

Appendix A

Quality Assurance Information

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The tables presented in this appendix address the acceptance criteria (FY 98 Planning and Control System [PACS], Participant Planning Sheet, Work Package 11017030M3, Activity ID WP20BM3] for the Level 3 deliverable *Waste Form Characteristics Report, Version 1.3*. **Table A-1** is the required “roadmap” that indicates where the criteria are met in this report. **Table A-2** is a list of the codes used for calculations discussed in this report, including the versions used and whether the codes are qualified.

Table A-3 lists the significant data in the sections included in Version 1.3 and the related data-tracking numbers (DTNs) from the Technical Data Management System (TDMS).

Because this CD-ROM version of the *Waste Form Characteristics Report* includes the 10 sections updated in Version 1.3 and all the remaining unchanged sections published in Version 1.2, **Table A-4** has been added to indicate the QA status of significant data used in the unchanged sections included from Version 1.2. QA requirements and document guidelines have changed significantly since Versions 1.0 and 1.2 were published; consequently, the qualified status of materials in those two versions has not been identified nor verified, although some of the data may meet the definition of qualified data, as defined in the glossary of the Office of Civilian Radioactive Waste Management (OCRWM), U.S. Department of Energy (DOE) Quality Assurance Requirements and Description (QARD) document, DOE/RW-0333P, Version 8.

Also, relevant DTNs from the TDMS have not been identified nor technical data information forms (TDIFs) submitted for data in Versions 1.0 or 1.2., although they may have been submitted for the same data when included in other documents. Because of this uncertainty in the qualification status of significant data in those older versions, they been defined conservatively in Table A-4 as “existing data,” as defined in the previously cited QARD. Literature references for the data in Version 1.2 are listed in captions or as footnotes. Material and references from Versions 1.0 and 1.2 may have changed since their original publication.

Table A-1 "Roadmap" table identifying where the deliverable (WP20M3) acceptance criteria are met in the *Waste Form Characteristics Report, Version 1.3*

Criteria Description	Section	Comment
<p>Provide preliminary degradation process models and up-to-date supporting test data that describe the performance, consistent with applicable expected environmental conditions, of commercial spent fuel and high-level, radioactive waste (HLW) immobilized in borosilicate glass for each applicable performance parameter and identified in the Waste Package Development Document (WPDD) [BBA000000-01717-5705-00009 Rev. 1].</p>		<p>There are 10 sections in this update, version 1.3. Six of the sections include data and are in Chapter 2. Those revised sections are 2.1.3.1, 2.1.3.2, 2.1.3.5, 2.2.1.5, 2.2.2.2, and 2.2.2.3. The remaining four sections (3.22, 3.4.2, 3.5.1, and 3.5.2) are in Chapter 3 and contain material on model development for spent nuclear fuel (SNF) and HLW glass waste forms.</p>
<p>WPDD Performance Parameters</p> <ul style="list-style-type: none"> • Process models for cladding failure from strain failure, delayed hydride cracking, and mechanical failure <p>Section also discusses cladding dry oxidation and chemical corrosion. Pit penetration/localized corrosion is not addressed.</p> <ul style="list-style-type: none"> • Higher SNF oxide formation rate data • SNF dissolution/corrosion and release data <p>Addresses RN concentrations in contacting water</p> <ul style="list-style-type: none"> • Glass fracture data; radionuclide (RN) release from glass; and colloidal species <p>Addresses RN concentrations in contacting water</p> <ul style="list-style-type: none"> • Higher SNF oxide formation rate models • SNF dissolution/corrosion and release models <p>Addresses RN concentrations in contacting water</p> <ul style="list-style-type: none"> • Glass dissolution data/experimental parameters and glass dissolution models <p>Addresses RN concentrations in contacting water.</p> <p>The HLW glass canister is stainless steel, which has a high corrosion rate. Consequently, no protective credit is taken for the canister.</p>	<p>2.1.3.1</p> <p>2.1.3.2</p> <p>2.1.3.5</p> <p>2.2.1.5 2.2.2.2 2.2.2.3</p> <p>3.2.2</p> <p>3.4.2</p> <p>3.5.1 3.5.2</p>	
<p>Provide available information related to the degradation behavior of additional spent fuel and waste forms proposed for disposal per the program baseline (e.g., DOE SNF, U.S. Navy fuel, and surplus weapons-usable fissile materials)</p>		<p>Information not currently available</p>

