Online Waste Library (OWL) and Waste Forms Characteristics Annual Report

Spent Fuel and Waste Disposition

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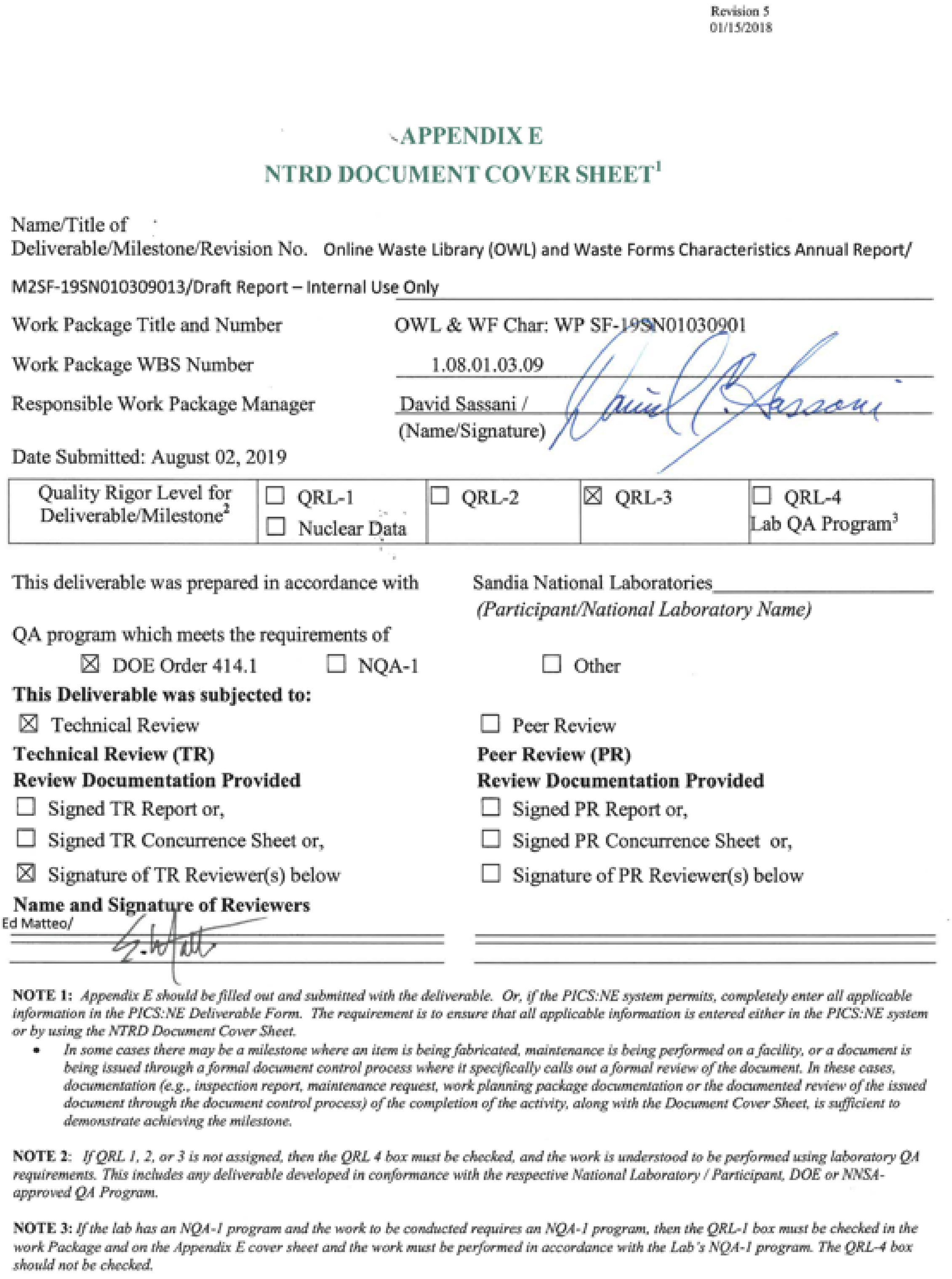

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APPENDIX E
NTRD DOCUMENT COVER SHEET[1]

Name/Title of Deliverable/Milestone/Revision No. Online Waste Library (OWL) and Waste Forms Characteristics Annual Report/ M2SF-19SN010309013/Draft Report – Internal Use Only

Work Package Title and Number	OWL & WF Char: WP SF-19SN01030901
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Quality Rigor Level for Deliverable/Milestone[2]	☐ QRL-1 ☐ Nuclear Data	☐ QRL-2	☒ QRL-3	☐ QRL-4 Lab QA Program[3]

This deliverable was prepared in accordance with Sandia National Laboratories
(Participant/National Laboratory Name)

QA program which meets the requirements of

☒ DOE Order 414.1 ☐ NQA-1 ☐ Other

This Deliverable was subjected to:

☒ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
☐ Signed TR Report or,	☐ Signed PR Report or,
☐ Signed TR Concurrence Sheet or,	☐ Signed PR Concurrence Sheet or,
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Name and Signature of Reviewers

Ed Matteo/

NOTE 1: *Appendix E should be filled out and submitted with the deliverable. Or, if the PICS:NE system permits, completely enter all applicable information in the PICS:NE Deliverable Form. The requirement is to ensure that all applicable information is entered either in the PICS:NE system or by using the NTRD Document Cover Sheet.*

- *In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity, along with the Document Cover Sheet, is sufficient to demonstrate achieving the milestone.*

NOTE 2: *If QRL 1, 2, or 3 is not assigned, then the QRL 4 box must be checked, and the work is understood to be performed using laboratory QA requirements. This includes any deliverable developed in conformance with the respective National Laboratory / Participant, DOE or NNSA-approved QA Program.*

NOTE 3: *If the lab has an NQA-1 program and the work to be conducted requires an NQA-1 program, then the QRL-1 box must be checked in the work Package and on the Appendix E cover sheet and the work must be performed in accordance with the Lab's NQA-1 program. The QRL-4 box should not be checked.*

AKNOWLEDGEMENTS

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This report benefitted from internal technical review by Ed Matteo (SNL).

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ACRONYMS

ASTM	American Society for Testing and Materials
C.E.	common era
CSSF	Calcine Solids Storage Facilities
DOE	U.S. Department of Energy
DOE-EM	DOE Office of Environmental Management
DOE-NE	DOE Office of Nuclear Energy
DHLW	DOE-managed (as) high-level radioactive waste
DSNF	DOE-managed spent nuclear fuel
EA	environmental assessment
EBR-II	Experimental Breeder Reactor II
ECN	External Collaboration Network
EFTEM	energy-filtered TEM mapping
EELS	electron energy-loss spectroscopy
EMT	electrometallurgical treatment
EP	Extraction Protection
ER	electrorefiner
FFTF	Fast Flux Test (Reactor) Facility
FRG	Federal Republic of Germany
FY	fiscal year
GDSA	geologic disposal safety analyses
GRAAL	Glass Reactivity with Allowance for the Alteration Layer
HIP	hot isostatic press (ed/ing)
HLW	high-level radioactive waste
INL	Idaho National Laboratory
INTEC	Idaho Nuclear Technology and Engineering Center
IPyC	inner dense pyrolytic carbon
ISG	International Simple Glass
LA	license application
MCC	Materials Characterization Center
MOX	mixed oxide (fuel)
MRWFD	Materials Recovery and Waste Form Development

N/A	not applicable
NMR	nuclear magnetic resonance
NQA-1	Nuclear Quality Assurance-1
NRC	U.S. Nuclear Regulatory Commission
OoM	orders of magnitude
OPyC	outer dense pyrolytic carbon
OUO	official use only
OWL	Online Waste Library
PA	performance assessment
PCT	Product Consistency Test
PRI	passivating reactive interphase
PWR	pressurized water reactor
RCRA	Resource Conservation and Recovery Act
R&A	review and approval
R&D	research and development
SAR	Safety Analysis Report
SBW	sodium-bearing waste
SiC	silicon carbide
SFDB	Spent Fuel Database
SNF	spent nuclear fuel
SNL	Sandia National Laboratories
SRS	Savannah River Site
SFWST	Spent Fuel and Waste Disposition
STEM-HAADF	scanning transmission electron microscopy with a high-angle annular dark-field detector
TRISO	tristructural-isotropic
TRU	transuranic
UNF	used nuclear fuel
UNF-ST&DARDS	Used Nuclear Fuel-Storage, Transportation & Disposal Analysis Resource and Data Systems
U.S.	United States
UUR	unlimited, unrestricted release
WFDOE	waste form disposal options evaluation
WG	waste group

WIPP	Waste Isolation Pilot Plant
WTP	Waste Treatment and Immobilization Plant
WTP-SW	WTP secondary waste
YM	Yucca Mountain

Selected Units

Bq	becquerel
ft	foot
GWd	gigawatt·days
in.	inch
lb	pound
MT	metric ton
MTHM	metric ton of heavy metal
MWd	megawatt·days
MTU	metric ton of uranium
wt %	weight percent
W	watt

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SPENT FUEL AND WASTE DISPOSITION/SPENT FUEL AND WASTE SCIENCE AND TECHNOLOGY

1. INTRODUCTION

This report represents completion of milestone deliverable M2SF-19SN010309013 "Online Waste Library (OWL) and Waste Forms Characteristics Annual Report" that reports annual status on fiscal year (FY) 2019 activities for the work package SF-19SN01030901 and is due on August 2, 2019. The online waste library (OWL) has been designed to contain information regarding United States (U.S.) Department of Energy (DOE)-managed (as) high-level waste (DHLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible; note that no classified or official-use-only (OUO) data are planned to be included in OWL). There may be up to several hundred different DOE-managed wastes that are likely to require deep geologic disposal.

This annual report on FY2019 activities includes evaluations of waste form characteristics and waste form performance models, updates to the OWL development, and descriptions of the management processes for the OWL. Updates to the OWL include an updated user's guide, additions to the OWL database content for wastes and waste forms, results of the beta testing and changes implemented from it. Also added are descriptions of the management/control processes for the OWL development, version control, and archiving. These processes have been implemented as part of the full production release of OWL (i.e., OWL Version 1.0), which has been developed on, and will be hosted and managed on, Sandia National Laboratories (SNL) systems. The version control/update processes will be implemented for updates to the OWL in the future. Additionally, another process covering methods for interfacing with the DOE SNF Database (DOE 2007) at Idaho National Laboratory on the numerous entries for DOE-managed SNF (DSNF) has been pushed forward by defining data exchanges and is planned to be implemented sometime in FY2020. The INL database is also sometimes referred to as the Spent Fuel Database or the SFDB, which is the acronym that will be used in this report. Once fully implemented, this integration effort will serve as a template for interfacing with additional databases throughout the DOE complex.

In FY2018, the OWL team pursued three studies to evaluate/redefine waste form characteristics and/or performance models (Sassani et al. 2018). The first study evaluated characteristic isotopic ratios for various waste forms included in postclosure performance studies to delineate isotope ratio tags that may quantitatively identify each waste form. In the second study, the team evaluated the basis for using the glass waste degradation rate models to simulate degradation of the hot isostatic pressed (HIP) calcine waste form. The third study is an ongoing investigation of the performance behavior of tristructural-isotropic (TRISO) particle fuels. The effort includes development of a stochastic model for the degradation of those fuels that accounts for simultaneous corrosion of the silicon carbide (SiC) layer and radionuclide diffusion through it.

Previously, Sassani et al. (2017) provided an update to Sassani et al. (2016) and included the following:

- An updated set of inputs (Sassani et al. 2017, Section 2.3) on various additional waste forms covering both DSNF and DHLW for use in the inventory represented in the geologic disposal safety analyses (GDSA)
- Summaries of evaluations initiated to refine specific characteristics of a particular waste form for future use (Sassani et al. 2017, Section 2.4)
- Updated development status of the Online Waste Library (OWL) database (Sassani et al. 2017, Section 3.1.2) and an updated user guide to OWL (Sassani et al. 2017, Section 3.1.3)
- Status updates (Sassani et al. 2017, Section 3.2) for the OWL inventory content, data-entry checking process, and external OWL beta testing initiated in FY2017

Sassani et al. (2017) updated the preliminary FY2016 inventory by adding the additional possible waste forms (DOE 2014) that were not previously included in GDSA representations, for which GDSA evaluation of thermal or radionuclide inventory aspects may be somewhat expanded compared to the previous analyses. Specifically, this expansion included the following:

- 340 Hanford Cs and Sr vitrified glass canisters (Wilson 2016, Table 2-6)
- 34 glass canisters of Hanford Federal Republic of Germany (FRG) glass, which has been designated as remote-handled transuranic (TRU) waste (Bounini and Anderson 2000), though it may be disposed in a deep geologic repository with other heat-producing waste
- The planned waste form for calcine waste, which is a HIP waste form (glass ceramic) can, with ~10 HIP cans loaded/stacked into naval canisters for a total of ~320 canisters (~5.5-ft diameter × ~15-ft height naval canisters/waste packages containing ~10 HIP cans each; SNL 2014)

Although most of these updates are relatively small from the standpoint of inventory mass, they may have some implications for analyses of thermal effects. The reason is that some of these added wastes tend to have higher average thermal loads per canister than the inventory previously evaluated in GDSA. Additionally, some of these waste forms represent larger waste packages, which may expand handling and emplacement considerations (e.g., planned calcine HIP waste form waste packages).

In Sassani et al. (2017), a number of questions regarding the characteristics of various waste forms led to three studies on waste form characteristics details. The first study assessed the potential sinks for ^{129}I in the various processes at the SRS that form the HLW glass and estimated the ^{129}I content of the SRS glass. The second study assessed the quantity of ^{135}Cs contained in the Cs capsules and in the FRG glass at Hanford. Estimates of the quantities of ^{135}Cs and ^{129}I are documented in Price (2018) and Savannah River Remediation (2018), respectively. The third study validated characteristic isotopic ratios for various waste forms included in postclosure performance studies (Section 3.4.1). This aspect arose due to questions regarding the relative contributions of radionuclides from disparate waste forms in GDSA results, particularly, radionuclide contributions of DSNF versus DHLW glass.

Sassani et al. (2017) reported OWL database updates in three areas. First, additional data for waste types (and their potential waste forms) and source documentation had been added to the OWL to flesh out its content covering DHLW and SNF. Second, in conjunction with further data entry, a process of checking the data entry into the OWL against the source documentation was launched to search for and rectify any errors in data entry. This checking was performed by technical individuals independent of the data-entry process. These individuals documented any issues noted and resolved the issues with the data-entry staff. Third, because the OWL was modified throughout the year in terms of its interface and features, another process to assess the usability of the OWL was completed. This process is referred to here as the external OWL beta test and involved technical staff from within the DOE Office of Nuclear Energy (DOE-NE) and DOE Office of Environmental Management (DOE-EM), as well as at other national laboratories, using the OWL and providing feedback on its utility and content.

1.1 Purpose and Scope

In 2014, SNL lead an analysis of the disposal of both commercial SNF and DHLW and DSNF in the variety of disposal concepts being evaluated within the previous Used Fuel Disposition Campaign and generated a report titled *The Evaluation of Options for Permanent Geologic Disposal of Used Nuclear Fuel and High-Level Radioactive Waste Inventory in Support of a Comprehensive National Nuclear Fuel Cycle Strategy* (SNL 2014). For convenience, that report is referred to herein as the WFDOE, an acronym for *Waste Form Disposal Options Evaluation*. That Used Fuel Disposition Campaign work covered a comprehensive inventory and a wide range of disposal concepts and provided the impetus for developing the OWL and for evaluating waste form characteristics.

The scope of the inventory and waste form characteristics work in this area covers DSNF and DHLW, with the current intent to dispose of these in a deep geologic repository. It is noted that the DHLW includes wastes that may be dispositioned in the future with a waste classification different than HLW (which would perhaps entail a different disposal pathway). In this work, the theoretical geologic repository for wastes, including DSNF and DHLW, is a deep mined geologic repository. The purpose of the work directly on OWL is to provide the inventory data for GDSA analyses of generic repositories for these wastes and their waste forms. Additional work on specific waste form characteristics includes assessing the inventory data and ensuring information exists for disposal relevant radionuclides, as well as evaluating the waste form degradation behavior of various waste forms for implementation into GDSA models of postclosure safety performance assessments.

This report does not attempt to reproduce the OWL content. Rather, Sections 2 and 3 summarize and describe the development of the OWL and its content, to provide an understanding of the OWL capabilities development and content coverage, as well as an overview of the processes applied to during the OWL development.

1.2 Background

The WFDOE (SNL 2014) provided part of the technical basis for the DOE (2014) assessment of disposal options. The WFDOE (SNL 2014) work provides the starting point for information consideration of inventory for disposal in a generic repository. Both the wastes and waste forms considered in the previous work, as well as summaries of disposal concepts evaluated, are given below (Section 1.2.2). For convenience, a list of key definitions is presented first in Section 1.2.1.

1.2.1 Key Definitions

The following key definitions clarify the meaning of certain terms that are used in a specific manner within OWL and this status report. These terms may or may not be defined in the same manner in other reports cited herein.

Waste Type—The currently existing materials (in whatever form, abundance, and location they occupy) that either are or will be processed into some waste form to be disposed of a deep geologic repository. Some waste types may have more than one possible waste form depending on the processing needed, whereas waste types that require no processing other than packaging may equate to a single waste form.

Waste Form—The end-state material, as packaged, that is to be disposed of in a deep geologic repository. Examples include commercial SNF and HLW glass. For this report, a vessel that cannot be separated easily from the waste form is considered to be part of the waste form. For instance, a glass pour canister is essential for making the glass waste form. The HLW glass is poured into the canister; the canister is not easily removed and it is not intended to contain other waste forms or waste types. Therefore, the glass pour canister is considered part of the waste form.

Vessel—A canister, container, cask, overpack, etc. that can serve as a single layer in a nested system designed to surround and contain the waste form for the purposes of storage, transportation, and/or disposal.

Disposal Form—The waste form plus the nested system of vessels needed to meet the requirements for disposal of the waste form.

Waste Group—A set of waste forms with similar disposal characteristics such as expected postclosure degradation behavior; radionuclide inventory; thermal output; physical dimensions; chemical reactivity; packaging of the waste form; and safeguards and security needed for handling, transporting, and disposing of the waste form in the context of the disposal concepts. The groupings used in this report are consistent with the ten groups defined in WFDOE (SNL 2014) and discussed further in Section 1.2.2.

1.2.2 Waste Types and Waste Forms Considered

The scope of the waste in the WFDOE (SNL 2014) includes all existing SNF from commercial, defense, and research reactors, and SNF from reasonably foreseeable operations of existing reactors (projected to exist in year 2048). That study’s scope also includes existing HLW forms (e.g., vitrified HLW at SRS and West Valley Demonstration Project) and waste forms projected to be generated in the future from existing process waste (e.g., projected vitrified HLW from HLW currently in tanks at Hanford, SRS, and the INL). In addition, the WFDOE (SNL 2014) considers both direct disposal of waste forms that are not currently planned for disposal without further treatment (e.g., calcine waste at the INL) and alternatives to planned treatments. The WFDOE (SNL 2014) acknowledges existing plans, commitments, and requirements when applicable, but evaluates options for disposal based primarily on technical, rather than programmatic or regulatory constraints.

The WFDOE (SNL 2014) waste inventory was categorized into 43 different waste types. Considering the alternative treatment options for some of these 43 waste types, the WFDOE (SNL 2014) defined 50 waste forms, which were aggregated into the 10 waste groups (SNL 2014, Table ES-2) with similar disposal characteristics (listed in the definition in Section 1.2.1). The aggregation into waste groups allowed a high-level identification of waste forms that have unique qualities in any one of those disposal characteristics. The 10 groupings listed in Table ES-2 of SNL (2014), except those groups consisting solely of commercial SNF (waste group 1 (WG1) and WG2), are utilized below in this study to consider information needs regarding features of any repository concept.

Major assumptions and considerations used in the WFDOE (SNL 2014) include the following:

- HLW and SNF considered are restricted to existing materials and those materials that can be reasonably expected to be generated by existing or currently planned facilities and processes.
- The inventory of HLW and SNF is intended to include existing materials in the U.S. requiring deep geologic isolation. It is based on the best available information.
- Technologies under consideration, including both for waste treatments and disposal concepts, are limited to those that can be deployed in the near future.
- Programmatic constraints, including legal, regulatory, and contractual requirements, are acknowledged when applicable, but are not considered in the technical evaluations, consistent with the goal of the study to provide technical input to strategic decisions. For example, the identification of wastes requiring deep geologic isolation is based on consideration of overall risk, rather than on specific U.S. legal and regulatory requirements.
- Evaluations are primarily qualitative and are based in large part on insights from past experience in waste management and disposal programs in both the U.S. and other nations.

The assumptions above apply also to the present work, which builds on the WFDOE (SNL 2014) but the focus herein for the OWL is more oriented on the DHLW and DSNF, although postclosure waste form degradation behavior is considered for all waste forms to be disposed in deep geologic repository systems. This assessment of the DHLW and DSNF inventories is working to provide disposal inventories for GDSA for analyses of generic repository concepts and to develop the online waste library (OWL) to manage the waste types/forms information (including any potential additions to the inventory to be added to the previous list; SNL 2014, Tables C-1 and ES-1), and develop constraints on waste form postclosure degradation performance.

