combining the residence time for waste in the melt pool, and the residence time in the pour spout and discharge trough. The glass properties can be defined as those of a real fluid that exhibits finite viscosity and non-uniform velocity distribution, and experiences friction and turbulent flow.

Based on chemical kinetics and reactor design, joule-heated ceramic melter technologies can be described as a combination of a well-stirred reactor and a plug-flow reactor (Bickford and others 1990a). The melt chamber, which contains a majority of the glass product, behaves as a well-stirred reactor. This has behavior been confirmed with feed turnover measurements conducted by WTP research facilities with pilot-scale melters (Matlack and others 2002b). While the residence time distribution in a simple well-stirred reactor model mathematically (but not physically) includes zero (Cooper and Jeffreys, 1973), the mean residence time of glass in the melt chamber, 20 hours (HLW) and 7.5 hours (LAW), is very large. It must also be noted that the HLW and LAW glass melters operate with a cold cap where chemical transition from slurry to glass occurs. However, residence time analysis for the cold cap is not considered in the analysis below since, theoretically, the melter can be operated without the use of a cold cap. The melter pour spout, on the other hand, is expected to approximate plug-flow reactor kinetics.

The calculations and discussions that follow describe the theoretical residence time of the melt pool and pour spout. Cold cap residence time is not considered in the analysis below.

These simple calculations are based on the assumption that the pour stream undergoes uniform flow and the melter behaves like a well-stirred reactor. Corrections can be made to account for the fact that the pour stream in the pour trough undergoes non-uniform flow due to the pour stream accelerating, thus increasing in velocity slightly. However, the calculations for both LAW and HLW clearly show that the glass undergoes a residence time significantly greater than any error that would be induced by the assumption of uniform flow, thus a detailed analysis of non-uniform flow is unwarranted. Literature from the Environmental Sciences and Engineering Group of the University of Dayton Research Institute (UDRI) states that the pyrolysis of organic constituents is kinetically (reaction rate), not thermodynamically, controlled (UDRI 1989). Therefore determination of the exact, time, temperature and stoichiometry history of all molecules in a melter is necessary to determine the absolute destruction efficiency of organic compounds. Given the uncertainties concerning exact quantities of organics in Hanford tank waste, such an approach is not practical, and would likely have little value in light of what is already known about organics pyrolysis during vitrification. However, an approximate residence time for the major components of the HLW and LAW melter can be computed, and is provided below to provide reasonable assurance that residence time in the melter is sufficient for pyrolysis to occur.

3.1 Melt Pool Mean Residence Time

The following provides calculations of mean residence time in the HLW and LAW melter chambers (for a continuous pour at the maximum pour rate):

$$\begin{aligned}\text{HLW Mean Residence Time} &= \text{Melt Pool Weight} \div \text{Pour Rate} \\ &= 10 \text{ MT} \div 0.5 \text{ MT/h} \\ &= 20 \text{ h}\end{aligned}$$

$$\begin{aligned}\text{LAW Mean Residence Time} &= \text{Melt Pool Weight} \div \text{Pour Rate} \\ &= 22.7 \text{ MT} \div 3.0 \text{ MT/h} \\ &= 7.5 \text{ h}\end{aligned}$$

3.2 Melt Pool Residence Time Distribution

As previously discussed, melter technologies can be described as a combination of a well-stirred reactor (melt pool) and plug-flow reactor (discharge spout). For the melt pool, theoretically, a minimum residence time of zero is possible, and a residence time distribution can be approximated by knowing the mean residence time (\bar{t}). This approximation is useful in that it can be used to predict, using conservative assumptions, a residence time that corresponds with the lower 99th percentile. That is, the shortest time increment for which 99 % of the feed material is in the melter, can be approximated. Cooper and Jeffreys show that for a single well-stirred reactor, the proportion of mass exiting the reactor at time "t" can be approximated as follows:

$$\frac{c_1}{c_0} = 1 - e^{-Qt/V}$$

Where:

c_1 is the concentration exiting the melter at time t
 c_0 is the concentration exiting the melter at time $t = \infty$, or the final concentration
Q is the volumetric flowrate
V is the melter volume

Recognizing that c_1/c_0 is also the proportion of molten glass exiting the system, and the relationship of $V/Q = \bar{t}$ (the mean residence time) for a constant density fluid, the equation above can be simplified to:

$$\frac{c_1}{c_0} = 1 - e^{-t/\bar{t}}$$

Solving for "t" at $c_1/c_0 = 0.01$, the time at which only 1 % of the molten glass has passed into the pour spout under maximum continuous pour rate (assumed condition), the following results:

$$t = -\ln(1 - c_1/c_0) \times \bar{t}$$

For HLW, $\bar{t} = 20$ hours, after 12 minutes only 1 % of the molten glass has passed into the pour spout. The remaining 99 % of the molten glass has a residence time distribution greater than 12 minutes.

For LAW, $\bar{t} = 7.5$ hours, after 4.5 minutes only 1 % of the molten glass has passed into the pour spout. The remaining 99 % of the molten glass has a residence time distribution greater than 4.5 minutes.

From these theoretical computations, it is clear that essentially all glass exiting the melter has sufficient residence time at the nominal melter temperature, and for purposes for evaluating organics destruction

and removal, may be considered a well-mixed reaction system. Not only is there substantial residence time in the melt pool, but there is additional residence time in the pour spout as discussed below.