Criteria Description	Section	Comment
Q and non-Q (NQA) data used and cited in this deliverable are appropriately noted and clearly identified.	Appendix A	Significant data are identified as Q or NQA in Table A-3 and Table A-4.
Every effort has been made to ensure that qualified data are used in this deliverable.	2.1.3.1 through 3.5.2	
Technical data contained in the deliverable and not already incorporated in the GENISES will be submitted, if appropriate, for incorporation. Submittal compliance will be demonstrated by including in this report a copy of the TDIF and the transmittal letter to the GENISES administrator.	Appendix A	Data actually used in this report are identified in Appendix A.
Record accession numbers and automated tracking numbers will be included, as appropriate, for all data used or cited in this deliverable.	Chapters 3 through 7; Appendix A	Accession numbers are provided in the reference lists for sources for which they are available. Data-tracking numbers are provided in Appendix A for data used.

Table A-2 Simulation codes and chemical databases used in the *Waste Form Characteristics Report, Revision 1.3*

Section	Code	Version	Description	Application	Qualified?	Reference
2.1.3.5.3 3.5.1.7 3.5.1.9	EQ3/6	7.2b	Thermodynamic and reaction-path model	Equilibrium water composition and reaction-path modeling	Yes	Wolery 1992a; Wolery 1992b; Wolery and Daveler, 1992
3.5.1.7 3.5.1.9	GEMBOCHS	EQ3/6 V. 6	Thermodynamic database and maintenance software	Derive, enter, and test thermo-dynamic data files	No	Wolery 1992a; Wolery 1992b
3.4.2.3	RS/1 Explore	2.1	Data analysis software	Multiple regression analysis	No; commercial software	BBN Software Products, 1990

Table A-3 Summary of significant data used in the *Waste Form Characteristics Report, Revision 1.3*

Data Description	Reference	LLNL Data?	Related DTNs	Q/NQ*
Section 2.1.3.1 Cladding Degradation				
Tables 2.1.3.1-2 and 2.1.3.1-3	Siegmann, 1998	No	LL981106851021.070	NQ
Section 2.1.3.2 UO₂ Oxidation in Fuel				
Tables 2.1.3.2-1, 2.1.3.2-2, and 2.1.3.2-3 Figures 2.1.3.2-2 and Figures 2.1.3.2-9 through 2.1.3.2-13	Hanson, 1998	No	LL980608251021.046	Q

Data Description	Reference	LLNL Data?	Related DTNs	Q/NQ*
Section 2.1.3.2 UO₂ Oxidation in Fuel (continued)				
Figure 2.1.3.2-1 and Figures 2.1.3.2-3 through 2.1.3.2-8 Figure 2.1.3.2-A.1 through Figure 2.1.3.2-A.23	Hanson, 1998	No	LL980601851021.044	Q
Section 2.1.3.5 Dissolution Radionuclide Release from UO₂ Fuel				
Table 2.1.3.5-1	Wilson, 1984	No	LL980710651021.049	Q
Table 2.1.3.5-2	Wilson, 1990	No	LL980710651021.049	Q
Data on pages 2.1.3.5-5 and 2.1.3.5-6	Wilson, 1990	No	LL980710651021.049	Q
Tables 2.1.3.5-3 and 2.1.3.5-6	Gray, 1998	No	LL980711051021.048	Q
Table 2.1.3.5-4	Steward and Gray, 1994	Yes	LL980601551021.042	Q
Table 2.1.3.5-4a	Gray, 1996; 1998	No	LL980704251021.045 LL980711051021.048	Q
Table 2.1.3.5-5	Steward and Mones, 1997	Yes	LL961210151021.027	Q
Tables 2.1.3.5-7 and 2.1.3.5-8	Wronkiewicz et al., 1996	No	LL980710651021.049	Q
Tables 2.1.3.5-9 through 2.1.3.5-13	Finn et al., 1997	No	LL980710651021.049	Q
Tables 2.1.3.5-14 through 2.1.3.5-22	Finn et al., 1997	No	LL980710551022.012	Q
Section 2.2.2.2 Dissolution Radionuclide Release from Glass				
Table 2.2.2.2-1	Finn, 1997	No	LL980710651021.049 LL980710551022.012	Q
Tables 2.2.2.2-2 through 2.2.2.2-5	Finn, 1997	No	LL980710551022.012	Q
Figures 2.2.2.2-1 through 2.2.2.2-10	Finn, 1997	No	LL980913251021.060	Q
Section 2.2.2.3 Soluble-Precipitated/Colloidal Species				
Table 2.2.2.3-1	Finn, 1997	No	LL980710551022.012	Q
Section 3.2.2 Oxidation Models				
Tables 3.2.2-1 through 3.2.2-11	Version 1.3 of this report	Yes	LL980912451021.055	Q
Figures 3.2.2-6 through 3.2.2-8	Version 1.3 of this report	Yes	LL980912351021.054	Q
Figures 3.2.2-9 through 3.2.2-34	Version 1.3 of this report	Yes	LL980912451021.055	Q
Section 3.4.2 Spent-Fuel Dissolution Models				
Tables 3.4.2-5 through 3.4.2-7	Version 1.3 of this report	Yes	LL980912251021.053	Q
Figures 3.4.2-1 through 3.4.2-4 Figures 3.4.2-6 through 3.4.2-8	Version 1.3 of this report	Yes	LL980912251021.053	Q