The set of mined disposal concepts used in the WFDOE (SNL 2014) work is the same as that identified by DOE’s Used Fuel Disposition Campaign as a primary target for further research and development. These same disposal concepts are presented here as a useful and representative, rather than a comprehensive, set of concepts, and are also the concepts being used in this work.

1.3 Disposal Concepts Considered

The WFDOE (SNL 2014) considered the four representative disposal concepts selected for further research and development activities by the DOE-NE’s Used Fuel Disposition Campaign (Rechard et al. 2011). These four concepts are mined repositories in three geologic media—salt, clay/shale rocks, and crystalline (e.g., granitic) rocks—and deep borehole disposal in crystalline rocks. As summarized by

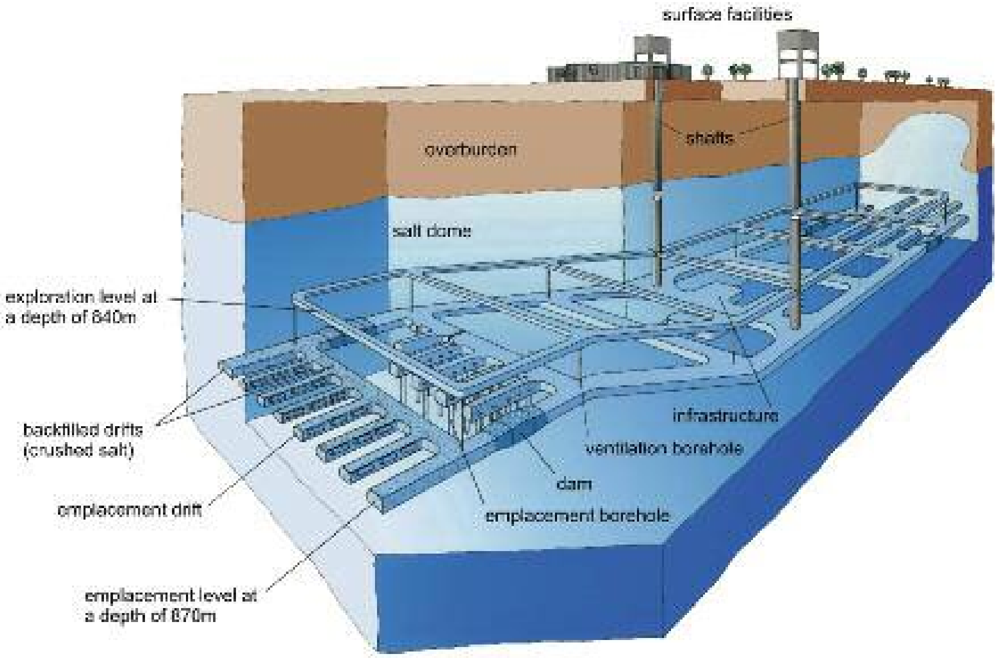
Rechard et al. (2011), selection of these four concepts begins with the observation that options for disposal of SNF and HLW have been evaluated in multiple nations for decades, and deep geologic disposal was recognized as early as the late 1950s to be the most promising approach (NA/NRC 1957). By the 1980s, the U.S. waste management program concluded that multiple geologic media had the potential to provide robust isolation, and that conclusion remains valid today. Experience gained in waste management programs in other nations reinforces that conclusion (NWTRB 2009). For example, Finland has been granted a construction license and Sweden has a license application (LA) pending for proposed mined repositories for SNF in crystalline rock. The U.S. has an operating repository in salt for TRU waste at the Waste Isolation Pilot Plant (WIPP), and Germany has extensive experience with the design of a mined repository for SNF and HLW in salt (e.g., BMWi 2008). France, Switzerland, and Belgium have completed detailed safety assessments for proposed SNF and HLW repositories in clay and shale media. Although no nations are currently planning deep borehole repositories, the concept has been evaluated in multiple programs since the 1970s, and remains viable for waste forms small enough for emplacement in boreholes (e.g, Brady et al. 2009). However, given that the DOE decided to not continue to pursue deep borehole disposal in FY2017, this disposal option is not included in this report; only mined geologic repository concepts are considered.

Variants of the three primary mined geologic disposal concepts are also considered as appropriate. For example, as described by Hardin et al. (2012), some mined repository concepts can be implemented in an open mode, that is, a mode that includes active ventilation during the operational period. The choice between an open mode implementation versus a closed mode with early emplacement of backfill would depend, in part, on thermal load management needs.

Other mined geologic disposal concepts have been proposed and are potentially viable. For example, Canada is currently evaluating a mined repository for intermediate-level radioactive waste in carbonate rocks (NWMO 2011) and the U.S. has evaluated a potential mined repository concept in volcanic tuff (DOE 2008).

1.3.1 Mined Repositories in Salt

The primary information sources for mined repositories in salt come from the U.S. WIPP program (DOE 1996, 2009), which is an operating repository accepting and emplacing defense-related TRU waste, and the proposed German repository at Gorleben (e.g., BMWi 2008). Figure 1-1 shows a representative design for a salt repository. Emplacement of waste would occur in horizontal tunnels (referred to as “drifts” in mining terminology), or in subhorizontal boreholes drilled along the drifts, at depths between 500 and 1,000 m below the land surface. As proposed, access to the emplacement areas would be by hoists in vertical shafts. Primary isolation would be provided by the essentially impermeable nature of intact salt.



Source: BMWi 2008, Figure 15.

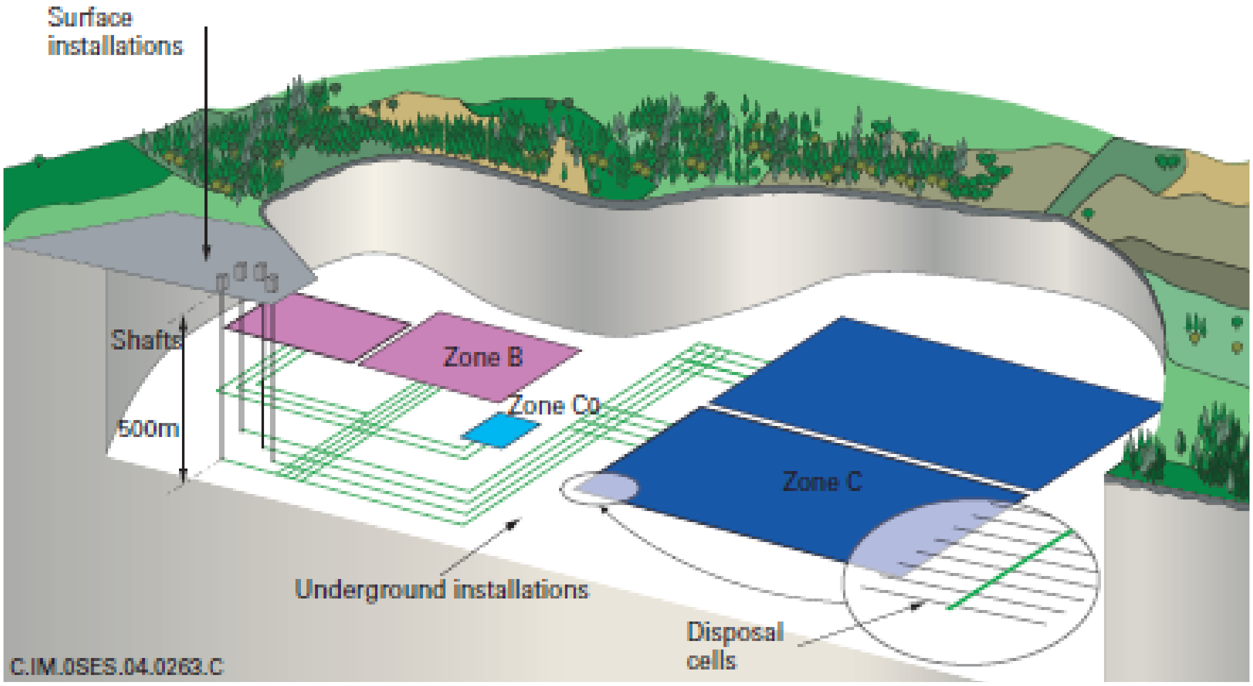
Figure 1-1. Schematic Representation of a Mined Repository in Salt

Other attributes of salt relevant to repository design and waste disposal include relatively high thermal conductivity, which allows conductive transfer of heat away from the waste, relatively low water content, and viscoplastic mechanical response (e.g., Hansen et al. 2016). This viscoplastic behavior of salt allows creep behavior under differential stress that causes salt to slowly flow. This slow flow leads to closing and healing of fractures and open spaces, allowing for the use of access shaft seal systems that will compact under lithostatic load to achieve extremely low permeability. The salt creep will tend to close emplacement regions relatively rapidly on geologic time scales (perhaps within decades) after waste emplacement, potentially complicating the implementation of extended periods of ventilation without significant drift support. However, the relatively high thermal conductivity of salt significantly reduces the need to remove heat with ventilation and allows more flexibility of thermal loading to meet temperature limits, which are generally higher than those for concepts that include an in-drift clay backfill/barrier.

There are two major end-member types of salt systems being examined (Hansen et al. 2016). One system is bedded salt, which occurs in horizontal layers of nearly pure sodium chloride originally deposited from shallow, evaporating salt-saturated seawater. Bedded salt can contain both small quantities of trapped brine and interbedded layers of clays and other evaporite minerals such as anhydrite (calcium sulfate). The second system is domal salt, which has moved from its original bedded form into dome-shaped structures due to viscoplastic flow over geologic time. Domal salt tends to have less water, and fewer impurities and intact interbeds than bedded salt, but domal salt is more restricted geographically. To the extent that sufficient water may be present to saturate a repository waste emplacement region in either bedded or domal salt, it will form salt-saturated brine and chemical conditions will be reducing. Any free oxygen introduced would be consumed by corrosion of metal in the waste packages or other engineered systems. Because of the essentially impermeable nature of the salt host rock and the very low potential for advective transport of radionuclides away from the disposal region, little or no reliance for the long-term performance is given to the waste form or the waste packaging.

1.3.2 Mined Repositories in Clay and Shale Rocks

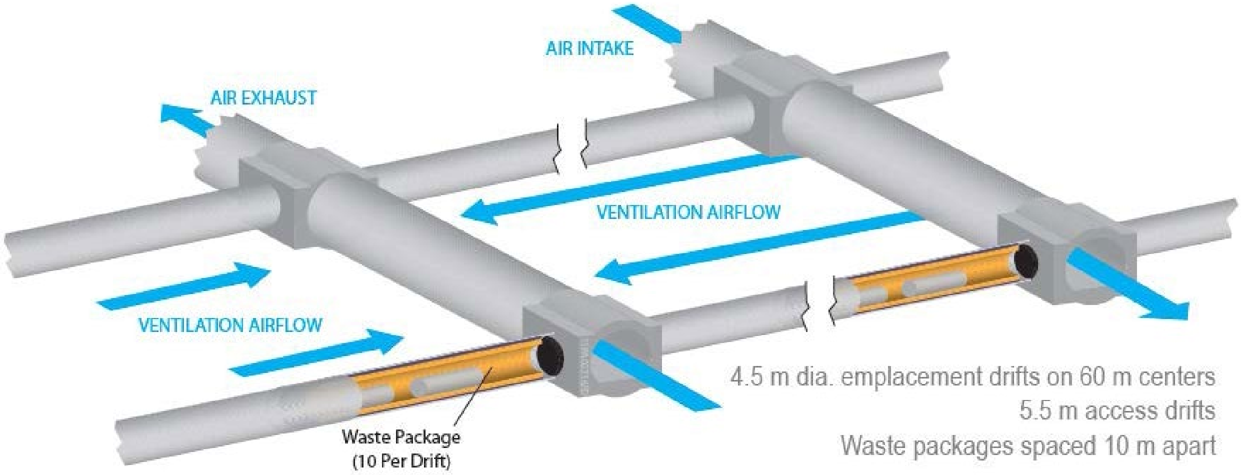
The primary information sources for mined repositories in clay and shale rocks come from the French, Swiss, and Belgian national programs, each of which is evaluating disposal in argillaceous host rocks (ANDRA 2005a, 2005b; NAGRA 2002; ONDRAF/NIRAS 2011). Figure 1-2 shows a representative design for a mined repository in clay or shale. Emplacement of waste would occur in horizontal holes bored laterally from access drifts at a nominal depth of 500 m below the land surface. As proposed, access to the underground emplacement region would be by hoists in vertical shafts. Isolation would be provided by long-lived waste packages, waste forms that are long-lived in the chemically reducing environment, and by the extremely slow rate of diffusion through the low-permeability host rock. Sorption of radionuclides on clay minerals within the backfill and the host rock would effectively prevent long-term releases of all but the most mobile radionuclides, such as ^{129}I and ^{36}Cl, and long-term releases of these species would remain very low because transport is diffusion dominated.



Source: ANDRA 2005b.

Figure 1-2. Schematic Representation of a mined Repository with Various Waste Form Zones in Argillaceous Rock

Argillaceous rocks display a broad range of physical properties from weakly indurated clays capable of viscoplastic flow (e.g., the formation being evaluated for a repository in Belgium), to strongly indurated and massive argillites such as that being evaluated for disposal in France, to laminated shales common in many sedimentary basins, especially in the U.S. All these lithologies are characteristically extremely low permeability, which will lead to diffusion-dominated release pathways and contain an abundance of clay minerals that contribute to radionuclide sorption. All argillite varieties have lower thermal conductivity than salt. Mined repository concepts in clay and shale rocks must be designed accordingly to accommodate thermal loads. The most widely adopted approach to manage decay heat in clay/shale rocks is to use relatively small waste packages (up to four spent fuel assemblies per package) and to space the emplacement drifts relatively far apart. Hardin et al. (2012) evaluated the potential for increasing the thermal loading capacity of a mined repository in shale by considering an “open-emplacement” design concept in which emplacement drifts remain completely open to allow extended ventilation to remove decay heat, as illustrated in Figure 1-3. Backfilling and sealing of access drifts would occur at repository closure, with the option of leaving the emplacement drifts open permanently, without backfill, if the operational constraints so dictate. Some argillites would require ground support for maintaining the openings for long durations.

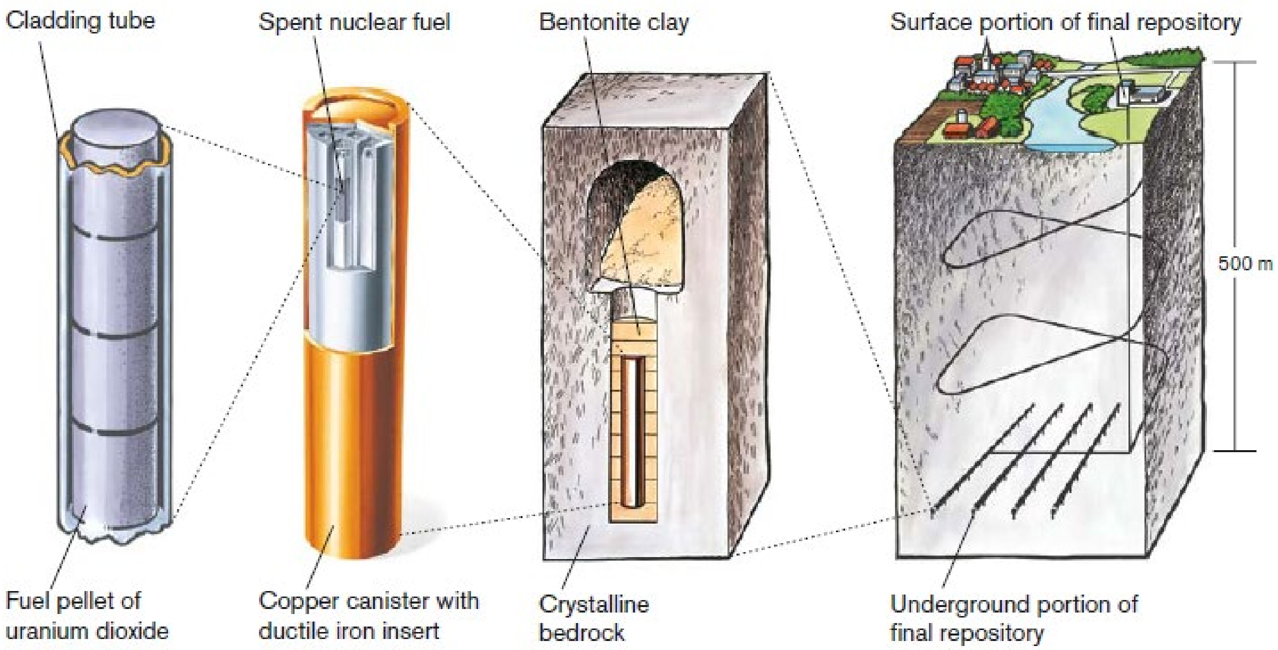


Source: Hardin et al. 2012, Figure 1.5-3.

Figure 1-3. Schematic of Shale Open (i.e., no backfill) Emplacement Repository Concept

1.3.3 Mined Repositories in Crystalline Rock

The primary sources of information for mined repositories in crystalline rock come from the Swedish and Finnish programs (SKB 2011; Posiva Oy 2013), which are in various stages of seeking and obtaining licenses to construct and operate facilities for the permanent disposal of SNF. Other nations are also conducting research on mined repositories in crystalline rock, including Canada, Japan, Korea, China, and the Czech Republic. Figure 1-4 shows a representative disposal concept developed for the Swedish program. Wastes (SNF in this example) are emplaced in vertical boreholes drilled in the floor of



Source: SKB 2011, Figure S-1.

Figure 1-4. Schematic Representation of a Mined Repository in Crystalline Rock

horizontal drifts at a nominal depth of 500 m below the land surface. Alternative design options call for emplacing waste in horizontal tunnels drilled into the sides of the access drifts. In either case, access to the waste disposal region is by an inclined ramp in this concept, rather than vertical shafts and hoists.

Generally, crystalline rock repository systems provide isolation by long-lived corrosion-resistant copper waste packages, by the durability of the uranium oxide SNF waste form, and by the high sorption capability of the bentonite clay buffer that would surround the waste packages in the Swedish repository concept (SKB 2011). Both the copper waste package and SNF planned for disposal in the Swedish repository are more durable under chemically reducing conditions. Other reduced waste forms (e.g., metallic fuels) would be closer to their equilibrium conditions and would corrode more slowly than in oxidizing environments. Still other waste forms (e.g., HLW glass) may not benefit from the reducing environment as much in terms of waste form lifetimes in such a disposal concept, but many radionuclide solubility limits would be very low and substantial performance would be expected based on the waste package lifetime and the bentonite backfill capabilities. Open and interconnected fractures, which can occur in crystalline rocks at these depths, have the potential to provide pathways for advective transport of radionuclides from the repository to the near-surface environment if the near-field barriers were to be breached. Design concepts therefore avoid emplacement in areas intersected by fractures and surround waste packages with a low-permeability bentonite clay buffer (SKB 2011; Posiva Oy 2013).

Because bentonite undergoes durable physical changes at elevated temperatures, crystalline repository concepts generally have defined a peak temperature constraint at the waste package surface of approximately 100°C. Existing design concepts meet this constraint with relatively small waste packages, accommodating four spent fuel assemblies per package.

As discussed by Hardin et al. (2012, 2013), alternative design concepts for mined repositories in crystalline (or other hard) rocks can address thermal load management issues by emplacing waste in large tunnels or vaults that remain open, without backfill, for extended periods of ventilation prior to permanent closure. In unsaturated rocks above the water table, the limited availability of water for advective transport has the potential to allow permanent disposal without backfill emplacement, although the oxidizing conditions in an unsaturated environment will require alternative robust designs for waste packaging and could allow for more rapid degradation of UO_2 waste forms once exposed. The same would be true for other reduced waste forms, especially metallic waste forms, which would also have higher potential for exothermic oxidation phenomena. Additionally, the HLW glass waste form may undergo different degradation mechanisms in a humid environment versus saturated conditions (Cunnane et al. 1994). In saturated environments, emplacement of a clay backfill will be desirable after extended ventilation to reduce the potential for advective transport away from the waste packages.

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2. INVENTORY FOR DISPOSAL ANALYSES

The WFDOE (SNL 2014) reached two overarching conclusions:

- The full inventory of DOE-managed and commercial HLW and SNF is diverse, and DOE has a broad range of viable options for disposing of it.
- The selection of preferred options will involve policy and programmatic considerations outside the scope of the report. The selection will be influenced by, and may help inform decisions about, multiple factors that could include future storage and packaging of commercial SNF, treatment and packaging of existing DOE wastes, and progress in repository siting.

All of the disposal concepts evaluated in that study have the potential to provide robust long-term isolation for specific wastes. In addition, each of the three mined repository concepts could accommodate essentially all of the identified waste groups. The only exception was for direct disposal of untreated sodium-bonded (Na-bonded) SNF, for which information is insufficient to support evaluation for disposal in any geologic disposal concept. The report also concluded that deep boreholes are feasible for disposal of small waste packages and provide flexibility to any disposal strategy. Additional generic and site-specific research and development (R&D) is needed before any disposal options can be implemented, although no recommendations were made with respect to specific R&D activities.