3.3 Pour Spout Residence Time

For simplicity of discussion, the pour spout discussed here is meant to include the riser throat at the bottom of the melter, the vertical airlift riser, and the pour trough housed in the heated discharge chamber (refer back to Figure 2-1). See Section 2 for the description of how molten glass is discharged via an airlift riser and discharge trough, located in a heated discharge chamber mounted adjacent to the melt chamber. The melter is designed such that the glass enters the vertical airlift riser through the slightly angled riser throat near the bottom of the glass melter pool. The molten glass is lifted by the air bubbles into the pour trough which is attached at the top of the riser. The entire pour spout section is operated under a vacuum at temperatures greater than 950 °C to maintain the glass viscosity at less than 10 Pa·s. This is necessary to ensure the glass flows and exits the melter pour spout.

In the HLW melter, the glass near the melter bottom is discharged through a 7.6 cm (3 inch) diameter pour throat and travels at a slight upward angle 41 cm (16 inch). The glass then travels in the vertical direction for 65 cm (25.6 inch) through the airlift riser before exiting into the pour trough. The glass travels 91 cm (36 inch) through the angled pour trough prior to exiting the pour spout into the glass storage canister.

Knowing that for plug-flow reactors, residence time is simply the length of travel divided by linear flow velocity, the residence time can be computed.

$$\text{HLW Pour Spout Residence Time} = \text{Total Pour Spout Length} \div \text{Pour Rate Velocity}$$

Pour Throat/Riser Diameter	= 0.0762 m	
Pour Throat Length	= 0.4106 m	
Airlift Riser Length	= 0.6513 m	
Pour Trough Length	= 0.9163 m	
Total Pour Spout Length	= 1.978 m	
Maximum Pour Rate	= 0.50 MT/h	
Glass Density	= 2.43 MT/m ³	
Pour Rate Velocity	= $0.50 \div (2.43 \times \pi \times (0.0762 \div 2)^2)$	= 45 m/h
Glass Residence Time	= 1.978 ÷ 45	= 0.044 h
		= 2.6 min
		= 158 s

The LAW melter pour spout design is very similar to the HLW melter pour spout and operates in the same manner. The glass near the bottom of the melter pool enters a 10 cm (4 inch) diameter pour throat. The glass travels at a slight upward angle approximately 46 cm (18 inch) in length before transitioning into the airlift riser. The glass travels vertically for approximately 64 cm (25 inch) before the glass exits and travels into the pour trough. The pour trough is angled downward approximately 30 degrees where the glass travels 1.4 m (56 inch) prior to exiting the melter pour spout into the glass storage canister.

LAW Pour Spout Residence Time = Total Pour Spout Length ÷ Pour Rate Velocity

Pour Throat/Riser Diameter	= 0.102 m	
Pour Throat Length	= 0.4602 m	
Airlift Riser Length	= 0.6429 m	
Pour Trough Length	= 1.429 m	
Total Pour Spout Length	= 2.532 m	
Maximum Pour Rate	= 3.0 MT/h	
Glass Density	= 3.0 MT/m ³	
Pour Rate Velocity	= $3.0 \div (3.0 \times \pi \times (0.102 \div 2)^2)$	= 122 m/h
Glass Residence Time	= 2.532 ÷ 130	= 0.021 h
		= 1.2 min
		= 74 s

The HLW residence time in the pour spout is approximately 158 seconds; the LAW residence time in the pour spout is approximately 74 seconds. These residence times represent the minimum residence times (the pour rate is assumed to be at the maximum and continuous), and don't take into account the residence time for the melt pool. In actuality, melter discharge will not be continuous because the glass canisters must be allowed time for thermal expansion, and each canister must be cycled (replaced with an empty canister) after being filled. Additionally, the melter discharge rate will most likely be held at nominal flow rates. The melter holdup time (melt pool weight divided by the nominal production, refer to Section 2.1) is a more representative value for melter residence time.

4 Precedents for Organics Destruction

Both Savannah River's Defense Waste Processing Facility (DWPF) and New York's West Valley Demonstration Project (WVDP) are treating high level radioactive waste using a joule-heated ceramic lined melter, which is the same technology being implemented at WTP. The successful startup and operation of vitrification facilities at the DWPF and the WVDP have direct relevance to WTP. Both the WVDP and the DWPF have successfully treated high level wastes via vitrification that satisfy the federal repository requirement that the canistered waste forms do not contain detectable amounts of organic materials. This vitrification experience represents an important piece in WTP's overall strategy for demonstrating organics will not be detectable in the vitrified waste forms, and is briefly discussed here.

Both the DWPF and the WVDP melter systems operate such that the melter material achieves temperatures of approximately 950 – 1250 °C, and are producing qualified borosilicate waste forms for permanent storage at a federal repository. The melter feeds at both sites contain organic materials, primarily hydrocarbons, organoborates, and amines. Like WTP, the WVDP's primary source of organic is sucrose, which is purposely added to control the oxidation state of the glass. This material is oxidized during the melting process and is not present as prohibited material in the glass product (WVDP 1997). It was found through laboratory testing by Savannah River Technology Center (SRTC) that organic materials present in DWPF waste either oxidize or boil away in the melter plenum space (the space in the melter above the molten glass pool, see Figure 2-1), and thus, do not survive the vitrification process (Bickford and others 1986, 1990b).

The time necessary to destroy organic materials, including the pyrolytic carbon formed from initial decomposition reactions, was found to be temperature dependent. These test results indicate that at melt pool temperatures exceeding 900 °C all organics, including pyrolytic carbon, were destroyed in times less than one hour. WVDP and SRTC obtained glass samples from pilot plant operations using surrogate wastes that included organic materials. The analysis performed on WVDP glasses resulted in less than 10 mg/kg total carbon in the glass (Bickford and others 1986). The analysis performed on SRTC glasses resulted in less than 52 mg/kg total carbon in the glass (Bickford and others 1990b). In both cases, these concentrations represented the method detection limits for the tests.