Data Description	Reference	LLNL Data?	Related DTNs	Q/NQ*
Section 3.5.1 Experimental Parameters for Glass Dissolution				
Table 3.5.1-1	Knauss et al., 1990	Yes	LL980710651021.049	Q
Table 3.5.1-3, Table 3.5.1-5, and Table 3.5.1-7	Version 1.3 of this report	Yes	LL980710651021.049	Q
Table 3.5.1-10	Version 1.3 of this report	Yes	LL980710651021.049	Q
Figure 3.5.1-3	Delage et al., 1992	No	LL980710651021.049	Q
Figure 3.5.1-8	Fortner and Bates, 1995	No	LL960101651022.008	Q
Figure 3.5.1-9	Version 1.3 of this report	Yes	LL980710651021.049	Q
Section 3.5.2 Glass Dissolution Models				
Figure 3.5.2-2	Bourcier et al., 1990	Yes	LL980912551021.056 LL981010251021.063	NQ
Figure 3.5.2-4	Bourcier et al., 1994	Yes	LL980608351021.041 LL980912551021.056 LL980912551021.057 LL981010451021.065 LL981010551021.066	Q
Figure 3.5.2-5	Bourcier et al., 1992	Yes	LL980912551021.056 LL980912551021.057 LL981010651021.067	Q
Figure 3.5.2-6	Bourcier, 1997	Yes	LL980912551021.056 LL981010751021.068 LL981010851021.069	Q

* The Q/NQ status of the significant data is identified in the TDIFs associated with each DTN.

Table A-4 Summary of significant data used in the *Waste Form Characteristics Report, Version 1.2*

Section	QA Status of Significant Data
1. Introduction	No Significant Data
2. Design Data for Waste Forms	
2.1.1 and 2.1.2	Existing data
2.1.3.1 and 2.1.3.2	See Table A-3
2.1.3.3 and 2.1.3.4	Existing data
2.1.3.5	See Table A-3
2.1.3.6 and 2.1.3.7	Existing data
2.2.1.1, 2.2.1.2, 2.2.1.3, and 2.2.1.4	Existing data
2.2.1.5	See Table A-3
2.2.2.1	No significant data
2.2.2.2 and 2.2.2.3	See Table A-3
2.3.1 and 2.3.2	Existing data

Section	QA Status of Significant Data
3. Scientific Basis for Predictive Model Development	
3.1.1	Existing data
3.1.2	No significant data
3.2.1	Existing data
3.2.2	See Table A-3
3.3.1 and 3.3.2	Existing data
3.4 and 3.4.1	Existing data
3.4.1.1	Existing and qualified data*
3.4.1.2	No significant data
3.4.1.3	Existing data
3.4.2	See Table A-3
3.5.1 and 3.5.2	See Table A-3
3.6.1	Existing data
3.6.2	No significant data
3.6.3	Existing data

* See Section 2.1.3.5 (Table A-3) for additional and up-to-date spent-fuel and UO₂ dissolution data, and see Section 3.4.2 (Table A-3) for models.

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