The results of the WFDOE (SNL 2014) study indicate that some disposal options for mined repository concepts may provide greater flexibility or fewer challenges than others. Specifically,

- Salt provides greater flexibility for disposal of heat-generating wastes because of the high thermal conductivity and high temperature limit. Disposal in this medium provides greater confidence in estimates of long-term performance because it limits radionuclide transport (low permeability) and reduces the reliance on the waste form and waste package lifetimes. The relative lack of water and the high cross-section of chlorine for capture of thermal neutrons make it easier to address criticality concerns. In some cases, it may be appropriate to directly dispose of some untreated waste types, potentially reducing cost and risks associated with waste treatment. The operational experience at the WIPP provides additional confidence in this disposal concept.
- Clay/shale, a disposal medium for which there is a significant amount of world-wide experience, has shown strong results as a disposal option for most waste groups with respect to most metrics. It is an attractive disposal option because it limits far-field radionuclide transport (low permeability and high sorption) and, therefore, reduces the reliance on the waste form and waste package lifetimes, compared to a crystalline disposal concept. However, compared to salt, there is more reliance on source-term performance and the thermal constraints are more stringent.
- Mined repositories in crystalline rocks may offer operational advantages because of the rock strength, which allows easy maintenance of the robust openings for long periods without substantial support. This strength provides the potential flexibility of possible ramp access. However, for fractured crystalline systems, high reliance on clay barriers immediately surrounding the waste package poses additional challenges for high thermal loads that may

> degrade such barriers. Because of the need for robust performance of the source-term, confidence in system performance may be directly dependent on very conservative thermal management.

In addition to the WFDOE (SNL 2014), a number of previous studies have evaluated the full inventory for storage and transportation purposes (Carter and Leduc 2013; Carter and Vinson 2014) as well as the more restricted inventory and smaller volume of generally cooler waste forms (e.g., Carter et al. 2012; Carter et al. 2013). These studies also inform the analyses done in FY2016 for the Used Fuel Disposition Campaign (Sevougian et al. 2016). The previous inventory estimates (Carter et al. 2012; Carter et al. 2013) were synthesized and integrated by Wilson (2016) to provide a preliminary inventory for use in those Used Fuel Disposition Campaign scoping analyses. It should be noted that the inventory defined in Wilson (2016) was considered preliminary and was developed for use in the prototype analyses (Sevougian et al. 2016). The preliminary inventory (covered in Section 2.1) is updated/expanded in the OWL. Given the major characteristics of the OWL inventory, the broad generalities for mined disposal concepts defined above have differences for system performance reliance on natural features versus variations on design concepts. Discussion is given also for potential additional wastes/waste forms for future inventories considered for deep geologic disposal (Section 2.2).

2.1 DHLW and DSNF Included in Inventory for Analyses

This section provides an overview of the inventory included for engineering and system performance analyses for FY2016 and summarizes the FY2017 updates to that inventory from Sassani et al. (2017). The included set of materials for the inventory may change in the future based on the designation decisions made by DOE and/or updated technical information about the wastes/waste forms. The included inventory in this report is only for use in analyses of a potential generic repository, and there is no intent to indicate how to classify any of the wastes/waste forms included herein.

Initial GDSA work (Sevougian et al. 2016) represented the major high-level waste (HLW) groups (Savannah River Site (SRS) and Hanford HLW Glasses) and DOE(-managed) spent nuclear fuel (DSNF) materials in the inventory to evaluate potential releases from both generic salt and generic crystalline (granitic) repositories. Wilson (2016) provides the preliminary inventory for the GDSA analyses including both DHLW and DSNF waste canister counts and thermal information (Wilson 2016, Tables 2-1 and 2-3 to 2-6). The Wilson (2016) report describes each waste form in terms of both average radionuclide content and average thermal output evolution. The tabulation includes canister counts and thermal characteristics for each DHLW and DSNF waste form considered (Wilson 2016). For that preliminary DSNF inventory, the detailed list of DSNF types is given in Appendix A of Sassani et al. (2016, 2017) to show the specific DSNF groups/items included in the ~2,485 canisters (Wilson 2016, Table 2-1).

Wilson (2016) provides the preliminary inventory for the analyses of a generic repository and includes both DHLW and DSNF waste canister counts and thermal information (Wilson 2016, Tables 2-1 and 2-3 to 2-6). Wilson (2016) describes each waste form in terms of both average radionuclide content and average thermal output evolution for each thermal category. That tabulation includes canister counts and ranges of thermal characteristics for each DHLW and DSNF waste form considered (Wilson 2016). For the preliminary inventory assembled in this report, the various specific DSNF types contained in the

~2,485 DSNF canisters (Wilson 2016, Table 2-1) are listed in Appendix A of Sassani et al. (2017). The included DHLW canister counts are given in Wilson (2016) in Tables 2-3 to 2-6, respectively, for SRS glass (7,824 canisters), Hanford glass (11,800 canisters), INL HIP calcine (4,391 canisters), and Hanford vitrified Cs and Sr capsules (340 canisters; SNL 2014).

The major updates in FY2017 (Sassani et al. 2017, Section 2.3) to the preliminary detailed inventory include (1) the 34 glass canisters of "German" (generated for FRG testing) glasses (SNL 2014), (2) the planned HIP calcine waste form cans loaded into ~320 large canisters (~5.5-ft diameter × ~15-ft height, naval canisters; SNL 2014); and (3) the revised list of DSNF materials included in the inventory based on any applicable DOE decisions and/or new technical data. Though most of these updates are relatively small from the standpoint of inventory mass, they may have some implications for thermal analyses (e.g., FRG glasses) and handling considerations (e.g., planned calcine waste forms).

2.1.1 Discussion of Current Included Inventory for Analyses Versus Previous Inventory Data Sets

Major variations in the inventory considered for any particular repository concept may influence more than just the total radionuclide content of that repository. The inventory also affects the total thermal input, the temporal and spatial thermal distribution, the numbers of packages to be handled, and the ranges of size and mass of packages to be handled in a repository concept. A comprehensive compilation and analysis of waste form information was conducted for the Safety Analysis Report (SAR) prepared in support of the Yucca Mountain (YM) Project (DOE 2008). The SAR inventory slated for a repository at YM included a large portion of commercial SNF, only ~46% of the SAR-projected DHLW canisters, and nearly all of the DSNF.

The details of the waste inventory (in addition to commercial SNF covered in SNL 2014) for GDSA analyses are listed at the end of Section 2.1. This inventory differs from the SAR inventory primarily in two ways:

- Larger quantities of the various DHLW Glass included
- Smaller quantities of DSNF included (this has been updated in FY2017, but still does not include all DSNF that was in the SAR inventory)

The inventory from Wilson (2016) includes about 2.5 times as many DHLW canisters as were planned for the YM repository[a]. The *Nuclear Waste Policy Act of 1982* placed a legal limit on the amount of radioactive waste (in metric tons heavy metal, or MTHM) that could be disposed of in the YM repository.

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[a] Note that this means the SAR projected inventory of total DHLW canisters is only about 40% of the inventory from Wilson (2016). However, the SAR projected inventory of total DHLW canisters is about 46% of the estimated total number of canisters for DHLW given in SNL (2014)—about 20,340 canisters. The difference between Wilson (2016) and SNL (2014) relates mainly to ~1,200 more Hanford glass canisters and ~4,000 more HIP calcine canisters (smaller sized, alternative waste form) projected in Wilson (2016) versus SNL (2014).

A portion (4,667 MTHM) of this limit was allocated to DHLW glass (DOE 2008, Table 1.5.1-1). The SAR projected a total of 21,228 DHLW canisters to be delivered to the YM site from Hanford, SRS, and INL (DOE 2008, Section 1.5.1.2.1.2). Of this total, the SAR projected that only ~9,300 DHLW canisters would be included in the YM inventory (DOE 2008, Table 1.5.1-1 and Section 1.5.1.2.1.1). At the time that the SAR was completed, this amount of DHLW represented less than half of the projected DHLW inventory. The current inventory includes a higher number of total projected DHLW canisters (~24,400) than the SAR projections, with the specific differences between those two inventory projections discussed below.

2.1.1.1 Included DHLW Inventory Compared to SAR Inventory

HLW has been generated as a by-product of reprocessing SNF. Currently these wastes are stored primarily as liquid tank wastes at DOE facilities at Hanford, SRS, and INL (SNL 2014). Processing of the various DHLW wastes into their final planned waste forms has not been uniform at the various sites. As a result, the wastes currently have different physical characteristics depending on the details of the processes used, or planned to be used, for a given waste. These characteristics may be quite different for the existing waste versus the planned waste forms (SNL 2014).

The DHLW is grouped here into the following categories:

- SRS tank waste, which is currently in the process of being vitrified into glass logs
- SRS existing vitrified glass logs
- Hanford tank waste, which is planned to be vitrified into glass logs
- Calcine waste at INL, which is planned to be change into a glass ceramic waste form with a HIP process (note that direct disposal of untreated calcine was being considered potentially for Deep Borehole Disposal: SNL 2014; DOE 2014)
- FRG glass logs stored at Hanford, which have no further planned treatment (added to inventory in FY2017)
- Sodium-bearing waste (SBW) at INL, which is to be treated by fluidized bed steam reforming (to be added to inventory in the future)
- Cs and Sr capsules at Hanford, which are planned to be vitrified (note that direct disposal of these untreated capsules was being considered potentially in the Deep Borehole Disposal concept: SNL 2014; DOE 2014)

The number of waste canisters that will ultimately be available to be disposed for each these unprocessed wastes is uncertain. In some cases, the planned waste form pathway has changed, which leads to further variation in estimated numbers of canisters for a projected waste form. For example, calcine waste at INL was planned to be vitrified for delivery to YM in ~2-ft diameter × ~10-ft height canisters (DOE 2008, Section 1.5.1.2.1.2), but is now planned for HIP treatment (DOE 2010, Record of Decision (ROD)

75 FR 137)[b]. Further, some projections include additional smaller volume wastes (e.g., SBWs, German glass canisters), whereas others do not. All of these aspects have led to some variability in the projected canister totals in different reports (e.g., DOE 2008; Carter et al. 2012; SNL 2014; Wilson 2016), so it should be kept in mind that the values are approximate, and that projected canister counts should be explicit regarding which wastes are included to facilitate comparisons.

The YM SAR (DOE 2008, Section 1.5.1.2.1.2) included projections based on the best information available at the time. Wilson (2016) developed the inventory for supporting design/engineering analyses, including thermal evolution, and safety assessments of a generic repository. The two sets of projected canister values are presented in Table 2-1. There is some variability between the estimated values for Hanford and SRS DHLW glass canister projections, but the largest difference is in the values for the INL canisters. The difference in numbers of INL canisters is largely explained by the change to the planned waste form from vitrified calcine (SAR) to HIP calcine (current disposal pathway).

Table 2-1. Comparison of Numbers of Projected HLW Canisters from the Full Received (though not to be disposed) Inventory from the SAR (DOE 2008) and the Current Estimates from Wilson (2016)

Projected HLW Canisters		
Site	**YM SAR Projection[a]**	**Current Projection[b]**
Hanford	13,205 canisters	12,140 canisters
SRS	6,833 canisters	7,824 canisters
INL	1,190 canisters[c]	4,391 canisters[c]

NOTE: [a]These values represent best estimates of projected numbers of canisters that were to be delivered to the YM site at the time of the SAR (DOE 2008), however only about 46% of them were to be disposed with the remainder slated for a second repository.

[b]These estimates were developed by Wilson (2016) for the inventory in support of preliminary design thermal and postclosure safety calculations for FY2016. They are based on current planning assumptions for waste treatment.

[c]The estimate for INL HLW from the SAR included vitrification of calcine waste, whereas that from Wilson (2016) includes the assumption of an alternative calcine waste form that would be packaged for disposal in standard ~2-ft × ~10-ft cylindrical DSNF canisters.

HLW = high-level radioactive waste

INL = Idaho National Laboratory

SAR = Safety Analysis Report

SRS = Savannah River Site

YM = Yucca Mountain

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[b] The baseline canister dimensions for the planned HIP calcine waste form are ~5.5-ft diameter × ~15-ft height (Kluk et al. 2011), whereas the HIP calcine from Wilson (2016) includes the assumption of an alternative waste form packaged for disposal in a standard ~2-ft × ~10-ft cylindrical DSNF canister.

2.1.1.2 Included DSNF Inventory Compared to SAR Inventory

DOE production reactors, as well as foreign and domestic research reactors, have produced SNF with a very large range of physical characteristics. The Spent Fuel Database (SFDB) for DSNF contains hundreds of entries with a wide range of fuel types that are managed by DOE currently, or are to be received by DOE at a later date from, for example, foreign research (DOE 2007). Early SFDB work for the YM SAR led to a grouping system that categorized the total DSNF inventory into 34 groups of DSNF based in part on fuel matrix, cladding, cladding condition, and enrichment. These 34 DSNF fuel groups were the starting point for work leading up to the LA (DOE 2008) that DOE submitted to the U.S. Nuclear Regulatory Commission (NRC). The naval SNF, for example, is DOE SNF Group 32, separate from other DSNF. This DSNF grouping has proven to be very effective and is still in use today (DOE 2007; SNL 2014).

The canister counts and thermal output of the included inventory of DSNF for FY2016 analyses are given in Wilson (2016). Appendix A in Sassani et al. (2017) presents a detailed tabulation of DSNF items that are included in this inventory. That table is organized using the 34 DSNF groups. The information was extracted from the supporting data for the inventory and thermal characteristics reported by Wilson (2016). The right-hand column of the table identifies each DSNF item by name. The left-hand column identifies the DOE fuel group for each item, the mass (MTHM) of items within the fuel group, and the projected or estimated number of waste containers within each DSNF group.

2.2 Identifying Potential Additional Waste Types and Waste Forms

Reviewing the materials on radioactive waste types within the DOE-managed realm has produced a number of potential candidates to add to those waste types and waste forms that were evaluated in the WFDOE (SNL 2014). At this point in time, these candidates have only been identified but not added into the evaluations. Further consideration of these wastes in the future would determine which would be added to the list of DHLW and DSNF to be populated in the OWL database. A brief summary is given here of the waste types that are presently identified.

Within the DOE-managed waste complex, many of the waste types have been included in SNL (2014), as well as their proposed disposition as waste forms. The WFDOE (SNL 2014) inventory of wastes is a superset of the inventory discussed in Section 2.1. Inclusion of additional wastes into the OWL database would be only a first step as new waste types would only be added to the inventory based on input from the DOE.

Active research is being performed to evaluate a variety of HLW glass compositional variations to address limitations of glass formulations due to chemical components such as Fe, Al, Cr, Bi, P, Zr, and S (e.g., Kruger et al. 2012, 2013). In many of these cases, each compositional variation of the glass does not yet appear to warrant specific tracking because these glass compositions are still within the R&D stage. One exception included below is a glass composition from the high sulfur waste streams.

Advanced fuels are being developed that will at some point need disposal dispositioning, for example at research reactors like the Transient Reactor Test Facility (e.g., Pope et al. 2014). Given the wide range of fuel types existing within the DOE complex, such advanced fuels will only be considered after they are included into the DOE-managed SFDB as they would provide no immediate substantive difference for consideration.

Lastly, investigators are working to identify candidate waste forms for separated Tc waste streams, either directly from tank waste or from off-gassing as tank wastes are processed into glass (e.g., Westsik et al. 2014). Such waste forms include a wide variety of solids: borosilicate and iron phosphate glasses, cementitious grouts, geopolymers, phosphate-bonded ceramics, the fluidized bed steam reforming aluminosilicate waste form, the crystalline ceramic Synroc waste form, iron-technetium oxides, metal alloys, technetium oxides, silicate minerals, titanates, sulfides, phosphates, layered double hydroxides, and sulfur-based aerogels. One such waste form is included here because it has already been separated specifically, and is planned to be formed into the future. Additional tracking of potential waste types/forms for disposal disposition should only begin once the waste types/forms are actually generated.

Potential additions to the WFDOE (SNL 2014) inventory include the following waste types/forms from Hanford tank waste:

- **Existing Separated Waste**—Demonstration of Cs-Tc removal from tank waste brines via ion exchange resins to be incorporated into high activity waste glass (existing separated waste; Hassan et al. 2000).
- **Potential Separated Waste**—Potential new glass formulations for projected high sulfur HLW streams from Hanford Tank Waste (likely separated waste; Kruger et al. 2013).
- **Potential Separated Waste Type and Waste Form**—Off-gas condensate from the Waste Treatment and Immobilization Plant (WTP) low activity waste vitrification facility. The condensate, also known as WTP secondary waste (WTP-SW), will be generated and enriched in volatile components such as ^{137}Cs, ^{129}I, ^{99}Tc, Cl, F, and SO_4 that volatilize at the vitrification temperature of 1,150°C in the absence of a continuous cold cap (that could minimize volatilization). The current waste disposal path for the WTP-SW is to process it through the Effluent Treatment Facility. Fluidized Bed Steam Reforming is being considered for immobilization of the Effluent Treatment Facility concentrate that would be generated by processing the WTP-SW (Crawford et al. 2014).

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3. STATUS OF MANAGING INVENTORY DATA AND POSTCLOSURE PERFORMANCE ASSESSMENTS OF REPOSITORY CONCEPTS

This section summarizes the progress made on designing and developing the OWL database to manage the information of the wastes and waste forms from the WFDOE (SNL 2014). It also describes the status of constraints on waste form degradation for postclosure performance assessments (PAs). In Section 3.1, the OWL database is described with updated status information about the changes since FY2018. Both the OWL database model (Sassani et al. 2017) and an updated version of the *OWL User's Guide* (Section 3.1.3 and Appendix B) describe the architecture and usage of the OWL. Section 3.2 provides descriptions of the new additions to the inventory content of OWL, the status of the data-entry checking process, the updates from the beta testing of OWL, and the processes being developed for OWL interfacing with the DOE SFDB (DOE 2007) at INL and for versioning controls on OWL. Section 3.3 provides waste form performance constraints for postclosure PA in the context of the GDSA effort, and Section 3.4 includes ongoing evaluations of waste form characteristics and performance behavior.

3.1 Developing the OWL

The OWL has two primary purposes. One purpose, already mentioned, is providing a consolidated single source for information on the many different DOE-managed wastes that are likely to require deep geologic disposal, such that one can easily query the data. A second purpose is to be the primary source for information on the waste types, inventory, and waste form characteristics necessary to develop a database of parameters for a PA analysis for a repository safety assessment. The initial focus in this activity is to develop the database with a user-friendly interface and to populate it with the information on waste types and waste forms. The second purpose—linking OWL directly to performance modeling through a parameter database in order to facilitate PA analysis—will occur in subsequent activities after the OWL is populated more comprehensively for waste types and forms.

Although the goal is to make OWL available through the world-wide web, initial FY2016 prototype development was restricted to the internal SNL network until FY2017 when the OWL has been put on an external interface (for testing by limited DOE and national laboratory staff). The OWL is now functioning on the SNL External Collaboration Network (ECN). The ability to display various attributes of the information on waste forms is an important function of OWL. The level of support for active databases will determine the type of arrangements that may be practical. As much as possible, the OWL will leverage existing databases to minimize duplication of effort.

3.1.1 Description

The OWL has been designed to contain information on radioactive wastes and waste forms with links to the current supporting documents for the data. Note that no classified or OUO data or supporting documents are planned to be included at this point since the intent is to ensure OWL is suitable for unclassified unlimited release (i.e., UUR designation). There may be up to several hundred different DOE-managed wastes that are likely to require deep geologic disposal. The DOE has a database, the SFDB, that contains information regarding the SNF that DOE manages. OWL is not intended to replicate this database and the information in it; the idea is to take advantage of that existing data set by incorporating it into the OWL, so it is available for use in postclosure PA.

In addition to the data received from the SFDB, each waste (and its alternative waste forms) listed in the OWL *could* include (many already incorporated):

- Waste Characteristics
    - Narrative description of waste (some wastes that have variable processing characteristics, e.g., SRS tank waste, some of which has been processed and some of which has not; Na-bonded fuel, some of which has been treated and some of which has not; Hanford tank waste once treatment starts such that some of it is treated and some is not)
    - Type of waste (HLW or SNF or other)
    - Origin of waste (commercial, DOE-managed (as), foreign, research, other?)
    - Total quantity of waste (volume and/or mass as appropriate)
    - Physical form of waste (e.g., rods, plates, powder, liquid, glass)
    - Dimensional characteristic of waste (if a solid waste)
    - Radionuclide inventory and thermal information at specified times (e.g., at inception, at 2015, at 2048)
    - Bulk chemistry of the waste (noting hazardous constituents)
    - Resource Conservation and Recovery Act (RCRA) considerations (e.g., not an issue, characteristic, listed)
- Current storage information
    - Current storage location (e.g., INL, Hanford)
    - Description of current storage method (e.g., tanks, canisters, high-integrity canisters, capsules)
    - Number of current containers
    - Dimensions of current storage method (per container, as appropriate)
    - Volume of current storage method (per container, as appropriate)
    - Mass of packaged waste as it currently exists (per container, as appropriate)
    - Radionuclide inventory and thermal information at specified times on a per-container basis (or as available)
    - Current status (e.g., awaiting treatment, awaiting packaging, ready for disposal)
- Planned or alternative processing and packaging options for final disposition
    - Description of baseline/alternative processing and/or packaging for disposal, including options for processing and/or packaging
    - Number of baseline/alternative packages
    - Dimensions of baseline/alternative package
    - Volume of baseline/alternative package
    - Mass of baseline/alternative package
    - Status of baseline/alternative planned processing (e.g., none, in progress, under development)

  - Status of baseline/alternative packaging (e.g., ready, being developed)
  - Radionuclide inventory and thermal information for treated/packaged waste at specified times on a per-package basis (or as available)

- Transportation considerations (e.g., certified transport canister exists (yes/no))
- Current base-line disposition pathway (e.g., deep geologic disposal in a repository for HLW and/or SNF, WIPP, or to be determined)
- Copies of any RODs or agreements affecting the waste and its associated plans (linked to the specific data provided)
- Effects of ROD on waste (e.g., date of promised removal from state)
- Further information by request passed along to responsible contacts currently in charge of the waste types and forms for storage oversight, for processing, etc.