Based on previous test results performed by SRTC and the WVDP, nearly all the organics are destroyed in the melter primarily via pyrolysis. Pyrolysis is defined as the breaking apart of complex molecules into simpler units by the use of heat or combustion (Parker 1994). These data are consistent with the EPA Vitrification Handbook (EPA 1992) which concludes that vitrification is generally an effective treatment technology for organic-containing wastes, and may achieve destruction or removal efficiencies of greater than 99.99% for most organic compounds. The handbook states that the destruction of organic constituents occurs primarily via pyrolysis in the melt and combustion in the plenum. This high organic destruction efficiency is due to the high melting temperature of the glass and operating temperatures in the melter plenum.

EPA recently granted exclusion (also known as delisting) to DOE's Savannah River Site (SRS) for vitrified glass product made from F006 and F028 listed waste (67 FR 54124). In its petition to delist, SRS presented analytical data from small-scale melter tests in which actual SRS waste was vitrified. Included with the analytical data were the results for the total constituent analysis for all constituents in Appendix VIII of 40 CFR 261 and Appendix IX of 40 CFR 264. The data provided showed no detectable

quantities of any organic compounds in the SRS glass (Pickett 2000). The only organic compound identified as a constituent of concern by EPA was acetonitrile. Although acetonitrile was not a component of the SRS waste streams, it is a known offgas component that is a byproduct of the vitrification process. Acetonitrile was not detected in any of the glass samples analyzed by SRS.

5 WTP Glass Testing Results

5.1 Fate of Hazardous Organics Study

In late 1998 and early 1999, the Vitreous State Laboratory (VSL) of the Catholic University of America conducted small-scale melter tests at their research facility for determining the fate of hazardous organics during vitrification of both HLW and LAW wastes (Matlack and Pegg 1999). Independent analytical laboratories were contracted to perform emissions sampling and analysis of offgas, glass, and feed samples for hazardous organic compounds and metals using Environmental Protection Agency (EPA) sampling and analytical methods and procedures. The tests were performed on a small-scale vitrification system with WTP waste simulants representing two LAW feeds and one HLW feed.

The feed was injected continuously into the feed stream immediately upstream of the melter feed tube and mixed using an in-line mixing cell (closed system). The organic injection system consisted of a liquid reservoir, an HPLC-type metering pump, an injection nozzle, and a static mixer. The static mixer is located in the feed line between a pinch-valve assembly and the melter feed tube. The injection nozzle is located at the inlet of the static mixer. The HPLC pump operates continuously and the incoming feed pulse sweeps the accumulated organics into the static mixer, where the two are blended before flowing into melter. See Figure 5-1 for a simplified schematic showing the organics injection and melter feed system.

The glass in the small-scale melter was held at 1150 °C for several hours prior to being discharged. Glass samples were collected for analysis by SW-846 Methods 8260B, 8270C, and 8280A by General Engineering Laboratories in Charleston, NC. One-hundred-eighty-two individual organic compounds were analyzed for in 20 tests (20 glass samples collected) resulting in over 3600 records. In only 20 instances (0.5 % of the data points) were organics detected in the glass, most of which corresponded to common laboratory contaminants also found in laboratory method blanks, or suspected cross-contamination from shipping. The results are discussed below, and presented in Table 5-1 and Table 5-2.

None of the glass samples showed the detectable amounts of the spiked organic constituents by either Toxicity Characteristic Leaching Procedure (TCLP, SW-846 Method 1311 [EPA1997]) or total analysis. For the TCLP analysis, chlorobenzene and chloroform were detected above the minimum detection limits, but below the reporting limits. Chloroform was also detected in one associated TCLP laboratory blank sample. Chlorobenzene detected in the TCLP analysis was not detected in corresponding total glass analysis.

For the totals analysis, acetone, chloroform, chlorobenzene, methylene chloride, vinyl acetate, carbon disulfide, and naphthalene were detected above the minimum detection limits, but only acetone, methylene chloride, and vinyl acetate were detected above reporting limits (all less than 20 µg/kg, by totals analysis). Acetone, chloroform and methylene chloride were detected in laboratory blanks in excess of 10 % of their corresponding sample concentrations. These compounds are known, common laboratory contaminants due to their use in SW-846 offgas sample recovery procedures. Although chlorobenzene was not detected in laboratory blanks, chlorobenzene is a component of the laboratory control standard (LCS). Chloroform, methylene chloride, and carbon disulfide were also found to be associated with sample shipments, although trip blanks were not submitted with the glass samples. Carbon disulfide was also detected in the standard reference glass, an environmental assessment (EA) glass produced by Corning Engineering Services in 1992.

These data are summarized in Table 5-1, and analytical batch quality control (QC) sample results are summarized in Table 5-2.

5.2 Active ILAW and IHLW Glass Tests

In February 2001, WTP fabricated LAW and HLW glasses from actual tank waste to show compliance with the RPP-WTP contractual requirements, e.g., dangerous waste limitations and volatile and extractable organic content. The LAW sources were generated from the processing of Hanford tank 241-AW-101 and 241-AN-107 pretreated wastes. The HLW sources were generated from pretreated tank sludge samples from tanks 241-C-104 (C-104) and 241-AZ-102 (AZ-102). These wastes were vitrified into borosilicate glasses by Pacific Northwest National Laboratory in Richland, Washington. Pacific Northwest National Laboratory used modified versions of SW-846 methods 8260B, 8270C, 8082, and 8280A to perform analyses. No volatile organics, semi-volatile organics, polychlorinated biphenyls/pesticides, and polychlorinated dibenzo-p-dioxins and dibenzofurans were detected in the glass samples. The waste compositions used during these tests were spiked with known quantities of volatiles and semivolatiles. None of the spiked organic compounds were detected in the final glass product. This research data is presented in detail in Urie (2001) and Goheen (2001), and is summarized in the WTP project document 24590-WTP-RPT-ENV-01-012.