3.1.2 OWL Development Status

Over the last few years, the OWL team has identified a number of wastes to include in OWL, developed a database structure, and populated the content of that structure using source documents linked to the data sets. Currently, the OWL database contains information for ten different wastes with seventeen potential (planned or proposed) waste form pathways, and three existing waste forms defined. Additionally, the OWL capabilities are being expanded (starting late in FY2018, expected to continue into FY2020). The expansion is to add data structures and data sets regarding the vessels (cans, canisters, containers, casks, waste packages, etc.) that the various wastes/waste forms could be put into primarily for generating inventories directly from OWL for studies of generic disposal systems. For DSNF and DHLW, the primary source of information for vessels used for storage and transportation is available at a DOE website (DOE n.d.). As this work progresses, data in OWL will be cross-checked against data at that website.

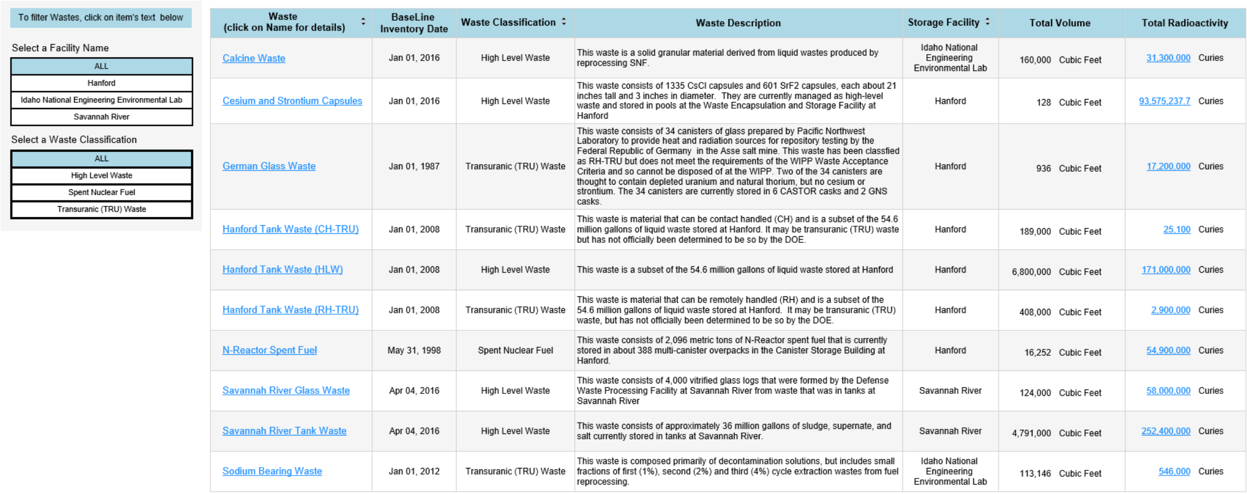
3.1.2.1 OWL Waste and Waste Form Information and Structure

Because of the way the database is structured, users can sort waste by facility (e.g., Hanford, INL, SRS), and waste classification (e.g., HLW, SNF). This feature makes it easy to identify all the HLW types that are currently at Hanford, for example, which is similar to the DOE SFDB capabilities.

Figure 3-1 is a screenshot of the visual display in which users can select wastes by Facility and/or Waste Classification as well as sort by Waste, Classification, or Storage Facility (using the up/down arrows). The total volume and total radioactivity of each waste are also shown.

Because there is a large variety of waste information, the waste detail is organized into sections that can be selected for display.

Figure 3-2 provides a sample screenshot of the waste detail for “Savannah River Glass Waste” with “Waste Characteristics and Disposal Waste Form” information displayed.


To filter Wastes, click on item's text below

Select a Facility Name

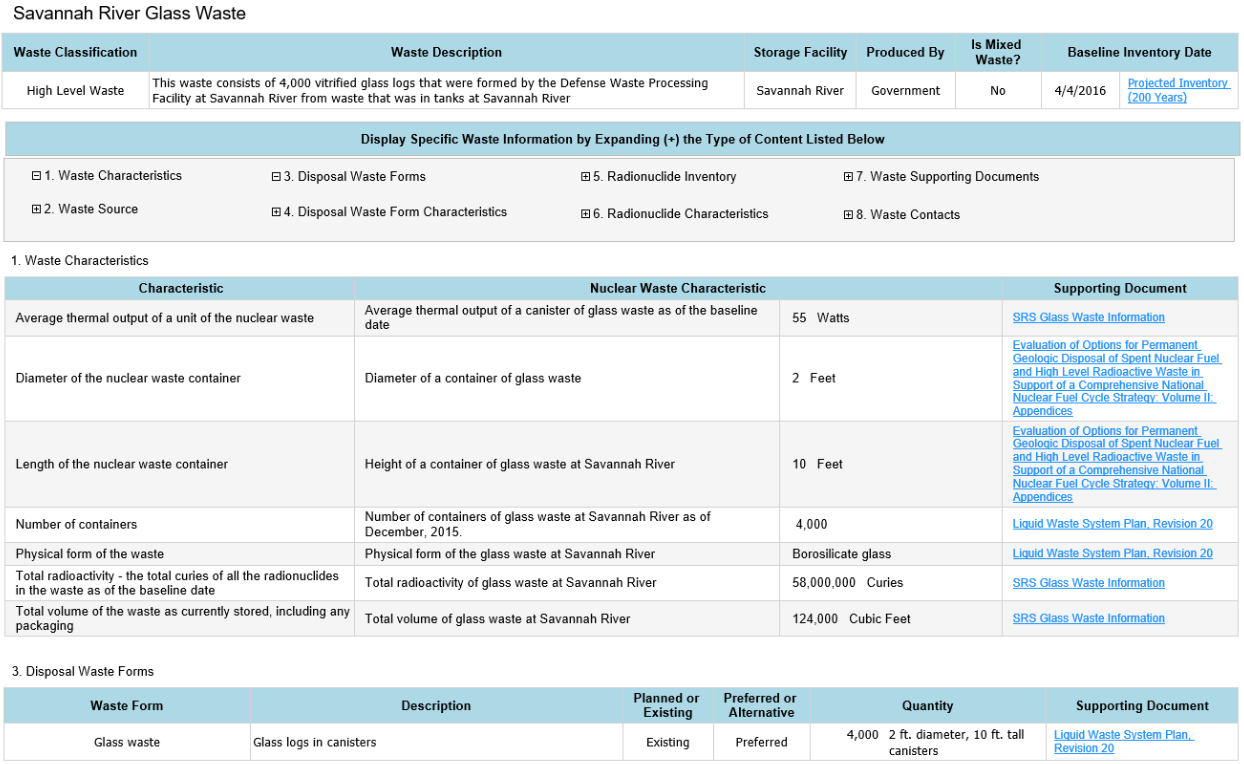
- ALL
- Hanford
- Idaho National Engineering Environmental Lab
- Savannah River

Select a Waste Classification

- ALL
- High Level Waste
- Spent Nuclear Fuel
- Transuranic (TRU) Waste

Waste (click on Name for details) ⇕	BaseLine Inventory Date	Waste Classification ⇕	Waste Description	Storage Facility ⇕	Total Volume	Total Radioactivity
Calcine Waste	Jan 01, 2016	High Level Waste	This waste is a solid granular material derived from liquid wastes produced by reprocessing SNF.	Idaho National Engineering Environmental Lab	160,000 Cubic Feet	31,300,000 Curies
Cesium and Strontium Capsules	Jan 01, 2016	High Level Waste	This waste consists of 1335 CsCl capsules and 601 SrF2 capsules, each about 21 inches tall and 3 inches in diameter. They are currently managed as high-level waste and stored in pools at the Waste Encapsulation and Storage Facility at Hanford	Hanford	128 Cubic Feet	93,575,237.7 Curies
German Glass Waste	Jan 01, 1987	Transuranic (TRU) Waste	This waste consists of 34 canisters of glass prepared by Pacific Northwest Laboratory to provide heat and radiation sources for repository testing by the Federal Republic of Germany in the Asse salt mine. This waste has been classfied as RH-TRU but does not meet the requirements of the WIPP Waste Acceptance Criteria and so cannot be disposed of at the WIPP. Two of the 34 canisters are thought to contain depleted uranium and natural thorium, but no cesium or strontium. The 34 canisters are currently stored in 6 CASTOR casks and 2 GNS casks.	Hanford	936 Cubic Feet	17,200,000 Curies
Hanford Tank Waste (CH-TRU)	Jan 01, 2008	Transuranic (TRU) Waste	This waste is material that can be contact handled (CH) and is a subset of the 54.6 million gallons of liquid waste stored at Hanford. It may be transuranic (TRU) waste but has not officially been determined to be so by the DOE.	Hanford	189,000 Cubic Feet	25,100 Curies
Hanford Tank Waste (HLW)	Jan 01, 2008	High Level Waste	This waste is a subset of the 54.6 million gallons of liquid waste stored at Hanford	Hanford	6,800,000 Cubic Feet	171,000,000 Curies
Hanford Tank Waste (RH-TRU)	Jan 01, 2008	Transuranic (TRU) Waste	This waste is material that can be remotely handled (RH) and is a subset of the 54.6 million gallons of liquid waste stored at Hanford. It may be transuranic (TRU) waste, but has not officially been determined to be so by the DOE.	Hanford	408,000 Cubic Feet	2,900,000 Curies
N-Reactor Spent Fuel	May 31, 1998	Spent Nuclear Fuel	This waste consists of 2,096 metric tons of N-Reactor spent fuel that is currently stored in about 388 multi-canister overpacks in the Canister Storage Building at Hanford.	Hanford	16,252 Cubic Feet	54,900,000 Curies
Savannah River Glass Waste	Apr 04, 2016	High Level Waste	This waste consists of 4,000 vitrified glass logs that were formed by the Defense Waste Processing Facility at Savannah River from waste that was in tanks at Savannah River	Savannah River	124,000 Cubic Feet	58,000,000 Curies
Savannah River Tank Waste	Apr 04, 2016	High Level Waste	This waste consists of approximately 36 million gallons of sludge, supernate, and salt currently stored in tanks at Savannah River.	Savannah River	4,791,000 Cubic Feet	252,400,000 Curies
Sodium Bearing Waste	Jan 01, 2012	Transuranic (TRU) Waste	This waste is composed primarily of decontamination solutions, but includes small fractions of first (1%), second (2%) and third (4%) cycle extraction wastes from fuel reprocessing.	Idaho National Engineering Environmental Lab	113,146 Cubic Feet	546,000 Curies

Figure 3-1. Visual Display of Wastes, Waste Classification, Description, Storage Facility, Total Volume, and Total Radioactivity


Savannah River Glass Waste

Waste Classification	Waste Description	Storage Facility	Produced By	Is Mixed Waste?	Baseline Inventory Date	
High Level Waste	This waste consists of 4,000 vitrified glass logs that were formed by the Defense Waste Processing Facility at Savannah River from waste that was in tanks at Savannah River	Savannah River	Government	No	4/4/2016	Projected Inventory (200 Years)

Display Specific Waste Information by Expanding (+) the Type of Content Listed Below

⊟ 1. Waste Characteristics
⊞ 2. Waste Source
⊟ 3. Disposal Waste Forms
⊞ 4. Disposal Waste Form Characteristics
⊞ 5. Radionuclide Inventory
⊞ 6. Radionuclide Characteristics
⊞ 7. Waste Supporting Documents
⊞ 8. Waste Contacts

1. Waste Characteristics

Characteristic	Nuclear Waste Characteristic		Supporting Document
Average thermal output of a unit of the nuclear waste	Average thermal output of a canister of glass waste as of the baseline date	55 Watts	SRS Glass Waste Information
Diameter of the nuclear waste container	Diameter of a container of glass waste	2 Feet	Evaluation of Options for Permanent Geologic Disposal of Spent Nuclear Fuel and High Level Radioactive Waste in Support of a Comprehensive National Nuclear Fuel Cycle Strategy: Volume II: Appendices
Length of the nuclear waste container	Height of a container of glass waste at Savannah River	10 Feet	Evaluation of Options for Permanent Geologic Disposal of Spent Nuclear Fuel and High Level Radioactive Waste in Support of a Comprehensive National Nuclear Fuel Cycle Strategy: Volume II: Appendices
Number of containers	Number of containers of glass waste at Savannah River as of December, 2015.	4,000	Liquid Waste System Plan, Revision 20
Physical form of the waste	Physical form of the glass waste at Savannah River	Borosilicate glass	Liquid Waste System Plan, Revision 20
Total radioactivity - the total curies of all the radionuclides in the waste as of the baseline date	Total radioactivity of glass waste at Savannah River	58,000,000 Curies	SRS Glass Waste Information
Total volume of the waste as currently stored, including any packaging	Total volume of glass waste at Savannah River	124,000 Cubic Feet	SRS Glass Waste Information

3. Disposal Waste Forms

Waste Form	Description	Planned or Existing	Preferred or Alternative	Quantity	Supporting Document
Glass waste	Glass logs in canisters	Existing	Preferred	4,000 2 ft. diameter, 10 ft. tall canisters	Liquid Waste System Plan, Revision 20

Figure 3-2. Waste Detail Sections Available for Display with Data Selected on Waste Characteristics and Disposal Waste Form

To support waste details, information on 86 radionuclides is also captured in the database. Figure 3-3 provides a screenshot from a database report showing a sample of the radionuclide information.

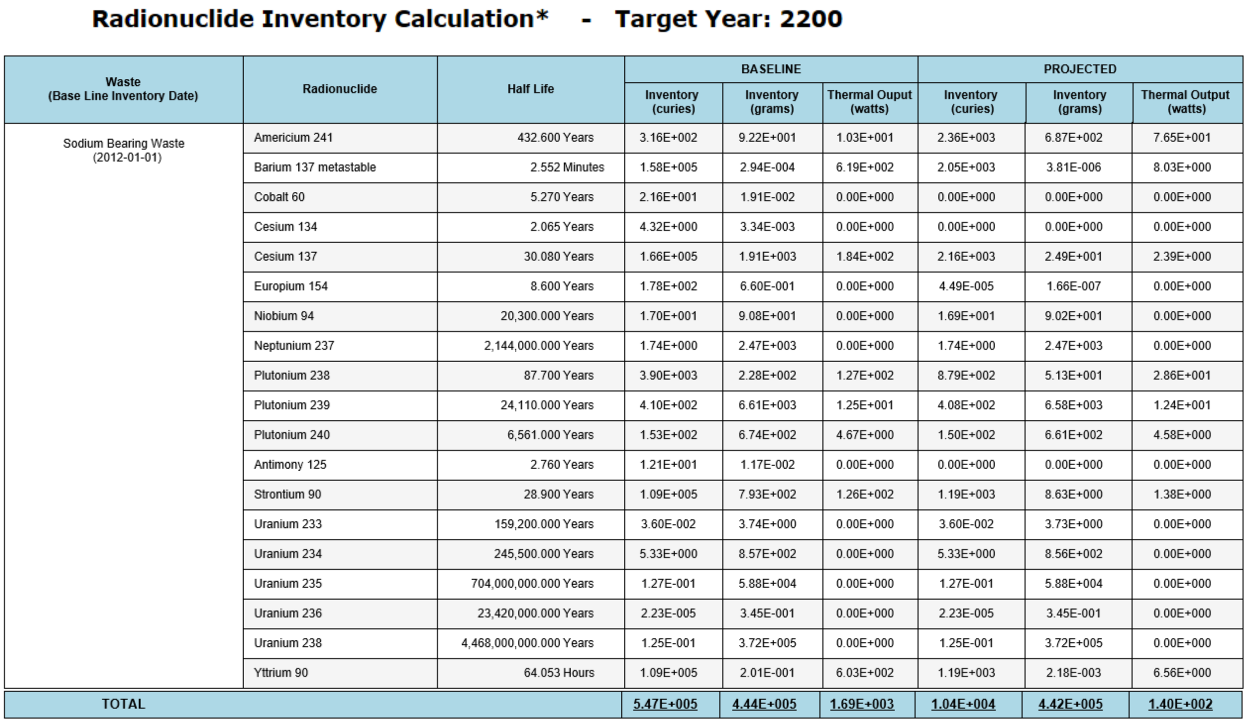
The OWL database can also calculate the inventory of a given waste in a given year (between the current year and 3000 C.E.). OWL database reports can be generated to provide the inventory in various units, such as volumes, radioactivity, and/or thermal output of wastes as they currently exist.

Figure 3-4 provides an example screenshot of the projected inventory database report for "Sodium Bearing Waste" from the baseline inventory date to the selected target year 2200.

In addition to providing the ability to calculate projected inventory for a specific target year, the database now provides a calculation of the projected inventory and thermal output by year for the next 200 years. The calculation is shown in charts (Figure 3-5) that allow selection by waste and radionuclide. The inventory can be displayed in both curies and becquerels.

Radionuclide	Description	Half Life			Atomic Mass (u)	Thermal Output (watts/kCi)	Parent Radionuclide	Inventory Ratio	Supporting Document
Ac-227	Actinium 227	21.77	Years	Projected Inventory (200 years)	227.00				Ac-227 Nuclear Data
Al-26	Aluminum 26	717,000.00	Years	Projected Inventory (200 years)	26.00				Al-26 Nuclear Data
Am-241	Americium 241	432.60	Years	Projected Inventory (200 years)	241.00	32.450	Pu-241		Am-241 Nuclear Data
Am-242	Americium 242	16.02	Hours	Projected Inventory (200 years)	242.00		Am-242m	0.995	Am-242 Nuclear Data
Am-242m	Americium 242 metastable	141.00	Years	Projected Inventory (200 years)	242.00				Am-242m Nuclear Data
Am-243	Americium 243	7,370.00	Years	Projected Inventory (200 years)	243.00				Am-243 Nuclear Data
Ba137-m	Barium 137 metastable	2.55	Minutes	Projected Inventory (200 years)	137.00	3.920	Cs-137	0.950	Ba-137m Nuclear Data
Bk-247	Berkelium 247	1,380.00	Years	Projected Inventory (200 years)	247.00				Bk-247 Nuclear Data
C-14	Carbon 14	5,700.00	Years	Projected Inventory (200 years)	14.00				C-14 Nuclear Data
Cd-113m	Cadmium 113 metastable	14.10	Years	Projected Inventory (200 years)	113.00				Cd-113m Nuclear Data
Ce-144	Cerium 144	284.91	Days	Projected Inventory (200 years)	144.00				Ce-144 Nuclear Data
Cf-249	Californium 249	351.00	Years	Projected Inventory (200 years)	249.00				Cf-249 Nuclear Data
Cf-251	Californium 251	898.00	Years	Projected Inventory (200 years)	251.00				Cf-251 Nuclear Data

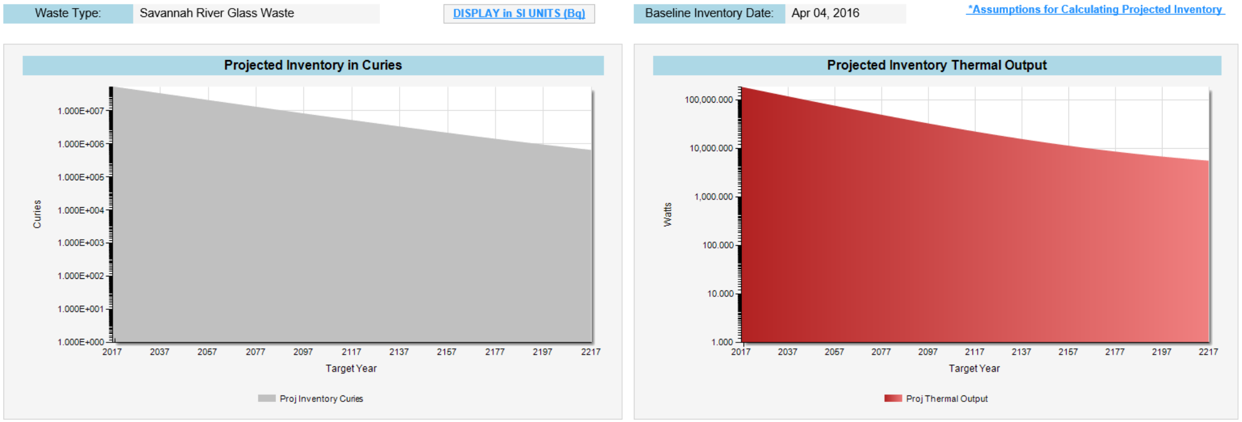
Figure 3-3. OWL Database Report Sample of Radionuclides