Cyanide was analytically detected in the both C-104 and AZ-102 tank wastes (Brooks 2000, Fiskum 2000). The AZ-102 and C-104 glass products were analyzed in duplicate for total cyanide. One of the four glass analyses did detect total cyanide above the estimated detection limit (Goheen 2001). However, cyanide was present at only 0.5% of the quantitation limit, this result is highly questionable. Since the data were provided from a research facility, method detection limits were not derived in accordance with SW-846 as would be the case for a commercial environmental laboratory. Although the EPA Vitrification Handbook states that cyanide will breakdown into carbon and nitrogen during vitrification (EPA 1992), the data suggest the additional research to confirm cyanide destruction during vitrification may be warranted.

5.3 Integrated Test Results

In January 2002 and March 2002 testing at VSL was conducted with simulated LAW sub-envelopes A1 and C1 with high levels of spiked organics (Matlack and others 2002a, 2002b). The objectives of these tests were to collect data for determining the system decontamination factors and destruction efficiencies using a scale model of the HLW melter system, the DM1200 vitrification system (melt surface area of 1.2 m²) and the pilot-scale prototypic offgas system components installed at VSL. Testing included processing feeds that were spiked with selected hazardous organic compounds while the offgas stream was sampled at four different locations. Glass sampling was performed to validate the complete destruction of organic compounds. To that end, all samples were collected in accordance with SW-846 protocols, and analyzed by a qualified commercial laboratory, specializing in environmental compliance sample analysis (Severn Trent Laboratories, Knoxville, TN).

The feed was spiked with large quantities of chlorobenzene, trichloroethylene, and naphthalene. The feed was injected continuously into the feed stream immediately upstream of the melter feed tube and mixed using an in-line mixing cell (closed system). The organic injection system consisted of a liquid reservoir, an HPLC-type metering pump, an injection nozzle, and a static mixer. The static mixer was located in the feed line between the pinch-valve assembly and the melter feed tube. The injection nozzle was located at

the inlet of the static mixer. The HPLC pump operates continuously and the incoming feed pulse sweeps the accumulated organics into the static mixer, where the two are blended before flowing into melter. The analytical results are presented below. The melter was run under nominal (steady state) conditions, with an average production rate¹⁰ of 1948 kg/m²/day, and 1639 kg/m²/day for sub-envelopes A1 and C1, respectively. Glass samples were collected for analysis by SW-846 Methods 8260B, 8270C, and 8290.

In the sub-envelope A1 glass analysis, acetone, methylene chloride, 1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin (HpCDD), octachlorodibenzodioxin (OCDD), 1,2,3,4,7,8-hexachlorodibenzofuran (HxCDF), 2,3,4,6,7,8-HxCDF, 1,2,3,4,6,7,8-heptachlorodibenzofuran (HpCDF), 1,2,3,4,7,8,9-HpCDF, and octachlorodibenzofuran (OCDF) were detected in samples and blanks. All detected quantities are estimates, and can be associated with laboratory contamination. All blanks contain these compounds in excess of 10% of the corresponding sample concentrations. Toluene was also detected (estimated quantity, well below LDR limits and proposed delisting levels) in a single sub-envelope A1 glass sample, however, toluene is also a component of the laboratory control sample. Toluene is not a combustion byproduct of the three spike constituents and is likely a lab contaminant that was not detected by blank or other analyses.

In the sub-envelope C1 glass analysis, acetone, methylene chloride, OCDD, and OCDF were detected in samples and blanks. All detected quantities are estimates, and are associated with laboratory contamination. All blanks contain these compounds in excess of 10% of the corresponding sample concentrations. Carbon disulfide also was detected (estimated quantity, well below LDR limits and proposed delisting levels) in a single sub-envelope C1 glass sample, however, since sulfur was not a component of any organic spike constituent, it is unlikely a direct result of partial combustion of the spiked organics.

All detected compounds (single-digit part-per-billion level for detected volatiles, and sub-part-per-billion levels for dioxins and furans) were far below LDR limits, and health-based delisting levels (refer to project document 24590-WTP-RPT-ENV-01-012, *Data Quality Objectives Process in Support of LDR/Delisting at RPP-WTP*, revision 0). Table 5-3 and Table 5-4 provide the results for compounds detected in simulated A1 glass, along with the relevant batch quality control sample results. Table 5-5 and Table 5-6 provides the results for compounds detected in simulated C1 glass, along with the relevant batch quality control sample results.

The constituents detected, and their reported concentrations, are indicative of the lower limits of laboratory cleanliness and the exceedingly low detection levels that are achievable for dioxin and furan analyses, rather than the actual presence of organic compounds in vitrified waste forms. This data, when coupled with the research data discussed in the preceding sections, provide evidence substantiating the volatilization and destruction of organic compounds as a byproduct of vitrification.

¹⁰ The production rates equate to 19.48 MT/day for sub-envelope A1, and 16.39 MT/day for sub-envelope C1, on a full sized LAW melter.

Table 5-1. Fate of Hazardous Organics Test: Glass Total Organic Analysis – Detected Results Only

Spiked Feed Concentration (mg/kg)								
benzene (C ₆ H ₆): 0 to 782								
phenol (C ₆ H ₆ O): 0 to 1,738								
naphthalene (C ₁₀ H ₈): 0 to 868								
Glass Sample	Shipment Number	Test Number	Spike Conc. (mg/kg)	Detected Compounds	Sample Result (µg/kg)	Lab Qualifiers	MDL (µg/kg)	RL (µg/kg)
OD-G-109A*	3	2	Benzene: 669 Phenol: 374 Naphth.: 289	Acetone	12.4	--	10.3	10.3
				Methylene chloride	6.37	J	1.40	5.00
OD-G2-37A*	3	5	Benzene: 264 Phenol: 565 Naphth.: 282	Chloroform	0.57	J	0.100	2.00
OD2-G-89C	4	4	Benzene: 262 Phenol: 562 Naphth.: 281	Methylene chloride	2.97	J	1.40	5.00
OD2-G-98B	4	6	Benzene: 49 Phenol: 106 Naphth.: 53	Methylene chloride	2.81	J	1.40	5.00
				Vinyl Acetate	2.24	J	2.10	10.0
OD2-G-100B	4	6	Benzene: 49 Phenol: 106 Naphth.: 53	Chloroform	1.33	J	0.100	2.00
				Methylene chloride	6.67	--	1.40	5.00
OD2-G-115A	4	7	Benzene: 79 Phenol: 168 Naphth.: 84	Methylene chloride	2.25	J	1.40	5.00
OD2-G-109B	4	8	Benzene: 56 Phenol: 119 Naphth.: 60	Methylene chloride	3.47	J	1.40	5.00
OD3-G-53B	5	13	Benzene: 141 Phenol: 314 Naphth.: 157	Chloroform	0.53	J	0.100	2.00
OD3-G-44B	5	14	Benzene: 254 Phenol: 788 Naphth.: 393	Chloroform	0.55	J	0.100	2.00
OD3-G-36B	5	15	Benzene: 782 Phenol: 1738 Naphth.: 868	Chloroform	0.50	J	0.100	2.00
OD3-G-88A	6	16	Benzene: 109 Phenol: 290 Naphth.: 85	Chloroform	0.57	J	0.100	2.00
OD3-G-76C	6	OP1	Benzene: 136 Phenol: 303 Naphth.: 151	Chloroform	0.54	J	0.100	2.00
OD3-G-67B	6	OP4	Benzene: 215 Phenol: 479 Naphth.: 239	Chloroform	0.53	J	0.100	2.00
OD3-G-121A	7	OP2	Benzene: 0 Phenol: 0 Naphth.: 0	Naphthalene	0.88	J	0.600	2.00
				Carbon Disulfide	0.79	J	0.300	10.0

Table 5-1. Fate of Hazardous Organics Test: Glass Total Organic Analysis – Detected Results Only

Spiked Feed Concentration (mg/kg)								
benzene (C ₆ H ₆): 0 to 782								
phenol (C ₆ H ₆ O): 0 to 1,738								
naphthalene (C ₁₀ H ₈): 0 to 868								
Glass Sample	Shipment Number	Test Number	Spike Conc. (mg/kg)	Detected Compounds	Sample Result (µg/kg)	Lab Qualifiers	MDL (µg/kg)	RL (µg/kg)
OD3-G-126B	7	OP3	Benzene: 0 Phenol: 0 Naphth.: 0	Carbon Disulfide	1.04	J	0.300	10.0
Environmental Assessment (EA) Reference Glass	7	N/A	Benzene: 0 Phenol: 0 Naphth.: 0	Carbon Disulfide	0.74	J	0.300	10.0
Blank Results:								
Lab Blank for Batch 139874: Samples: OD2-G-89C, OD2-G-98B, OD2-G-100B, OD2-G-109B, and OD2-G-115A			Chloroform		0.91	NR	0.100	2.00
			Methylene chloride		0.72	NR	1.40	5.00
Lab Blank for Batch 140865: Samples: OD3-G-53B, OD3-G-44B, OD3-G-36B, OD3-G-88A, OD3-G-76C, OD3-G-67B			2-Hexanone		0.76	NR	2.80	10.0
			Acetone		2.35	NR	10.3	10.3
			Methylene chloride		0.69	NR	1.40	5.00
Lab Blank for Batch 141882: Samples: OD3-G-121A, OD3-G-126B, EA Reference Glass			Chloroform		0.66	NR	0.100	2.00
			2-Butanone		25.9	NR	3.20	10.0

Analysis was performed by General Engineering Laboratories, Charleston, SC. No semivolatile, dioxin, or furan compounds detected.

MDL = Minimum Detection Limit

RL = Reporting Limit

NR = Not reported. Value was not provided by the analytical laboratory.

N/A = Not applicable.

* Blank results for associated samples OD-G-109A and OD-G2-37A were not reported.

J = Estimated Result. Result is less than the reporting limit or estimated quantitation limit.

-- = No qualifier reported. Data quantification is within standard method tolerances.