Radionuclide Inventory Calculation* - Target Year: 2200

Waste (Base Line Inventory Date)	Radionuclide	Half Life	BASELINE Inventory (curies)	BASELINE Inventory (grams)	BASELINE Thermal Ouput (watts)	PROJECTED Inventory (curies)	PROJECTED Inventory (grams)	PROJECTED Thermal Output (watts)
Sodium Bearing Waste (2012-01-01)	Americium 241	432.600 Years	3.16E+002	9.22E+001	1.03E+001	2.36E+003	6.87E+002	7.65E+001
	Barium 137 metastable	2.552 Minutes	1.58E+005	2.94E-004	6.19E+002	2.05E+003	3.81E-006	8.03E+000
	Cobalt 60	5.270 Years	2.16E+001	1.91E-002	0.00E+000	0.00E+000	0.00E+000	0.00E+000
	Cesium 134	2.065 Years	4.32E+000	3.34E-003	0.00E+000	0.00E+000	0.00E+000	0.00E+000
	Cesium 137	30.080 Years	1.66E+005	1.91E+003	1.84E+002	2.16E+003	2.49E+001	2.39E+000
	Europium 154	8.600 Years	1.78E+002	6.60E-001	0.00E+000	4.49E-005	1.66E-007	0.00E+000
	Niobium 94	20,300.000 Years	1.70E+001	9.08E+001	0.00E+000	1.69E+001	9.02E+001	0.00E+000
	Neptunium 237	2,144,000.000 Years	1.74E+000	2.47E+003	0.00E+000	1.74E+000	2.47E+003	0.00E+000
	Plutonium 238	87.700 Years	3.90E+003	2.28E+002	1.27E+002	8.79E+002	5.13E+001	2.86E+001
	Plutonium 239	24,110.000 Years	4.10E+002	6.61E+003	1.25E+001	4.08E+002	6.58E+003	1.24E+001
	Plutonium 240	6,561.000 Years	1.53E+002	6.74E+002	4.67E+000	1.50E+002	6.61E+002	4.58E+000
	Antimony 125	2.760 Years	1.21E+001	1.17E-002	0.00E+000	0.00E+000	0.00E+000	0.00E+000
	Strontium 90	28.900 Years	1.09E+005	7.93E+002	1.26E+002	1.19E+003	8.63E+000	1.38E+000
	Uranium 233	159,200.000 Years	3.60E-002	3.74E+000	0.00E+000	3.60E-002	3.73E+000	0.00E+000
	Uranium 234	245,500.000 Years	5.33E+000	8.57E+002	0.00E+000	5.33E+000	8.56E+002	0.00E+000
	Uranium 235	704,000,000.000 Years	1.27E-001	5.88E+004	0.00E+000	1.27E-001	5.88E+004	0.00E+000
	Uranium 236	23,420,000.000 Years	2.23E-005	3.45E-001	0.00E+000	2.23E-005	3.45E-001	0.00E+000
	Uranium 238	4,468,000,000.000 Years	1.25E-001	3.72E+005	0.00E+000	1.25E-001	3.72E+005	0.00E+000
	Yttrium 90	64.053 Hours	1.09E+005	2.01E-001	6.03E+002	1.19E+003	2.18E-003	6.56E+000
TOTAL			5.47E+005	4.44E+005	1.69E+003	1.04E+004	4.42E+005	1.40E+002

Figure 3-4. Visual Display of Calculated Projected Inventory from the Baseline Inventory to the Target Year 2,200



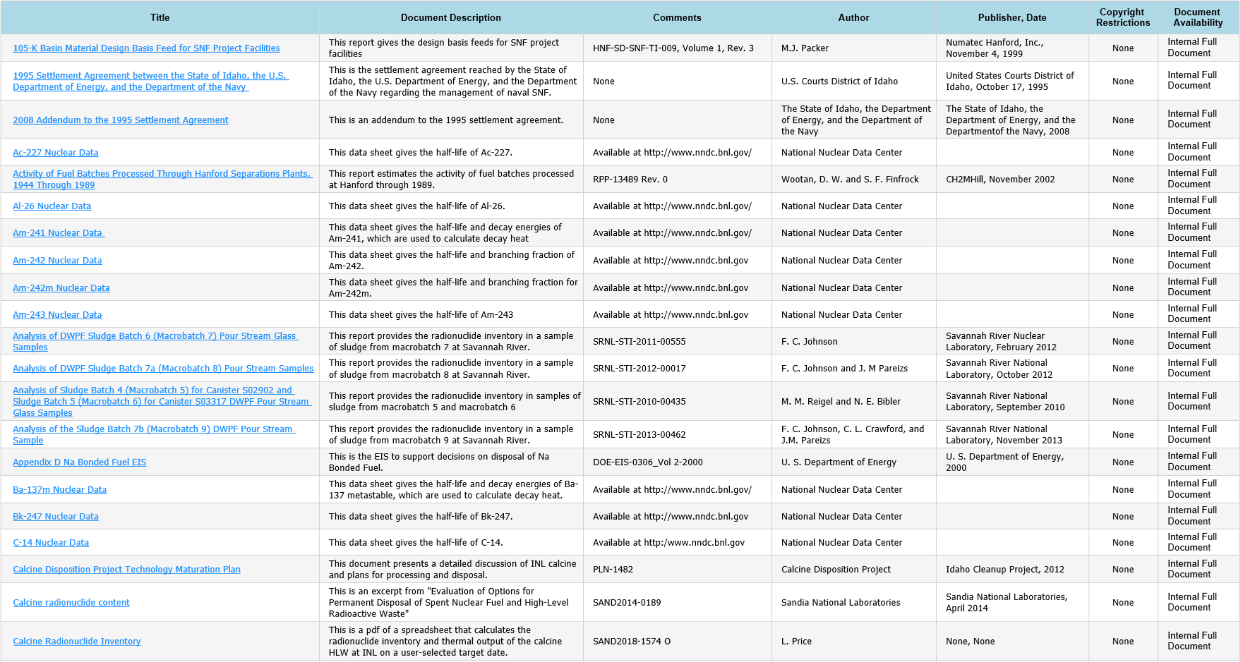
Waste Type: Savannah River Glass Waste

Baseline Inventory Date: Apr 04, 2016

Figure 3-5. Visual Display of Calculated Projected Activity and Thermal Output for a Waste by Year for the Next 200 Years

A further effort from FY2017 to FY2018 consisted of loading supporting documents into the OWL to provide the underpinning sources and to supplement the database content. There are currently 237 documents integrated with the database content and these can be viewed from within OWL. Figure 3-6 provides a screen shot sample of documents available.

As part of the effort to provide supporting documents for each waste, the Excel™ spreadsheet for each waste that can be used to calculate its inventory and thermal output and (in some cases) the volume of waste was turned into a pdf. Results from the beta test indicated that users sometimes had trouble opening or viewing the spreadsheets, so the spreadsheets were formatted appropriately, checked, and saved as pdf files before being sent through SNL's review and approval (R&A) process. Thus, each spreadsheet can be viewed and is referenceable. The original Excel™ spreadsheet is available upon request via an email to OWL@sandia.gov.



Title	Document Description	Comments	Author	Publisher, Date	Copyright Restrictions	Document Availability
105-K Basin Material Design Basis Feed for SNF Project Facilities	This report gives the design basis feeds for SNF project facilities	HNF-SD-SNF-TI-009, Volume 1, Rev. 3	M.J. Packer	Numatec Hanford, Inc., November 4, 1999	None	Internal Full Document
1995 Settlement Agreement between the State of Idaho, the U.S. Department of Energy, and the Department of the Navy	This is the settlement agreement reached by the State of Idaho, the U.S. Department of Energy, and the Department of the Navy regarding the management of naval SNF.	None	U.S. Courts District of Idaho	United States Courts District of Idaho, October 17, 1995	None	Internal Full Document
2008 Addendum to the 1995 Settlement Agreement	This is an addendum to the 1995 settlement agreement.	None	The State of Idaho, the Department of Energy, and the Department of the Navy	The State of Idaho, the Department of Energy, and the Departmentof the Navy, 2008	None	Internal Full Document
Ac-227 Nuclear Data	This data sheet gives the half-life of Ac-227.	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Activity of Fuel Batches Processed Through Hanford Separations Plants, 1944 Through 1989	This report estimates the activity of fuel batches processed at Hanford through 1989.	RPP-13489 Rev. 0	Wootan, D. W. and S. F. Finfrock	CH2MHill, November 2002	None	Internal Full Document
Al-26 Nuclear Data	This data sheet gives the half-life of Al-26.	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Am-241 Nuclear Data	This data sheet gives the half-life and decay energies of Am-241, which are used to calculate decay heat	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Am-242 Nuclear Data	This data sheet gives the half-life and branching fraction of Am-242.	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Am-242m Nuclear Data	This data sheet gives the half-life and branching fraction for Am-242m.	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Am-243 Nuclear Data	This data sheet gives the half-life of Am-243	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Analysis of DWPF Sludge Batch 6 (Macrobatch 7) Pour Stream Glass Samples	This report provides the radionuclide inventory in a sample of sludge from macrobatch 7 at Savannah River.	SRNL-STI-2011-00555	F. C. Johnson	Savannah River Nuclear Laboratory, February 2012	None	Internal Full Document
Analysis of DWPF Sludge Batch 7a (Macrobatch 8) Pour Stream Samples	This report provides the radionuclide inventory in a sample of sludge from macrobatch 8 at Savannah River.	SRNL-STI-2012-00017	F. C. Johnson and J. M Pareizs	Savannah River National Laboratory, October 2012	None	Internal Full Document
Analysis of Sludge Batch 4 (Macrobatch 5) for Canister S02902 and Sludge Batch 5 (Macrobatch 6) for Canister S03317 DWPF Pour Stream Glass Samples	This report provides the radionuclide inventory in samples of sludge from macrobatch 5 and macrobatch 6	SRNL-STI-2010-00435	M. M. Reigel and N. E. Bibler	Savannah River National Laboratory, September 2010	None	Internal Full Document
Analysis of the Sludge Batch 7b (Macrobatch 9) DWPF Pour Stream Sample	This report provides the radionuclide inventory in a sample of sludge from macrobatch 9 at Savannah River.	SRNL-STI-2013-00462	F. C. Johnson, C. L. Crawford, and J.M. Pareizs	Savannah River National Laboratory, November 2013	None	Internal Full Document
Appendix D Na Bonded Fuel EIS	This is the EIS to support decisions on disposal of Na Bonded Fuel.	DOE-EIS-0306_Vol 2-2000	U. S. Department of Energy	U. S. Department of Energy, 2000	None	Internal Full Document
Ba-137m Nuclear Data	This data sheet gives the half-life and decay energies of Ba-137 metastable, which are used to calculate decay heat.	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Bk-247 Nuclear Data	This data sheet gives the half-life of Bk-247.	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
C-14 Nuclear Data	This data sheet gives the half-life of C-14.	Available at http:/www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Calcine Disposition Project Technology Maturation Plan	This document presents a detailed discussion of INL calcine and plans for processing and disposal.	PLN-1482	Calcine Disposition Project	Idaho Cleanup Project, 2012	None	Internal Full Document
Calcine radionuclide content	This is an excerpt from "Evaluation of Options for Permanent Disposal of Spent Nuclear Fuel and High-Level Radioactive Waste"	SAND2014-0189	Sandia National Laboratories	Sandia National Laboratories, April 2014	None	Internal Full Document
Calcine Radionuclide Inventory	This is a pdf of a spreadsheet that calculates the radionuclide inventory and thermal output of the calcine HLW at INL on a user-selected target date.	SAND2018-1574 O	L. Price	None, None	None	Internal Full Document

Figure 3-6. Database Report Sample of Supporting Documents

3.1.2.2 *Expansion of OWL Capabilities*

From the beginning, the plan for OWL has been to allow the database to evolve over time in terms of both content and capability. One of OWL's primary functions is to provide access to information on DOE-managed wastes that are likely to be disposed of in a mined geologic repository. As a complement to this function, OWL is being expanded to include information on the vessels capable of disposing of that DOE-managed waste, with the ancillary aspects of storing and transporting those wastes/waste forms.

Note that certain "vessels" are considered a part of the waste form if that vessel cannot be separated easily from the waste form. As such, those vessels are already included in the descriptions in the waste form information of OWL and would not, in general, be added in this expanded OWL Vessel information. A good example is the glass pour canister that is essential for making the glass waste form. The glass pour canister contains the glass waste form, but is not easily removed, and is not intended to contain other waste forms or waste types. There are also exceptions such as when the vessel itself has an alternative use for a different waste/waste form—either existing or officially planned—that does not permanently bind it to the waste/waste form in that alternative. For example, glass canisters have no existing or planned alternative uses that would justify inclusion in OWL as a vessel (i.e., no planned or alternative use involving some other waste/waste form that would be contained therein). In summary, within OWL, the generic term “vessel” will be used to describe a can, canister, container, cask, overpack, waste package, etc. that can serve as a single layer in a nested system designed to surround and contain the waste form for potential disposal, storage, or transportation uses.

The focus of this OWL expansion addresses three different groups of vessels:

- **Group 1**—Vessels that exist and are used for DOE-managed wastes
- **Group 2**—Vessels that do not exist yet, but are part of official DOE planning for storage, transportation and/or disposal of DOE-managed waste
- **Group 3**—Vessels that exist and are available for use with commercial SNF

Groups 1 and 2 are currently the primary focus. Information on Group 3 is already part of the Used Nuclear Fuel-Storage, Transportation & Disposal Analysis Resource and Data Systems (UNF-ST&NDARDS) database at Oak Ridge National Laboratory, and a future effort is planned for integrating with that database.

Thus far, development efforts for the vessel area have emphasized mining the literature, determining which pieces of information (i.e., database fields) to capture for each vessel, and building the necessary database structure into OWL. The basic data model for the OWL database structure for vessels is shown in Appendix A.

The following list provides an indication of the types of database fields that will be available for each vessel. The data can be organized into two main categories as:

- Vessel General Information (primarily descriptive information)
    - Vessel Name
    - Vessel Category (waste package, canister, container, cask, overpack, etc.)
    - Purpose (storage, transportation, or disposal) and Purpose Type (primary or alternative)
    - Additional Vessel(s) (identifies the inner and outer Vessel layers needed in combination with the Vessel; each Additional Vessel is mapped to a Position relative to Vessel, a Purpose Type, and a Purpose)
    - Vessel Description (brief text about Vessel; can include content about components, configuration, basket, etc.)
    - Material(s)
    - Development Status (indicator of whether Vessel exists, is in some stage of planning, or is conceptual in nature)

  - Waste Form (identifies the Waste Form in OWL that is associated with the Vessel) or Waste Form Name and Description if the Waste Form is not in OWL (e.g., commercial SNF)
  - DOE facility (general facility identification only; specific locations within the site will not be given to help ensure information remains suitable for UUR designation)
  - License/Certification (confidence-building documentation; may specify alternative to license or certification such as DOE safety report as appropriate)
  - Relevant Regulations, Codes, and Standards (list reflects what is found in supporting document(s) and as such may or may not be comprehensive)
  - Disposal Licensing Considerations (description of any information, especially from the NRC, that pertains to disposal licensing of the Vessel)
  - Supplier (entity that supplied or may supply the Vessel to DOE; not necessarily the manufacturer)
  - Capacity
  - Other Loading Considerations (beyond properties given below)

- Vessel Properties (characterized by numbers and units)
  - Cavity Diameter
  - Cavity Length
  - Cavity Width
  - Cavity Height
  - Available Cavity Volume
  - Outer Diameter
  - Maximum Outer Diameter
  - Outer Length
  - Outer Width
  - Outer Height
  - Minimum Outer Length
  - Maximum Outer Length
  - Wall Thickness
  - Vessel Bottom Thickness
  - Vessel Lid Thickness
  - Top Shield Plug Thickness
  - Empty Weight
  - Loaded Weight
  - Maximum Loaded Weight

The fact that some fields above have a maximum version or both a minimum and maximum version whereas others do not is simply an outgrowth of what has been found in the data mining. Of course, not every field will be applicable to every vessel, but the database structure accounts for this situation. Also, the database is not locked into the initial set of fields created before fields are populated. If need be, the person doing data entry can create new fields on the fly whether those fields are related to vessel general information or to vessel properties.

As is standard practice for OWL, the information for vessels will have clear ties to the associated supporting documents to ensure traceability. Those supporting documents will be integrated into OWL's existing supporting documents library with the links to source information contained in the data tables. In addition, any supporting document that is a diagram of the vessel will be flagged as such so that the user interface can provide easy access.

The goal is to have the initial set of OWL vessel database structures in place by the end of FY2019. Vessel information likely will be accessible to users sometime in FY2020. Future work includes continued data mining, refinement of the database structures as needed, data entry, and data checking. Eventually, when logistics for the DOE SFDB integration task are finalized, the related vessel information will be incorporated in a manner that ensures a consistent and coherent vessel data set within OWL. As mentioned previously, commercial vessel information from the UNF-ST&NDARDS database will also be integrated into OWL in the future.

3.1.3 Access to OWL and the *OWL User's Guide*

The OWL is accessed through the SNL ECN, which requires a username/password to login for accessing the SharePoint and network facilities on which the OWL is implemented. The detailed model structure of the OWL is given in Appendix B of Sassani et al. (2017), and an overview of the implementing architecture is shown in Figure 3-7.

The usage of OWL occurs via straightforward access to a homepage (Figure 3-8) within a SharePoint site. From this screen, the user can search for the information that is contained in the database. Note that the screen shots in Sections 3.1 and 3.2 are from the current ECN OWL development version and do not include the updates that are being implemented in preparation for posting OWL Version 1.0. Appendix B, which reproduces the bulk of the *OWL User's Guide*, also demonstrates the various options for queries and reports from the database. For the user's convenience, a link to the *OWL User's Guide* is provided on all database reports generated within OWL (Section 3.2.3.2).

Currently, users can do the following:

- Search on all the wastes as well as view waste details and supporting documents
- Search waste disposal forms, their related wastes, and supporting documents
- View radionuclides, their properties, and supporting documents
- Calculate the inventory of a selected waste in a chosen year

- Display the projected inventory of wastes and radionuclides by year for the next 200 years
- Display “List of Supporting Documents” with the ability to open the documents

These capabilities, as organized by the “Find Information About” report selectors shown in Figure 3-8, are described in more detail in the *OWL User’s Guide* given in Appendix B.