Table 5-2. Fate of Hazardous Organics Test: Glass Total Organic Analysis QC Summary

Batch Number and Associated Samples	Method	QC Results
QC Batch 139874: Samples: OD2-G-89C, OD2-G-98B, OD2-G-100B, OD2-G-109B, and OD2-G-115A	SW-846 8260B	<ul style="list-style-type: none"> • Chloroform and methylene chloride detected in the blank. • All surrogate recoveries within limits except for low recovery of bromofluorobenzene, dibromofluoromethane, and toluene-d8. • LCS recoveries within limits except chlorobenzene. • MS/MSD recoveries and relative percent difference within limits.
QC Batch 140865: Samples: OD3-G-53B, OD3-G-44B, OD3-G-36B, OD3-G-88A, OD3-G-76C, OD3-G-67B	SW-846 8260B	<ul style="list-style-type: none"> • 2-Hexanone, acetone, and methylene chloride detected in the blank. • All surrogate recoveries within limits. • LCS recoveries within limits except for low recovery of chlorobenzene. • MS/MSD recoveries and relative percent difference within limits.
QC Batch 141882: Samples: OD3-G-121A, OD3-G-126B, EA Reference Glass	SW-846 8260B	<ul style="list-style-type: none"> • Chloroform and 2-butanone detected in the blank. • All surrogate recoveries within limits. • LCS recoveries within limits. • MS/MSD recoveries and relative percent difference within limits.

Quality control batch results for associated samples OD-G-109A and OD-G2-37A were not reported.

Table 5-3. DM1200 A1 Glass Organic Test Results

Spiked Feed Concentration ($\mu\text{g}/\text{kg}$)							
		chlorobenzene ($\text{C}_6\text{H}_5\text{Cl}$):	462,073				
		trichloroethylene (C_2HCl_3):	612,097				
		naphthalene (C_{10}H_8):	126,020				
Glass Sample	Spike added to feed?	Detected Compounds ($\mu\text{g}/\text{kg}$)	Sample Result ($\mu\text{g}/\text{kg}$)	Lab Qualifiers	MDL ($\mu\text{g}/\text{kg}$)	RL ($\mu\text{g}/\text{kg}$)	Notes (SW-846 Method)
12T-G-95E	No	Acetone	9.1	B, J	6.6	20	8260B
		Methylene Chloride	6.9	B	0.70	5.0	8260B
		1,2,3,4,6,7,8-HpCDD	0.090	Q, B, J	0.078	NR	8290
		OCDD	0.45	B, J	0.091	NR	8290
		1,2,3,4,7,8,9-HpCDF	0.081	Q, B, J	0.075	NR	8290
		OCDF	0.25	B, J	0.086	NR	8290
12U-G-62C	Yes	Acetone	8.6	B, J	6.6	20	8260B
		Methylene Chloride	7.5	B	0.70	5.0	8260B
		Toluene	1.5	J	0.50	5.0	8260B
		OCDD	0.48	B, J	0.11	NR	8290
		OCDF	0.22	Q, B, J	0.12	NR	8290
12U-G-86A	Yes	Acetone	7.7	B, J	6.6	20	8260B
		Methylene Chloride	8.0	B	0.70	5.0	8260B
		Toluene	1.3	J	0.50	5.0	8260B
		OCDD	0.37	B, J	0.098	NR	8290
12U-G-94B	Yes	Acetone	7.7	B, J	6.6	20	8260B
		Methylene Chloride	8.6	B	0.70	5.0	8260B
		OCDD	0.41	B, J	0.15	NR	8290
12-U-101B	Yes	Acetone	6.9	B, J	6.6	20	8260B
		Methylene Chloride	8.0	B	0.70	5.0	8260B
		Toluene	1.2	J	0.50	5.0	8260B
		1,2,3,4,6,7,8-HpCDD	0.22	B, J	0.10	NR	8290
		OCDD	0.92	B, J	0.10	NR	8290
		1,2,3,4,7,8-HxCDF	0.14	B, J	0.050	NR	8290
		2,3,4,6,7,8-HxCDF	0.17	B, J	0.053	NR	8290
		1,2,3,4,6,7,8-HpCDF	0.11	B, J	0.072	NR	8290
OCDF	0.36	B, J	0.10	NR	8290		

Table 5-3. DM1200 A1 Glass Organic Test Results

Spiked Feed Concentration ($\mu\text{g}/\text{kg}$)							
chlorobenzene ($\text{C}_6\text{H}_5\text{Cl}$):		462,073					
trichloroethylene (C_2HCl_3):		612,097					
naphthalene (C_{10}H_8):		126,020					
Glass Sample	Spike added to feed?	Detected Compounds ($\mu\text{g}/\text{kg}$)	Sample Result ($\mu\text{g}/\text{kg}$)	Lab Qualifiers	MDL ($\mu\text{g}/\text{kg}$)	RL ($\mu\text{g}/\text{kg}$)	Notes (SW-846 Method)
Blank Results:							
Blank for Lot # H2C080241: Samples: 12T-G-95E, 12U-G-62C, 12U-G-94B, 12U-G-86A, 12U-G-101B		Acetone	10	J	6.6	20	8260B
		Methylene Chloride	12	--	0.70	5.0	8260B
		1,2,3,4,7,8-HxCDD	0.17	Q, J	0.12	NR	8290
		1,2,3,4,6,7,8-HpCDD	0.28	Q, J	0.17	NR	8290
		OCDD	1.4	Q, J	0.17	NR	8290
		1,2,3,4,7,8-HxCDF	0.30	J	0.65	NR	8290
		1,2,3,6,7,8-HxCDF	0.23	J	0.60	NR	8290
		2,3,4,6,7,8-HxCDF	0.20	Q, J	0.69	NR	8290
		1,2,3,7,8,9-HxCDF	0.20	Q, J	0.76	NR	8290
		1,2,3,4,6,7,8-HpCDF	0.33	J	0.96	NR	8290
		1,2,3,4,7,8,9-HpCDF	0.28	Q, J	0.12	NR	8290
		OCDF	1.2	J	0.20	NR	8290

Analysis was performed by Severn Trent Laboratory, Knoxville TN. All holding times and QC criteria were met. Test results met all NELAC requirements. No semivolatle compounds detected.