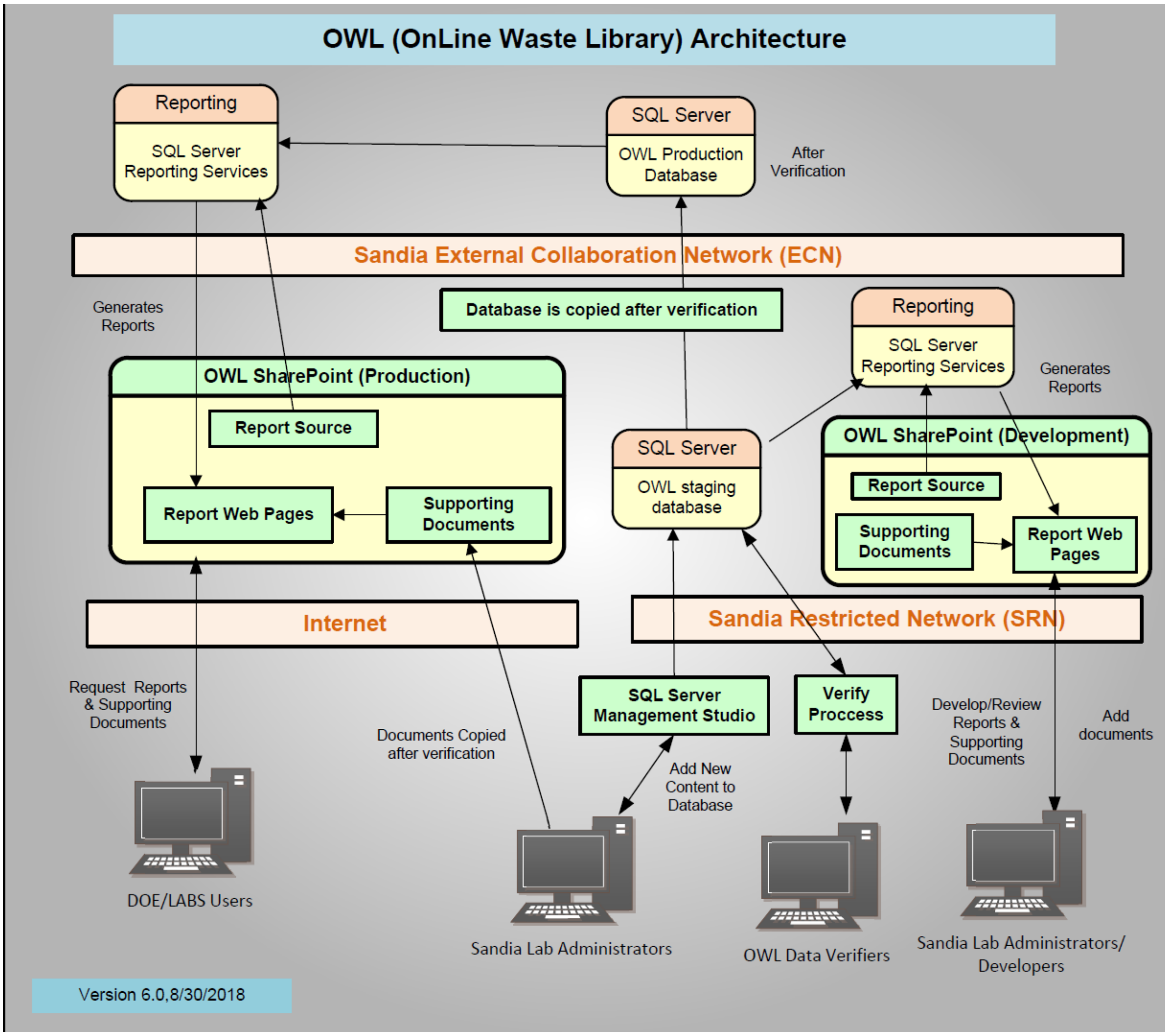
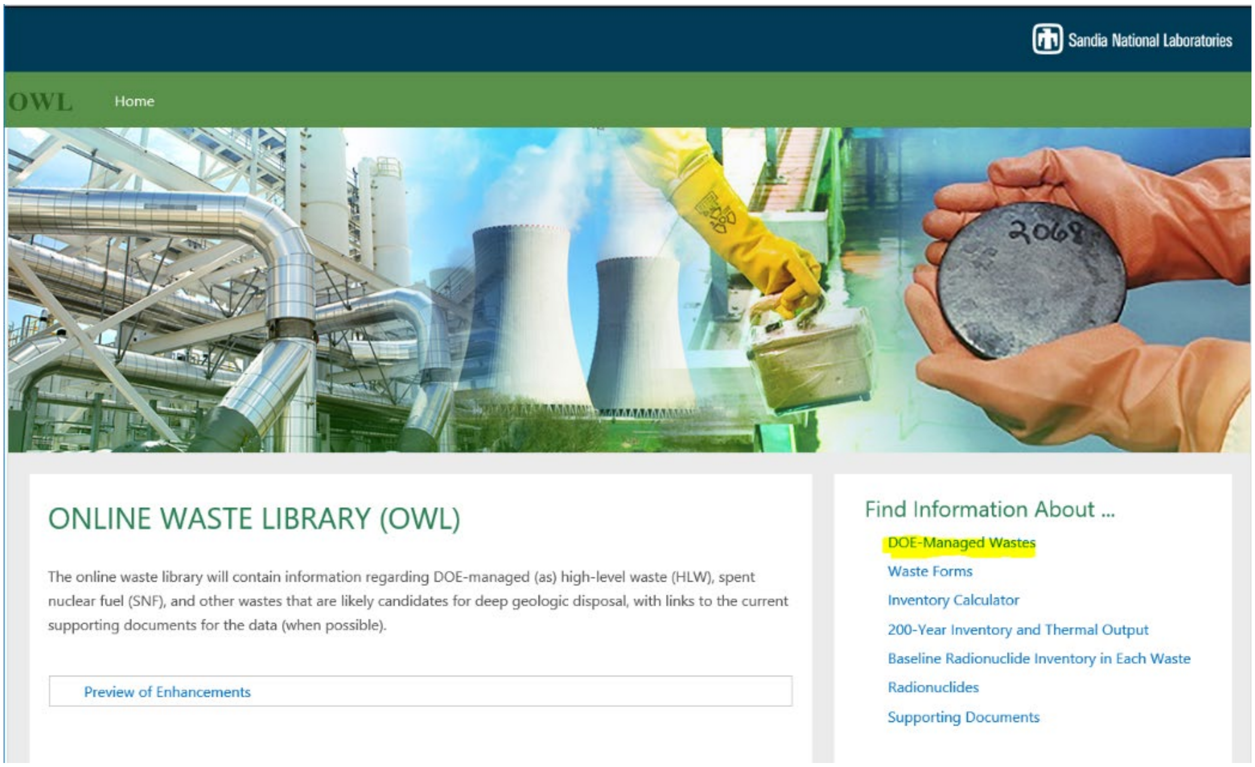


Figure 3-7. High-level Architecture of the OWL Implementation as Constructed on the SNL ECN



ONLINE WASTE LIBRARY (OWL)

The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Find Information About ...

- DOE-Managed Wastes
- Waste Forms
- Inventory Calculator
- 200-Year Inventory and Thermal Output
- Baseline Radionuclide Inventory in Each Waste
- Radionuclides
- Supporting Documents

Figure 3-8. Home Screen for OWL

3.2 Summary of Updates to OWL Status and Inventory Content

Throughout FY2017 to FY2019, the OWL database activities focused on four areas. First, additional data for waste types (and their potential waste forms) and source documentation have been added to the OWL to flesh out its content covering DHLW and DSNF. Second, in conjunction with further data entry, a process of checking the data entry into the OWL against the source documentation was launched to search for and rectify any errors in data entry. This checking was performed by technical individuals who were independent of the data-entry process. The technical checkers documented any issues noted and resolved the issues with the data-entry staff. Third, this data-entry checking process is being included in the delineation/development of the management processes for updating/controlling/archiving the OWL versions. Lastly, the external OWL beta test final input was collected and implemented in OWL from technical staff within the DOE as well as at other national laboratories. The subsections below summarize the data input (Section 3.2.1), the data checking (Section 3.2.2), the implemented beta testing changes to OWL (Section 3.2.3), and the refinement of delineated management processes (Section 3.2.4).

3.2.1 Update to OWL Inventory Content

The OWL database is itself the documentation and deliverable of the full array of information/data for the waste types and potential waste forms for use in GDSA evaluations for generic repository analyses. Because of its formative stature, the OWL database is updated continuously to add additional content, and capabilities to improve usability and facilitate research and development needs of the back end of the fuel cycle. The version of the OWL available to users will be updated at most twice per year: a minor update consisting of data revisions and a major update consisting of data revisions and structural content changes. The major update will occur at most once a year. Section 3.2.4 contains more information on the OWL update/archival processes.

The FY2019 data entry focused on the Na-bonded spent fuel that was produced from DOE's experimental fast-neutron breeder reactor program. The data for the associated spent fuel wastes, electrometallurgical treatment (EMT) produced wastes/waste forms, and other planned waste forms that are being, or are planned to be, produced are being incorporated into OWL. These wastes represent a large number of waste types and waste forms in OWL because they have been classified based on the reactor of origin and the type of fuel (driver versus blanket) from each nuclear reactor. Additionally, the data on SRS glass waste (i.e., HLW glass logs formed at SRS) has been updated wih the most recent production data.

Na-bonded spent fuel wastes have been produced at three separate facilities, i.e., the Experimental Breeder Reactor II (EBR-II) facility in INL, the Hanford Fast Flux Test (Reactor) Facility (FFTF), and the Detroit Edison Fermi Nuclear Power Plant facility (DOE 2014). Waste types for the existing spent fuels have been defined in the OWL for each of these facilities. Operation of these reactors involved two types of fuel, i.e. driver fuel and blanket fuel. The EBR-II facility further differentiates between driver fuel and experimental driver fuel. Waste types have been defined in OWL for each of these fuel types.

Data entry has commenced on the waste types for Na-bonded fuels from reactors EBR-II, FFTF, and Fermi, and their potential wastes/waste forms generated via EMT (note that the DOE ROD (DOE 2000a) only directs EMT processing for the first two of these, with the Fermi Na-bonded blanket fuels awaiting further disposition). This procedure includes an electrorefiner (ER) process that produces salt waste and metallic waste (DOE 2014). The procedure also produces a uranium metal product that is intended for future beneficial use. Because the uranium product is an intended useful recovery of the uranium, it is ***not*** a waste or waste form listed within the OWL. The mass of the uranium product is included in the OWL supporting documentation for mass balance calculations of the various wastes/waste forms from the Na-bonded spent fuels.

DOE decided in 2000 to treat some of the Na-bonded SNF using electrochemical treatment in two ERs (DOE 2000a): the Mark-IV ER and the Mark-V ER. Both ERs are in the Hot Fuels Examination Facility of Fuel Conditioning Facility at INL. The Mark-IV ER has been used to treat some of the EBR-II and FFTF driver SNF, which have low quantities of Pu. The Mark-V ER has been used to treat a small portion of the EBR-II blanket SNF, which has high quantities of Pu.

At this point in time, there are multiple existing wastes associated with the NA-bonded fuels:

- EBR-II Driver SNF
- EBR-II Experimental Driver SNF
- EBR-II Radial Blanket SNF
- FFTF Driver SNF
- Fermi-1 Blanket SNF

- Mark IV Salt Waste
- Mark V Salt Waste
- Metallic Waste (includes material from both the Mark IV and Mark V ERs)

Each of these existing wastes is a "Waste Type" in OWL.

The definition of waste forms in OWL is structured around the eight waste types above and the planned future outputs of the EMT procedure. The metallic waste produced by the EMT process is itself an alloyed metallic waste form as described in DOE (2000a). Two waste form pathways have been proposed for the salt waste. The currently preferred option (DOE 2000a) is to create a glass-bonded sodalite (ceramic waste form) material that encapsulates the salt waste. An alternative calling for direct disposal of the salt waste without further treatment has been proposed (Wang et al. 2011; Lee et al. 2013; SNL 2014; Rechard et. al. 2017).

As a result of these complexities, there are three projected waste forms for each of the five SNF Waste Types. For example, the EBR-II Driver SNF Waste Type has three projected waste forms:

- EBR-II Driver SNF Salt Direct Disposed
- EBR-II Driver SNF Ceramic
- EBR-II Driver SNF Metallic

Each of the two existing salt waste types from the completed ER processing have two associated waste forms. The waste forms for the Mark IV Salt Waste Type are the Mark IV ER Salt Product Direct Disposed (existing) and the Mark IV Ceramic (projected). The waste forms for the Mark V Salt Waste Type are the Mark V ER Salt Product Direct Disposed (existing) and the Mark V Ceramic (projected). The existing Metallic Waste Type produced from the Mark IV and Mark V ERs is also a waste form (i.e., Mark IV Metallic and Mark V Metallic). As additional SNF is processed through the Mark IV and Mark V ERs the quantity, i.e., mass and volume, of the SNF waste type, and the associated waste forms, will decrease. The quantities, mass, and volume of the salt and metallic waste types and associated waste forms will correspondingly increase.

These factors led to the defining eight waste types for the Na-bonded spent fuel in OWL. Of the eight waste types, five are types of Na-bonded SNF and three are products from the Mark IV and Mark V ERs. The waste form section of OWL includes 17 projected waste forms and 3 existing waste forms. The three waste types produced by the ERs are also waste forms. Data input for the Na-bonded spent fuel waste types and waste forms will be ongoing until the EMT processing is complete, but data entry of the current information should be finished by the end of FY2019.

As of the summer of FY2017 (Sassani et al. 2017), the OWL beta version contained completed primary data sets for eight waste types (increased from two in the OWL prototype) and their planned/preferred and potential alternative waste forms. These essentially completed primary data sets for waste types address the following:

- Calcine waste at INL
- Cs and Sr capsules at Hanford
- DOE SNF from N-reactor (essentially DOE Group 1)
- Hanford tank wastes
  - HLW tank waste
  - Contact-handled tank waste
  - Remote-handled tank waste
- SRS HLW
  - Existing HLW glass logs
  - HLW tank waste

The SRS has continued to process its tank waste at the Defense Waste Processing Facility, producing more glass logs. The Defense Waste Processing Facility operates in batch mode; as of the summer of FY2017 the OWL had information regarding nine batches of tank waste that had been vitrified into glass logs. In the summer of FY2019, information regarding the tenth batch became available. As a result, the spreadsheet that calculates the radionuclide inventory, volume, and other properties of the glass logs was updated to include macrobatch number 10. This updated information was reviewed using processes described in Section 3.2.4 and will be available in the initial release of OWL (i.e., OWL Version 1.0).

The OWL contains information/data on physical form, bulk composition, and content of over 85 radionuclides for these waste types and their waste forms, including concentrations as well as the related thermal output. In addition to the included information/data, the OWL contains over 200 source documents that supplement and support the database content, and which are available for review through links directly included within database content.

Additional improvements made to the OWL in FY2017 include the following:

- New reporting capabilities
  - Waste searching by classification or facility with links to waste detail
  - Waste forms and characteristics with links to supporting documents
  - Radionuclide inventory search by facility, classification, or name
  - Radionuclide list with links to details
  - Supporting document list with links to documents
  - Radionuclide inventory calculation by selected target date (primarily for hundreds-of-years timeframe)
- Improved reporting capabilities
  - New color and formatting themes (lighter, easier to read)
  - Improved waste detail with selectable/customizable content types

The other primary capability/quality improvements made for the OWL are the data-entry checking process (Section 3.2.2), the summary and status of the external OWL beta testing (Section 3.2.3), and the preliminary development of management processes for OWL (Section 3.2.4).

3.2.2 Status of Data-Entry Checking

A primary aspect of the OWL database is to provide as comprehensive a compilation of current information/data for DHLW and SNF that simultaneously provides direct links to the source documentation that underlies the content. This combination offers both readily checkable/verifiable information/data entries, as well as clear information paths, which can be updated expeditiously as new information/data is/are collected. Also, this practice provides as clear as possible derivation of the values being utilized with traceability to the source documentation. All of this facilitates maintaining clear understanding of the information/data content, as well as a direct method for finding/correcting errors in data entry. Lastly, because of the explicit link to the source documentation, consideration of, comparison to, and inclusion of alternative data sources is simplified.

Given the additions to the content of the OWL, checking of the data-entry process was initiated in FY2017 to verify the validity of the information/data already included in primary data sets for the essentially complete waste types. The primary goal of this process of data-entry checking against the source documentation was to identify and rectify any errors in data entry using the database and source documents. This data-entry checking is a continuous and iterative process of improvement, which is needed to ensure the integrity of such a large set of information/data that is updated continuously. One key aspect of the checking process is that it is performed by technical individuals who are independent of the data-entry process. These individuals document any issues noted and resolve the issues with the data-entry staff using the aid of technical managers as needed.

The process for documenting any issues identified requires the checker to take the steps below:

1. Print the OWL report to a MS Word file.
2. Highlight in the file all data entries as verified or potentially at issue (e.g., green highlight => verified; red or yellow highlight => potential issue).
3. Summarize issues in an email to the data-entry staff and the technical manager (at least) with email documentation of resolution of each issue.

Potential issues were then clarified/corrected via discussion and definition of summary solutions, with involvement from technical management as needed to define the path for correction.

For the data-entry checking on the primary data sets for the essentially complete waste types, there were 147 specific comments on potential issues.

These fell into the following types of comments/corrections:

- 82 – Typographical errors
- 4 – Inconsistent units of measurement or presentation of information

- 6 – Information not in specified supporting document
- 31 – Supporting document not clearly referenced or incorrectly referenced (e.g. wrong date, wrong document number)
- 21 – Lack of agreement between information in OWL and corresponding information in the supporting document (in some cases, this issue arose for numerical values because of rounding of source values or because inventory content below a certain value was considered to be zero value)
- 2 – Information presented in an unclear fashion
- 1 – Link not functional

Virtually all comments were addressed directly and the issue was corrected. One issue is still being investigated for a solution. This issue involves assigning an inventory of zero for radionuclides with inventories less than about 10^{-7} curies. Only a few radionuclides fall into this issue category. The format of the data type for these values in OWL is floating point decimal and data entries can be input over the range from 10^{-7} to 10^{12} curies. Currently, work is ongoing to develop an approach that does not force an assumption of 0 curies for the inventory of those few radionuclides.

3.2.3 OWL External Beta Testing

The first external beta test of OWL was launched in late July 2017 to solicit input from a small group of knowledgeable individuals—DOE Technical Staff (in DOE-NE and DOE-EM) and staff at INL and SRNL—who would be likely candidates to use the OWL and its content. These staff members agreed to use the OWL as time allowed and provide input/feedback assessing OWL's usability including how straightforward it was to access the information and source materials. This beta test of the OWL continued into the first quarter of FY2018, and the feedback has been evaluated and addressed either by direct modifications/fixes for those issues that were straightforward, or by management processes planned in FY 2018 and implemented in FY2019. A summary of the feedback is provided below.

Example questions to the beta testers included the following:

1. What you found most likeable/easy about using the OWL?
2. What you do not like about the way it works/presents the information?
3. What improvements you would like to see in its usability?
4. What additions to data/information representation you would most like to see?
5. What aspects made using it more difficult than expected?

Although the focus of the OWL beta testing was on its utility/ease of use and information access/presentation, the OWL team welcomed comments/corrections of any nature from the beta testers. As discussed in Section 3.2.2, information in OWL goes through a data-entry checking process against the source information to mitigate the risk of data-entry errors. However, with any large set of information, there is still a chance that such errors may occur, so the team encouraged participants to note any errors detected during beta testing.

3.2.3.1 OWL External Beta Test Feedback and Status

The beta test feedback on the OWL consisted of 35 review comments, which are summarized as follows:

- 13 – Comments not requiring modifications to the OWL (e.g., compliments, connection problems that have already been resolved, general questions requiring a response but no change to the OWL)
- 8 – Problems with navigation (e.g., looking for an easy way to "Return to Home," finding the parameters with which to filter database reports, presence of SharePoint headers and links, size of the collapse/expand box)
- 6 – Suggestions and questions regarding content (e.g., additional background information regarding OWL, adding MTU as a waste characteristic, adding the remaining DSNF, whether information is current)
- 5 – Comments regarding information presentation and selection (e.g., selecting items with which to filter or sort a database report, the units used to describe parameter values)
- 1 – Link not working
- 1 – Problem opening Excel spreadsheet
- 1 – Typographical error

While most comment have been resolved, a few comments are the subject of ongoing efforts for expanding OWL content. One example is the inclusion of DSNF items in OWL, which will be handled by efforts to synchronize with the DOE SFDB at INL via a planned interface process (Section 3.2.4.1). Plans for OWL updates and version control management were developed in FY2018 and implemented in FY2019 (Section 3.2.4.2).

3.2.3.2 Additional Changes to OWL Based on Beta Test Input

Modifications to the OWL database reports were made based on feedback provided during the beta testing completed in the first quarter of FY2018. The following provides a synopsis of beta test comments in two general areas as well as the changes made in response.

Beta Test Comment Area 1

Issue Description—Problems with navigation were encountered. Examples include looking for an easy way to "Return to Home," trouble figuring out how to select parameters with which to filter database reports, and lack of easy-to-find links to supporting documents.

Response—The following changes were implemented for navigational clarity:

- Each database report now includes an OWL banner (Figure 3-9), which has links to the home page, the home report "DOE-Managed Wastes", and the *OWL User's Guide*.

- Text at top of parameter boxes has been added to instruct users to select their items, then to hit 'enter' or select 'apply' at the bottom (Figure 3-10).
- The title of each supporting document is now displayed as a link to that document (Figure 3-11).
- An electronic version of the *OWL User's Guide* (Figure 3-12) has been made available within OWL to provide the user with help in using the database and its content.

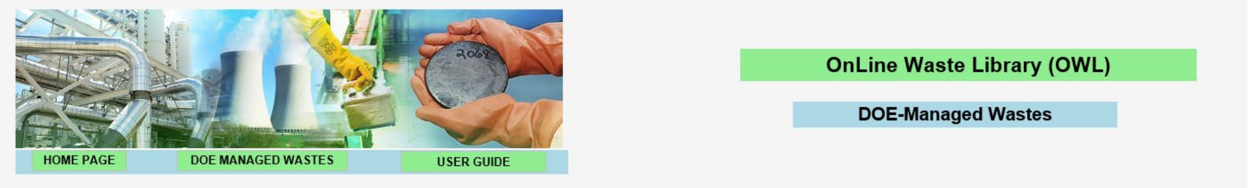
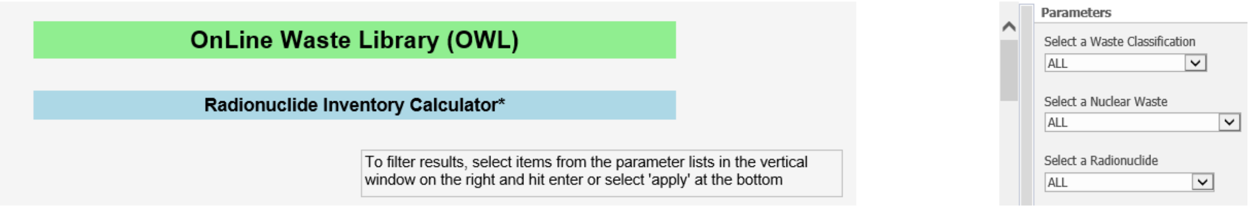


Figure 3-9. OWL Banner Added to Each Database Report To Improve Navigation



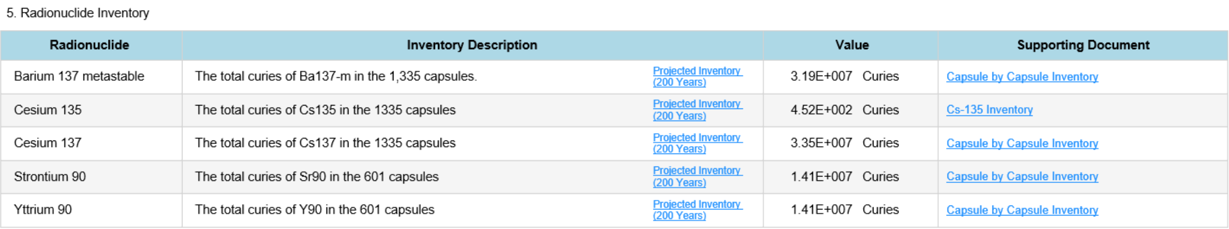
To filter results, select items from the parameter lists in the vertical window on the right and hit enter or select 'apply' at the bottom

Select a Waste Classification: ALL

Select a Nuclear Waste: ALL

Select a Radionuclide: ALL

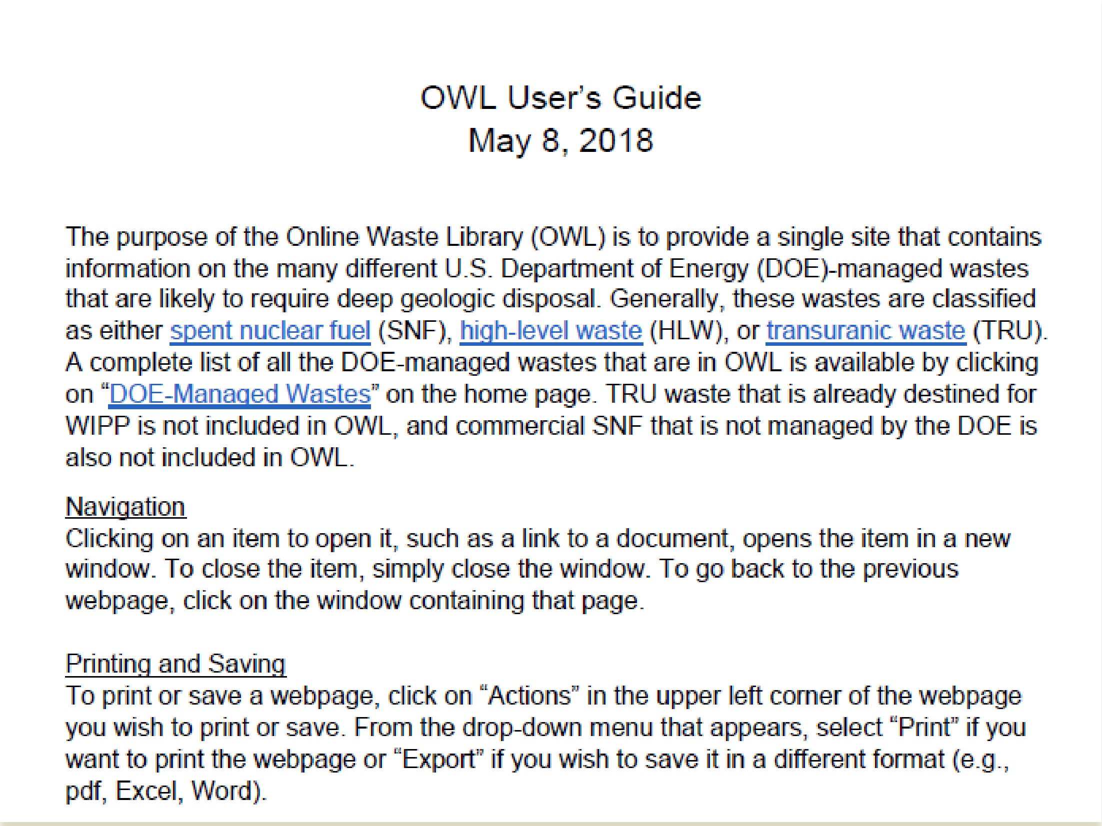
Figure 3-10. Verbiage Added to Top of Parameter Boxes To Provide Instructions to Users



5. Radionuclide Inventory

Radionuclide	Inventory Description		Value		Supporting Document
Barium 137 metastable	The total curies of Ba137-m in the 1,335 capsules.	Projected Inventory (200 Years)	3.19E+007	Curies	Capsule by Capsule Inventory
Cesium 135	The total curies of Cs135 in the 1335 capsules	Projected Inventory (200 Years)	4.52E+002	Curies	Cs-135 Inventory
Cesium 137	The total curies of Cs137 in the 1335 capsules	Projected Inventory (200 Years)	3.35E+007	Curies	Capsule by Capsule Inventory
Strontium 90	The total curies of Sr90 in the 601 capsules	Projected Inventory (200 Years)	1.41E+007	Curies	Capsule by Capsule Inventory
Yttrium 90	The total curies of Y90 in the 601 capsules	Projected Inventory (200 Years)	1.41E+007	Curies	Capsule by Capsule Inventory

Figure 3-11. Titles of Supporting Documents Link User to the Associated Documents



OWL User's Guide
May 8, 2018

The purpose of the Online Waste Library (OWL) is to provide a single site that contains information on the many different U.S. Department of Energy (DOE)-managed wastes that are likely to require deep geologic disposal. Generally, these wastes are classified as either spent nuclear fuel (SNF), high-level waste (HLW), or transuranic waste (TRU). A complete list of all the DOE-managed wastes that are in OWL is available by clicking on "DOE-Managed Wastes" on the home page. TRU waste that is already destined for WIPP is not included in OWL, and commercial SNF that is not managed by the DOE is also not included in OWL.

Navigation
Clicking on an item to open it, such as a link to a document, opens the item in a new window. To close the item, simply close the window. To go back to the previous webpage, click on the window containing that page.

Printing and Saving
To print or save a webpage, click on "Actions" in the upper left corner of the webpage you wish to print or save. From the drop-down menu that appears, select "Print" if you want to print the webpage or "Export" if you wish to save it in a different format (e.g., pdf, Excel, Word).

NOTE: The screenshot is provided as an example. While it reflects the 2018 version of the *OWL User's Guide*, this document was updated in FY2019 in preparation for the release of OWL Version 1.0.

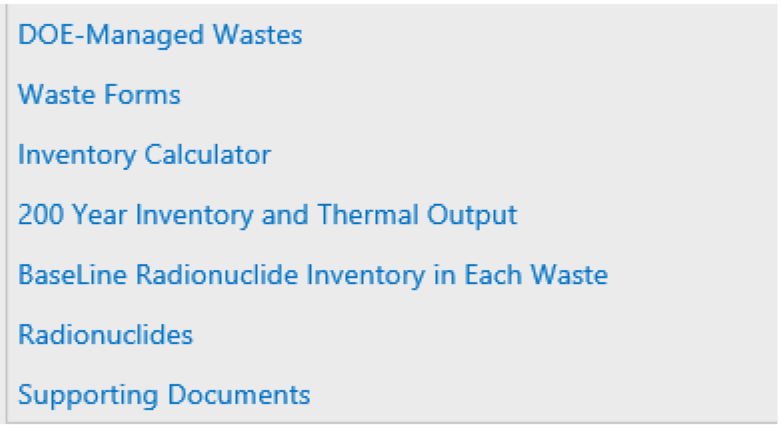
Figure 3-12. First Page of the *OWL User's Guide* Accessed within OWL

Beta Test Comment Area 2

Issue Description—Manner of item selection and presentation should be more user friendly. Examples of desired changes include making it easier to select items with which to filter or sort a database report and incorporating the ability to change the display to different units for parameter values.

Response—The following changes were made to make it easier for the user to select what information is to be accessed and how that information is to be displayed:

- Report selections on the home page were renamed for clarity, the goal being to make them more meaningful to the user (Figure 3-13).
- Radionuclide reports were modified to provide the capability to sort by half-life (Figure 3-14).
- On the "200 Year Inventory and Thermal Output" report, a controls were added allowing the user to request a change in the units displayed for the inventory. If the inventory graph is in curies, the user can request that SI units (Bq) be used (Figure 3-15). Similarly, if the inventory graph is in becquerels, the user can request that curies be used (Figure 3-16). In addition, the y-axis of the inventory graph was changed to be logarithmic.



DOE-Managed Wastes

Waste Forms

Inventory Calculator

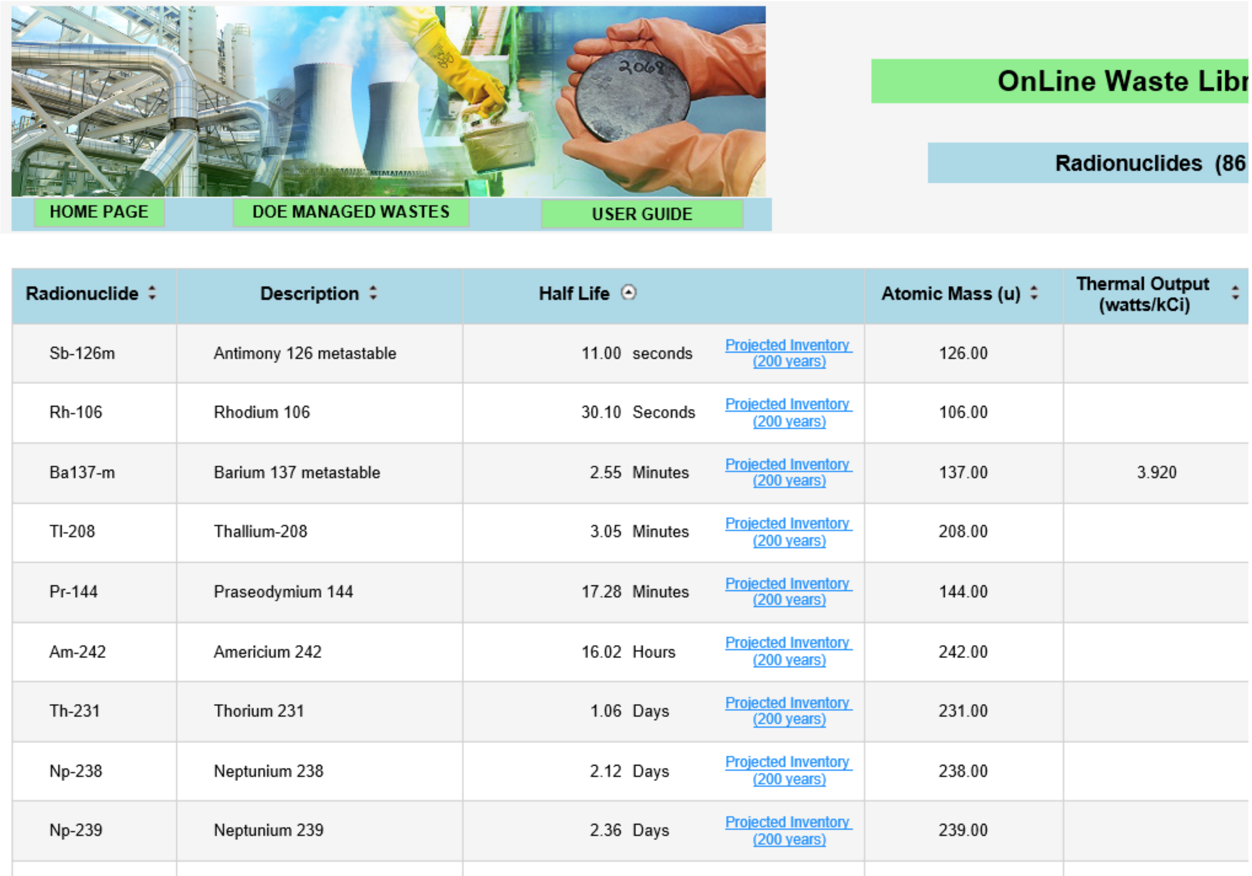
200 Year Inventory and Thermal Output

BaseLine Radionuclide Inventory in Each Waste

Radionuclides

Supporting Documents

Figure 3-13. Report Selections Renamed for Clarity



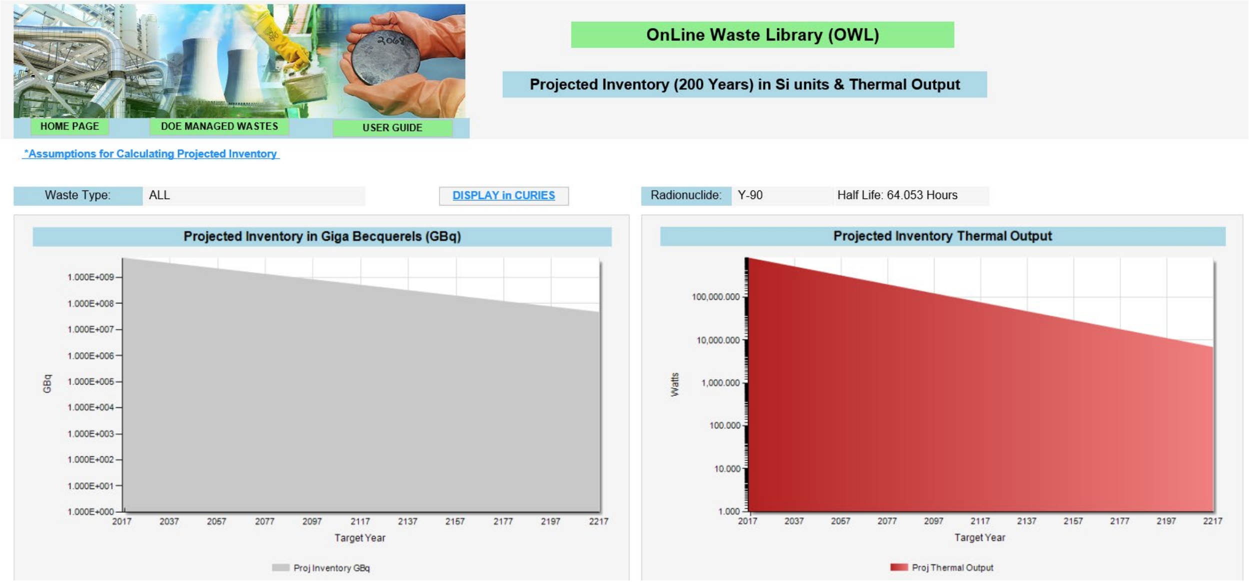
Radionuclide	Description	Half Life		Atomic Mass (u)	Thermal Output (watts/kCi)
Sb-126m	Antimony 126 metastable	11.00 seconds	Projected Inventory (200 years)	126.00	
Rh-106	Rhodium 106	30.10 Seconds	Projected Inventory (200 years)	106.00	
Ba137-m	Barium 137 metastable	2.55 Minutes	Projected Inventory (200 years)	137.00	3.920
Tl-208	Thallium-208	3.05 Minutes	Projected Inventory (200 years)	208.00	
Pr-144	Praseodymium 144	17.28 Minutes	Projected Inventory (200 years)	144.00	
Am-242	Americium 242	16.02 Hours	Projected Inventory (200 years)	242.00	
Th-231	Thorium 231	1.06 Days	Projected Inventory (200 years)	231.00	
Np-238	Neptunium 238	2.12 Days	Projected Inventory (200 years)	238.00	
Np-239	Neptunium 239	2.36 Days	Projected Inventory (200 years)	239.00	

Figure 3-14. Radionuclide Reports with Capability of Sorting by Half Life

Waste Type: ALL

Radionuclide: Y-90 Half Life: 64.053 Hours

Figure 3-15. Option Provided To Change Inventory Graph from Curies to SI Units (Bq)



Waste Type: ALL

Radionuclide: Y-90 Half Life: 64.053 Hours

Figure 3-16. Option Provided To Change Inventory Graph from SI Units (Bq) to Curies

3.2.4 Development of Management Processes for the OWL

This section provides a summary overview of two management processes developed for the OWL. One process addresses methods for interfacing with the DOE SFDB (DOE 2007) at INL on the numerous entries for DSNF, and the other process addresses the management of updates to, and version control/archiving of, the OWL database.

3.2.4.1 Interface with the DOE SFDB (INL)

Although the DSNF inventory for N-reactor has been entered directly into the OWL database for use directly in GDSA analyses (primarily because this represents the major mass of DSNF, it is not efficient, nor desirable, to re-enter the other 700+ entries of DSNF in the INL's SFDB, a Nuclear Quality Assurance-1 (NQA-1) quality assurance database (DOE 2007). As such, the OWL team is currently working with INL staff (primarily Layne Pincock and Brett Carlson) to develop a plan for the OWL to synchronize periodically with the SFDB. Note that both the Na-bonded SNF and the Canyon Stabilization SNF are each planned to be further treated in some fashion as opposed to directly disposed of as SNF, and as such will be entered into OWL to capture those non-SNF waste forms. Because of the nature of the SFDB content, care is being taken to select a subset of information fields to be supplied to the OWL that is sufficient for performance analyses of the back end of the fuel cycle (primarily disposal). The current work in this area is delineating exactly what the desired data fields from the SFDB are for use in the OWL. For example, numbers of DSNF elements, masses, and dimensions are all parameters that are desired for constraining numbers and types of canisters for storage or disposal. But there are many additional fields that would perhaps be useful beyond those. Location information would be limited to the DOE facility of storage (e.g., Hanford, INL) to help ensure the OWL can be made publicly available with no restrictions.

The preliminary mechanism identified for this interface synchronization is a spreadsheet output from the SFDB that would contain a listing of the ~700+ DSNF items and selected data fields (currently being identified). This mechanism would allow for a computer script to be constructed to read the SFDB spreadsheet information and enter that information into the OWL database automatically, obviating human-based data-entry checking via a checksum arrangement. Using such an automated process should facilitate wholesale replacement of the SFDB information upon each spreadsheet update (either with some notation in the spreadsheet on the data that have changed or via an automated file comparison process to highlight the changes. This process would also facilitate using a grouping structure for these DSNF items being input into the OWL as part of the assimilation process. That is, instead of listing each of the specific DSNF item separately, they may be assigned, for example, to their respective group of the 34 DSNF groups (Sections 2.1.1 and 3.2.2). Grouping in this manner will be evaluated for comparison of efficiency versus limitations for analyses. At this point, a draft set of characteristics have been sent to the INL SFDB staff who will generate a draft spreadsheet for evaluation by the OWL group.

Regardless of the ultimate representation in the OWL, the spreadsheet report generated from the SFDB would be listed as the source/supporting document from the SFDB. However, the spreadsheet itself would only be available upon request. During OWL beta testing, issues were encountered regarding opening actual spreadsheets online. As a result, only pdf versions of spreadsheets will be made available online through OWL.

Currently, the draft schedule calls for such synchronizations to occur twice annually with about two to three months lead time prior to OWL version updates to allow time to deal with any unforeseen issues with the file handling. This schedule will be finalized during initial implementation of this interface, currently planned for some time in FY2020.

3.2.4.2 Processes for OWL Development, Version Control, and Archiving

An important part of the infrastructure supporting OWL is a coherent suite of processes that preserve information integrity and traceability as the database evolves over time. The subsections below describe the processes governing (1) development methodology and version control, (2) information update mechanisms, and (3) error reporting.

Development Methodology and Version Control

The current OWL is the beta version, and it has been modified to address the input from the beta testing. The initial OWL production version, planned for release by the end of FY2019, is designated as Version 1.0. The numbering scheme is modeled after the recognized practice of "semantic versioning" (Preston-Werner, T. n.d.). While this scheme incorporates a three-part version (major.minor.patch), OWL will be using just the first two parts (major.minor). A version is considered major if it includes significant changes to any or all the three system components: (1) database, (2) supporting documents, and (3) reports. Minor version updates typically only involve changes to the OWL data such as data corrections and new data content, though minor fixes to new aspects of the previous major release are also possible. In any new version, all three system components are released together as one version. Individual components are not released separately. Changes to the database can include new or revised content as well as structure changes to accommodate new content. Changes to the supporting documents can include new documents or revisions to existing documents, and reporting function changes can include new or modified functionality. In general, major version updates are expected to occur at the end of a fiscal year. Minor version updates are expected to occur in the February to March time frame (if needed). Minor releases are optional and as such may or may not be issued during any particular year.

In addition to the version number (major.minor), the release date (mm/dd/yyyy) is suffixed to the version number. For example, if the first version is released on September 20, 2019, the full version stamp would be "Version 1.0, 9/20/2019". Note that this stamp is in addition to the current date and time that appears on every database report or output file that is produced. Any output files generated from the OWL are stamped internally with the full version stamp for traceability.

Development and implementation processes used for OWL are based on the SNL software development methodology documented on an internal SNL wiki site (Lane 2017). This methodology provides requirements for software documentation and version control, user access, and archival of system components. More detailed development processes and version control documentation for the OWL system components are currently being planned. The goal is to facilitate migration of the processes to programs for which higher graded quality assurance requirements are utilized beyond the current application of standard practices at SNL within the Spent Fuel and Waste Disposition (SFWST) Campaign.

SNL's development methodology utilizes multiple environments for developing systems (Lane 2017). For OWL, the applicable environments are a test environment (also referred to as a development environment), a release candidate environment, and a production environment. The test environment, which resides on Sandia Restricted Network (SRN), is where all modifications to OWL originate. These modifications include database content changes, structure changes, the addition or revision of supporting documents, and the addition or revision reports. Once the OWL administration team completes testing the environment and decides that the test environment is ready to be released as a new version, a version number is assigned to the environment and a release candidate of the components is created on the SNL ECN. The release candidate environment is used to conduct multiple reviews (including the SNL R&A process) and additional testing as appropriate. This environment is only accessible to the OWL team and OWL reviewers.