MDL = Minimum Detection Limit

RL = Reporting Limit

NR = Not reported. Value was not provided by the analytical laboratory.

Q = Estimated maximum possible concentration

B = Method blank contamination. The associated method blank contains the target analyte at a reportable level.

J = Estimated Result. Result is less than the reporting limit or estimated quantitation limit.

-- = No qualifier reported. Data quantification is within standard method tolerances.

HpCDD = Heptachlorodibenzo-p-dioxin

HpCDF = Heptachlorodibenzofuran

HxCDD = Hexachlorodibenzo-p-dioxin

HxCDF = Hexachlorodibenzofuran

OCDD = Octachlorodibenzodioxin

OCDF = Octachlorodibenzofuran

Table 5-4. DM1200 A1 Glass Organic Test QC Summary

Lot Number and Associated Samples	Method	QC Results
H2C080241: 12T-G-95E, 12U-G-62C, 12U-G-94B, 12U-G-86A, and 12U-G-101B	SW-846 8260B	<ul style="list-style-type: none"> • All surrogate recoveries within limits. • LCS recoveries within limits. • All MS & MSD recoveries within limits. • All MS & MSD RPDs within limits. • Acetone and methylene chloride detected in the blank. Methylene chloride was detected above the reporting limit
	SW-846 8270C	<ul style="list-style-type: none"> • All surrogate recoveries within limits. • LCS recoveries within limits. • All MS & MSD recoveries within limits. • All MS & MSD RPDs within limits. • Nothing detected in the blank.
	SW-846 8290	<ul style="list-style-type: none"> • All internal standard recoveries within limits. • LCS recoveries within limits, with the exception of 1,2,3,7,8,9-HxCDD and 1,2,3,4,6,7,8-HpCDF, which were just below (within 3%) of the recovery limits. The lab reports overall recoveries were low and thought to be caused by dilution of the native stock solution. • All MS & MSD recoveries within limits. • All MS & MSD RPDs within limits. • Multiple compounds were detected in the lab blank

LCS = Laboratory Control Sample
 MS = Matrix Spike
 MSD = Matrix Spike Duplicate
 RPD = Relative Percent Difference
 HpCDF = Heptachlorodibenzofuran
 HxCDD = Hexachlorodibenzo-p-dioxin

Table 5-5. DM1200 C1 Glass Organic Test Results

Spiked Feed Concentration (µg/kg)							
		chlorobenzene (C ₆ H ₅ Cl):	547,730				
		trichloroethylene (C ₂ HCl ₃):	724,992				
		naphthalene (C ₁₀ H ₈):	148,552				
Glass Sample	Spike added to feed?	Detected Compounds (µg/kg)	Sample Result (µg/kg)	Lab Qualifiers	MDL (µg/kg)	RL (µg/kg)	Notes (SW-846 Method)
12R-G-116B	No	Acetone	7.9	B, J	6.6	20	8260B
		Methylene Chloride	2.6	B, J	0.70	5.0	8260B
12S-G-20A	Yes	Acetone	8.1	B, J	6.6	20	8260B
		Carbon Disulfide	0.69	J	0.50	5.0	8260B
		Methylene Chloride	2.7	B, J	0.70	5.0	8260B
		OCDD	2.3	Q, B, J	0.45	NR	8290
		OCDF	1.8	Q, B, J	0.60	NR	8290
12S-G-37A	Yes	Acetone	7.5	B, J	6.6	20	8260B
		Methylene Chloride	2.7	B, J	0.70	5.0	8260B
		OCDD	0.39	Q, B, J	0.24	NR	8290
12S-G-74A	Yes	Methylene Chloride	2.2	B, J	0.70	5.0	8260B
12S-G-85C	Yes	Methylene Chloride	2.3	B, J	0.70	5.0	8260B
		OCDD	0.76	J	0.24	NR	8290

Table 5-5. DM1200 C1 Glass Organic Test Results

Spiked Feed Concentration ($\mu\text{g}/\text{kg}$)							
chlorobenzene ($\text{C}_6\text{H}_5\text{Cl}$):		547,730					
trichloroethylene (C_2HCl_3):		724,992					
naphthalene (C_{10}H_8):		148,552					
Glass Sample	Spike added to feed?	Detected Compounds ($\mu\text{g}/\text{kg}$)	Sample Result ($\mu\text{g}/\text{kg}$)	Lab Qualifiers	MDL ($\mu\text{g}/\text{kg}$)	RL ($\mu\text{g}/\text{kg}$)	Notes (SW-846 Method)
Blank Results:							
Blank for Lot # H2A160117 Samples: 12R-G-116B, 12S-G-20A, 12S-G-37A, 12S-G-74A		Acetone	7.8	J	6.6	20	8260B
		Methylene Chloride	1.7	J	0.70	5.0	8260B
Blank for Lot # H2A170254 Sample 12S-G-85C		Bromomethane	3.8	J	3.5	10	8260B
		Chloromethane	2.4	J	0.93	10	8260B
		Methylene Chloride	1.7	J	0.70	5.0	8260B
Blank for Lot # H2A170254 / H2A170126 Samples: 12R-G-116B, 12S-G-20A, 12S-G-37A, 12S-G- 85C, 12S-G-74A		1,2,3,4, 6,7,8- HpCDD	0.54	J	0.31	NR	8290
		OCDD	2.1	J	0.45	NR	8290
		1,2,3,4,7,8-HpCDF	0.44	J	0.24	NR	8290
		OCDF	1.7	J	0.48	NR	8290

Analysis was performed by Severn Trent Laboratory, Knoxville TN. All holding times and QC criteria were met. Test results met all NELAC requirements. No semivolatiles compounds detected.

MDL = Minimum Detection Limit

RL = Reporting Limit

NR = Not reported. Value was not provided by the analytical laboratory.

Q = Estimated maximum possible concentration

B = Method blank contamination. The associated method blank contains the target analyte at a reportable level.

J = Estimated Result. Result is less than the reporting limit or estimated quantitation limit.

HpCDD = Heptachlorodibenzo-p-dioxin

HpCDF = Heptachlorodibenzofuran

OCDD = Octachlorodibenzodioxin

OCDF = Octachlorodibenzofuran

Table 5-6. DM1200 C1 Glass Organic Test QC Summary

Lot Number and Associated Samples	Method	QC Results
H2A160117: 12R-G-116B, 12S-G-20A, 12S-G-37A, and 12S-G-74A	SW-846 8260B	<ul style="list-style-type: none"> All surrogate recoveries within limits. LCS recoveries within limits. All MS & MSD recoveries within limits. MS & MSD RPDs for benzene, 1,1-dichloroethene, trichloroethene were beyond control limits. Acetone and methylene chloride detected in the blank, but below RL.
	SW-846 8270C	<ul style="list-style-type: none"> All surrogate recoveries within limits. LCS recoveries within limits. All MS & MSD recoveries within limits. All MS & MSD RPDs within limits. Nothing detected in the blank.
H2A170254 / H2A170126: 12R-G-116B, 12S-G-20A, 12S-G-37A, 12S-G-85C, and 12S-G-74A	SW-846 8290	<ul style="list-style-type: none"> All internal standard recoveries within limits. LCS recoveries within limits. All MS & MSD recoveries within limits. All MS & MSD RPDs within limits. 1,2,3,4,6,7,8-HpCDD, OCDD, 1,2,3,4,7,8-HpCDF, OCDF detected in the blank, but below reporting limit.
H2A170254: 12S-G-85C	SW-846 8260B	<ul style="list-style-type: none"> All surrogate recoveries within limits. LCS recoveries within limits. All MS & MSD recoveries within limits. All MS & MSD RPDs within limits. Bromomethane, chloromethane, and methylene chloride detected in the blank, but below reporting limit.
	SW-846 8270C	<ul style="list-style-type: none"> All surrogate recoveries within limits. LCS recoveries within limits. All MS & MSD recoveries within limits. All MS & MSD RPDs within limits. Nothing detected in the blank.

Lot #H2A170254 (sample 12S-G-85C) was combined with Lot #H2A170126 to make a single batch for analysis by method 8290.

LCS = Laboratory Control Sample

MS = Matrix Spike

MSD = Matrix Spike Duplicate

RPD = Relative Percent Difference

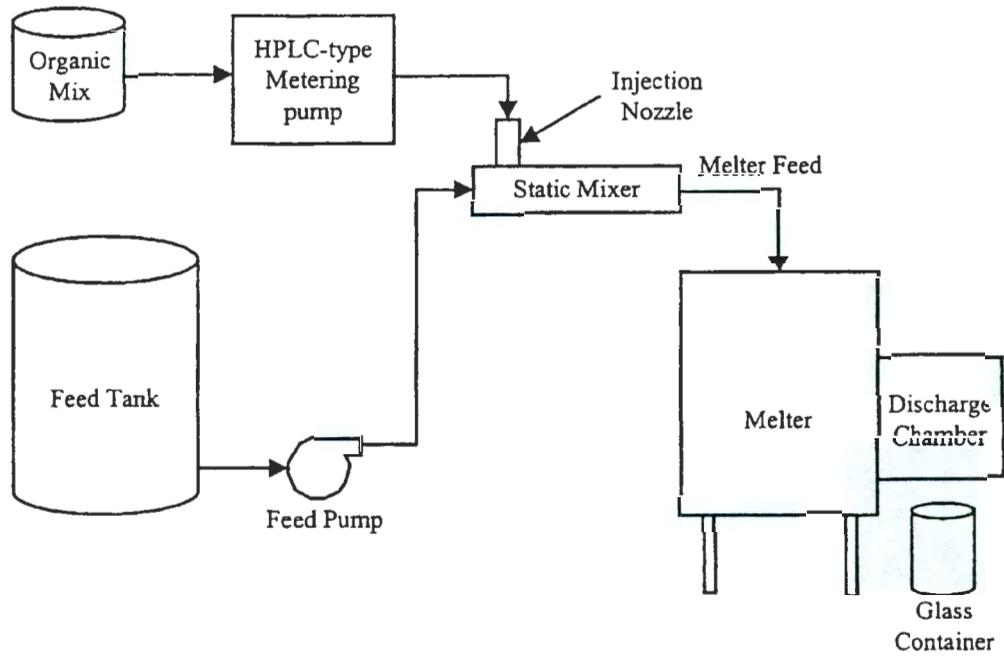
HpCDD = Heptachlorodibenzo-p-dioxin

HpCDF = Heptachlorodibenzofuran

OCDD = Octachlorodibenzodioxin

OCDF = Octachlorodibenzofuran

Figure 5-1 Simplified Schematic of VSL Research Melter and Feed System.



6 References

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40 CFR 261, Appendix VIII *Hazardous Constituents*, Code of Federal Regulations, as amended.

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