All changes made since the previous version are documented in a version release change document, which is included as a supporting document in the release candidate and becomes available for review within OWL. This document includes (1) content modifications/deletions/additions and (2) functionality changes/additions. For the convenience of OWL users, the document is added as an appendix to record the change history within the updated version of the *OWL User's Guide*, which is available from the OWL home page. With every version release, the corresponding version release change document is added to that appendix, the result being that the appendix contains a complete and continuous history of version changes.

If the OWL release candidate passes the reviews and final testing, it is moved into the production environment on the ECN. The release date for the version is entered in the database, where it is used to display the version/release date on reports, output files, and other OWL components. An archive of the released version is then created in the OWL Archive area of the production ECN environment. The archive consists of all the OWL components and is identified by version/release date. Archives of production releases are not deleted, and therefore the archive can be used to restore previous versions if necessary. The archive serves both as a backup for the current version and as a complete record of the modifications to all the OWL components. Users then have access to the new production release of OWL and the version release change document on the OWL home page (i.e., the new OWL is accessible to those with SNL ECN and OWL accounts).

Table 3-1 is a template of the high-level tasks used to develop a schedule for an OWL production release.

Information Update Mechanisms

The mechanisms triggering updates to information in the OWL include (1) discovery of newer published documents that supersede the supporting technical documents for data in the OWL, (2) receipt of updates from the SFDB as discussed above, (3) receipt of new information with supporting documentation from DOE/national laboratory staff responsible for the wastes, (4) identification of any types of issues by OWL users via the OWL email service, (5) changes to data used from the National Nuclear Data Center, and (6) internal discovery of errors. A user feedback process will be developed further as needed to enable users to ask questions, provide feedback, and report errors. The feedback information will be used to determine changes in new OWL versions.

The changes made to the OWL content are handled with the same data-entry checking process that is used for addition of new information. This data-entry checking process is described in Section 3.2.2, but it is summarized again below for convenience.

Table 3-1. High-Level Tasks Supporting OWL Production Release

Item	Task
1	Develop Schedule for Version Release • Identify a target production release time frame • Create schedule with assignments and dates
2	Stop All OWL Changes in Test Environment (SRN) • Software changes • Data content and structure changes • Document library changes
3	Assign Version and Create Release Candidate • Assign test environment with version number • Create candidate release in ECN candidate release environment from SRN test environment • Create version release change document
4	Team Review/Data Check
5	Technical Review of Candidate Release • Document review
6	Candidate Undergoes R&A • Prepare content for R&A • R&A review
7	Release Candidate to Production • Update database with release date • Archive new production release • Copy release candidate to ECN production environment • Release test environment for new changes

NOTE: ECN = External Collaboration Network
OWL = Online Waste Library
R&A = review and approval
SRN = Sandia Restricted Network

The checker documents any issues identified for the data reviewed and resolves those issues with the following steps:

1. Print the OWL report to a MS Word file.
2. Highlight in the file all data entries as verified or potentially at issue (e.g., green highlight => verified; red or yellow highlight => potential issue).
3. Summarize issues in an email to the data-entry staff and the technical manager (at least) with email documentation of resolution of each issue.

In this process, each potential issue is clarified and resolved via discussion and definition of summary solutions, with involvement from technical management as needed. Each issue and its resolution, including specific changes planned as a part of that resolution, are documented. That documentation is deposited in a supporting document data-entry checking folder for the relevant version of the OWL and archived with that version.

Error Reporting

Note that as the OWL is used, errors and suggested revisions can be identified either internally by the OWL team or externally by users via the OWL email address. Internally, "corrections" are tracked in a Change Request system, which can be used to identify required corrections as well as requested enhancements, prioritize the items, assign completion to a future version of OWL, maintain a status of completion, and provide other relevant information. Because such changes are not accessible until the next OWL version release, a list of the accepted corrections (i.e., an errata sheet) for the current OWL version is created and made available to users on the OWL Homepage. All such corrections are directly included in the next OWL version, and the errata sheet is reset to an initial blank state.

3.3 Waste Form Performance Constraints for Postclosure Safety Assessments

Each waste form included in a PA has characteristic degradation behavior assigned within the PA analyses to evaluate the release of radionuclides from the waste form (after waste packages are breached) over geologic time. In the current PA for the Generic Disposal System Analyses (GDSA), there are three types of degradation behavior: instantaneous degradation, used nuclear fuel (UNF; or UO_2 or SNF) degradation, and glass waste degradation. The constraints on applying these degradation behavior types to various waste forms along with the associated bases are given below.

3.3.1 Degradation of Potential Waste Forms

Waste form degradation rates of potential waste forms for current and future GDSA PAs have been constrained in detail for a number of waste forms in various disposal concepts (e.g., Sassani et al. 2017, Section 3.3.1). The waste forms considered include (1) UNF, (2) HLW glass (and other glass waste), and (3) DSNF. HIP calcine waste is treated currently as degrading similar to HLW glass. This treatment is further evaluated below to delineate any methods to refine it. Degradation constraints for other waste forms are also considered below, but not modeled in the current GDSA. These degradation models include untreated granular calcine waste (instantaneous degradation) in case it is determined that this waste should be included in future PA. Also included is the stage 3 glass degradation rate model being developed external to the SFWST Campaign, for which some summary literature information is given below. Details of the model approaches and implementations for the basic UNF (i.e., UO_2 spent fuels) and HLW glass degradation models are given in Sassani et al. (2017).

For example, the degradation model for UO_2 spent fuels includes measurements of instant release fractions for UNF at different burnups and for a variety of environmental conditions for PWR fuel at 60 MWd/kgHM burnup (Sassani et al. 2012). The Sassani et al. (2012) study recommends the instant release fractions summarized in Table 3-2.

Table 3-2. UNF Instant Release Fractions for PWR (60 MWd/kgHM burnup)

Source	Instant Release Fraction (%)	Comments
Johnson et al. (2005)	C: 10 Cl: 5 Sr, Tc: 7(11) I, Cs: 10(16)	Best estimates (pessimistic estimates in parentheses); Sassani et al. (2012) recommends using the best estimates for 60 MWd/kgHM burnup, pessimistic estimates for 75 MWd/kgHM burn-up, and a linear relationship for fuel with burnups that fall between

3.3.2 Evaluation of Bases for Assigning Postclosure Performance Constraints

The models for degradation of both UO_2 and HLW glass referred to above are currently being used within the GDSA for PA modeling of postclosure system evolution. The waste forms in the current analyses have been mapped into those models as either performing similarly or being bounded by a particular model degradation behavior. For example, the HIP calcine waste form is assigned to degrade as the HLW glass degradation. For waste forms that do not have substantial waste form lifetimes (i.e., generally only 10,000 years or less), the instantaneous degradation rate is used. In all cases the waste form degradation is the initial, kinetic step, and the dissolved radionuclides are evaluated against solubility limits based in part on the geologic environment.

The current assignments for degradation rates of the DSNF in the inventory are based on the work in the YM SAR (DOE 2008), which assigned virtually all the DSNF to the instantaneous degradation rate model except for the naval SNF. This assumption was based primarily on both that the primary mass of DSNF is N-reactor metallic uranium fuel, which would degrade effectively instantly in any system, and the small amounts of the other DSNF relative to the mass of commercial SNF represented in the YM SAR. The OWL team has been reviewing the bases for the PA groupings from the YM SAR and some prior analyses to see if there may be some of the DSNF waste forms that have a basis for better performance in postclosure. In addition, the assumption of glass degradation being assigned to the HIP calcine waste form is being evaluated as well.

3.3.2.1 DSNF Grouping and Associated Degradation Models

Background of DSNF Grouping in Support of PA and Disposal Concepts

A number of published reports and meeting documents have focused on the management of the more than 200 DSNF types into groups for specific purposes, such as disposition in geological repositories. A representative example of such attempts to selectively group DSNF was documented in 1997 in the report *Grouping Method to Minimize Testing for Repository Emplacement of DOE UNF* (DOE 1997). This report suggested the partition of DSNF into 11 groups for testing purposes, based on the examination of available data and information and associated degradation models of DSNF. The behaviour of DSNF in terms of time-to-failure and release rate was found to be primarily influenced by fuel matrix and cladding, while seven other parameters (i.e., burnup, initial enrichment, cladding integrity, fuel geometry, radionuclide inventory, fission gas release, and moisture content) had only limited impact on fuel behaviour (DOE 1997, 1998a). However, subsequent discussions suggested that this 11-group partition is not suitable for other analyses, such as criticality evaluations in support of DSNF repository disposal, and a new partition into 34 intermediate condensed DSNF groups was proposed based on fuel matrix, cladding, cladding condition, and enrichment (DOE 2002).

For the purpose of total system performance assessment (TSPA), those 34 DSNF groups could be reduced to 16 groups for the TSPA, with the seminal rationale for such partitioning documented in the report *DOE UNF Information in Support of TSPA-VA* (DOE 1998b, Figure 5-1). Further details for grouping are presented in the report *DOE UNF Grouping in Support of Criticality, DBE, and TSPA-LA* (DOE 2000b). According to the DOE grouping team assessment, the 34 intermediate condensed DSNF groups in support of the postclosure safety case could be further reduced to 13 groups for the purpose of postclosure PA analyses (DOE 2002), with a subsequent refinement to 11 DSNF groups for TSPA (by placing the plutonium/uranium nitride fuels in the "miscellaneous fuel" group (Group 10 below) due to their small quantity and the uranium beryllium oxide fuels into the "uranium oxide" group (Group 8 below) owing to their similarities). The final DSNF TSPA grouping in support of the YM SAR (DOE 2008) for the purpose of postclosure safety is given below:

- **Group 1**—Naval SNF (Classified UNF from surface ship/submarine assemblies)
- **Group 2**—Plutonium/uranium alloy (Fermi Core 1 and 2 UNF)
- **Group 3**—Plutonium/uranium carbide (FFTF-Test Fuel Assembly UNF)
- **Group 4**—Mixed oxide (MOX) and plutonium oxide (FFTF-Demonstration Fuel Assembly/FFTF-Test Demonstration Fuel Assembly UNF)
- **Group 5**—Thorium/uranium carbide (Fort St. Vrain UNF)
- **Group 6**—Thorium/uranium oxide (Shippingport light water breeder reactor UNF)
- **Group 7**—Uranium metal (N-Reactor UNF)
- **Group 8**—Uranium oxide (Three Mile Island-2 core debris)
- **Group 9**—Aluminum-based UNF (Foreign Research Reactor UNF)
- **Group 10**—Miscellaneous Fuel
- **Group 11**—Uranium-zirconium hydride (Training Research Isotopes–General Atomics (TRIGA) UNF)

The aforementioned 11 DSNF groups were also used in the TSPA-SR/LA in FY1999 (DOE 2002).

Recently, a new grouping of waste forms was introduced in the context of the various disposal concepts being considered in the WFDOE (SNL 2014). Those waste groups are based on expected postclosure performance, radionuclide inventory, thermal characteristics, chemical characteristics, physical characteristics, packaging, and considerations of safeguards and security. The WFDOE (SNL 2014) inventory included 43 waste types currently in existence and assigned them to 50 potential waste forms after taking into account alternative disposal pathways for several waste types (Section 1.2.1). The 50 waste forms were further sorted into 10 waste groups, which were used to assess design aspects for each repository concept based primarily on expected postclosure degradation behavior assigned to each of those groups. Two of the groups comprised of commercial SNF are not evaluated further here. The other eight waste groups contain waste types currently managed by DOE that are potentially part of an inventory for generic repository analyses. These eight waste groups are the following:

- **WG3**—Vitrified HLW (including vitrified Cs and Sr capsules)
- **WG4**—Other engineered HLW forms (including HIP calcine)
- **WG5**—Metallic and non-oxide spent fuel (N-reactor is the largest waste in this group)
- **WG6**—Untreated Na-bonded spent fuels (would be processed via EMT, but are not considered further as no direct disposal pathway was delineated)
- **WG7**—DOE-managed oxide spent fuels
- **WG8**—Salt, granular solids, and powders (including untreated calcine waste and untreated Cs and Sr capsules)
- **WG9**—Coated-particle spent fuel (e.g., TRISO particles)
- **WG10**—Naval spent fuel

Note that some waste types (e.g. calcine waste and Cs and Sr capsules) appear in more than one waste group due to alternative disposal pathways. Within these eight groups the relevant DSNF inventory is captured in WG5 (metallic SNF), WG7 (oxide spent fuels), WG9 (coated-particle spent fuel, e.g., TRISO particles) and WG10 (naval SNF).

Preliminary postclosure PA analyses within the GDSA for the various representative disposal concepts under consideration (i.e. mined repositories in salt, clay/shale rocks, and crystalline (e.g., granitic) rocks) are currently underway.

Degradation Models for the DSNF Groups

Actual postclosure analyses carried out as part of the FY1999 TSPA demonstrated that, for the aforementioned 11 DSNF groups considered for TSPA, a U-metal spent fuel surrogate can accurately represent DSNF properties for the base case in TSPA (DOE 2001b), except for naval SNF (Group 1). Owing to its significantly different and robust design, this UNF remains essentially intact beyond several hundred thousand years, therefore significantly delaying release from naval SNF (DOE 2002). In order to provide a conservative simplification for the TSPA, the commercial light water reactor UNF (i.e., UO_2-type UNF) was used as a surrogate for naval UNF under the range of expected repository environmental conditions (DOE 2004). Therefore, only two release/degradation models—instantaneous (Groups 2–11) and UO_2-type (Group 1) release/degradation models—were used to simulate radionuclide release from those 11 DSNF groups in the TSPA-LA model (DOE 2004). This approach has been adopted in the GDSA analyses being conducted, with some further evaluation of modifications as discussed in Section 3.4.5 below.

This conservative selection of only two upper-limit release/degradation models to represent the DSNF properties was specifically tied to the base case in TSPA (DOE 2001), for which inventory was dominated by commercial SNF. It is desirable to evaluate the degradation models to see if DSNF degradation properties are appropriately captured, or if additional degradation behavior would be appropriate to add into GDSA. Consequently, the OWL team re-examined closely the various initial release/degradation models for the 11 TSPA DSNF groups (DOE 2002). For each of the 11 TSPA DSNF groups from DOE (2004), summaries of their DSNF wet dissolution models (DOE 2002) of both bounding degradation models and best-estimate degradation models are presented in Table 3-3 and Table 3-4, respectively.

As shown in Table 3-3, eight variants of dissolution/degradation models (including multiples of those models) were considered:

- Commercial UO_2-type model (Groups 1, 4, 8)
- 0.1× commercial UO_2-type model (Group 11)
- U-metal model (Groups 7 and 10)
- 10× U-metal model (Group 7)
- 100× U-metal model (Group 3)
- U-<8 wt% Mo/water model (Group 2)
- Ceramic model (Group 6)
- Aluminum alloy model (Group 9)

Based on composition alone, those variants can be further regrouped into only five main dissolution/degradation models, namely, the commercial UO_2-type model (Groups 1, 4, 8, and 11), the U-metal model (Groups 3, 5, 7, and 10), the U-<8 wt% Mo/water model (Group 2), the ceramic model (Group 6), and the aluminum alloy model (Group 9). Details of these are given in Table 3-4 for the 11 DSNF groups.

Table 3-3. DOE UNF Wet Dissolution Models (bounding) for the 11 DSNF Groups

Fuel Group	Fuel Matrix	Typical Fuel in the Group	Wet Dissolution Model
1	Naval SNF	Surface Ship/Submarine Assemblies	Commercial model
2	Pu/U alloy	FERMI Core 1 and 2 standard fuel assembly fuel	U-<8 wt% Mo/water model
3	Pu/U carbide	FFTF (FFTF-TFA-AC-3) carbide fuel	100x U-metal model
4	MOX and Pu-oxide	FFTF (FFTF-DFA/TFA) oxide fuel	Commercial model
5	Th/U carbide	Fort St. Vrain fuel	10× U-metal model
6	Th/U oxide	Shippingport LWBR fuel	Ceramic model
7	U-metal	N-reactor fuel	U-metal/water model
8	U-oxide	Three Mile Island fuel, Shippingport PWR fuel	Commercial model
9	Al-based UNF	Foreign Research Reactor fuel	Aluminum alloy model
10	Miscellaneous fuel	Miscellaneous fuel	U-metal
11	U-Zr-Hx	Training Research Isotopes—General Atomic fuel	0.1× Commercial Model

NOTE: FFTF = Fast Flux Test (Reactor) Facility
MOX = mixed oxide (fuel)
PWR = pressurized water reactor
UNF = used nuclear fuel

Source: Adapted from DOE 2002.

Table 3-4. DSNF, Naval UNF, Plutonium Disposition Release/Degradation (best-estimate) Models

		Upper-Limit Model		Best-Estimate Model
Fuel Group	**Fuel Matrix**	**Model**	**Surrogate**	**Model**
1	Naval SNF	Commercial UNF	UO_2-type	Commercial UNF
2	Pu/U alloy	Instantaneous release upon exposure to groundwater	uranium - molybdenum	(semi-empirical) rate (mg metal/cm^2/h) = 1.15×10^8 exp{(−66,500 ± 12,200 J/mol)/RT} [100°C–178°C] rate (mg metal/cm^2/h) = 1.58×10^6 exp{(−80,500 ± 10,600 J/mol)/RT} [304°C–440°C] (Linear interpolation between 178°C and 304°C)
3	Pu/U carbide	Instantaneous release upon exposure to groundwater	uranium metal	100× Unirradiated uranium metal best-estimate: k (mg/m^2·day) = $100 \times \{1.21 \times 10^{15} \exp(-66.4 \pm 2.0\ \text{kJ/mol}\ /RT)\}$
4	MOX and Pu-oxide	Instantaneous release upon exposure to groundwater	light water reactor UNF	(semi-empirical) uranium oxide best-estimate model
5	Th/U carbide	Instantaneous release upon exposure to groundwater	SiC	(semi-empirical) R (kg/m^2·s) = 0.6×10^{-12}
6	Th/U oxide	Instantaneous release upon exposure to groundwater	Synroc	(semi-empirical) k (mg/m^2·day) = $82.0 \times 10^{(-1{,}000/TK)}$
7	U-metal	Instantaneous release upon exposure to groundwater	N-reactor	(semi-empirical) 2.52×10^{10}exp (−66,400/RT) mg/cm^2·hr R = 8.314 J/mol·K
8a	Intact U-oxide	Instantaneous release upon exposure to groundwater	light water reactor UNF	(semi-empirical) uranium oxide best-estimate model
8b	Damaged U-oxide	Instantaneous release upon exposure to groundwater	Three Mile Island-2 debris	(surface area enhancement factor of 100 is based on professional judgment) 100× uranium oxide best-estimate
9	Al-based UNF	Instantaneous release upon exposure to groundwater	SRS uranium/ aluminum UNF in J-13 well water	(empirical) 1.38 mg metal/m^2·day at 25°C 13.80 mg metal/m^2·day at 90°C

Table 3-4. DSNF, Naval UNF, Plutonium Disposition Release/Degradation (best-estimate) Models (continued)

		Upper-Limit Model	**Best-Estimate Model**	
Fuel Group	**Fuel Matrix**	**Model**	**Surrogate**	**Model**
10	Miscellaneous fuel	Instantaneous release upon exposure to groundwater	N/A	(empirical) rate (mg metal/cm^2/h) = 1.15 × 10^8 exp{(−66,500 ± 12,200 J/mol)/RT} [100°C–178°C] rate (mg metal/cm^2/h) = 1.58 × 10^6 exp{(−80,500 ± 10,600 J/mol)/RT} [304°C–440°C]
11	U-Zr-Hx	Instantaneous release upon exposure to groundwater	Training Research Isotopes–General Atomic	(empirical) 0.1× uranium oxide best estimate

NOTE: N/A = not applicable
UNF = used nuclear fuel

Source: Adapted from DOE 2004.

For the DSNF in WG5, WG7, WG9 and WG10, a potential remapping to the behaviors for the 11 groups is given in Table 3-5. The WG10 (naval SNF) corresponds to Group 1 and will continue to be represented with the UO_2-type degradation model. DSNF in WG5 (metallic and non-oxide spent fuels) comprise aspects of Group 2 (Pu/U alloy, with U-<8 wt% Mo/water degradation model), Group 7 (U-metal, with instantaneous degradation model), Group 9 (Al-based, with aluminum-alloy degradation model), Group 10 (miscellaneous UNF, with instantaneous degradation model), and Group 11 (U-Zr-Hx, with UO_2-type degradation model). There may be some waste forms within those groups that could have various models assigned in future GDSA PA analyses if desired. The DSNF in WG7 (DOE oxide spent fuels) will include fuel belonging to Group 4 (MOX, with UO_2-type degradation model), Group 6 (U/Th oxide, with ceramic degradation model), and Group 8 (U-oxides, with UO_2-type degradation model). Finally, DSNF from WG9 would correspond to Group 3 (U/Pu carbide, with instantaneous degradation model) and Group 5 (U/Th carbide, with instantaneous degradation model). This tentative remapping, with respect to degradation/dissolutions, of DSNF in WG5, WG7, WG9 and WG10 into Group 1 through Group 11 allows consideration of more specific assignments for PA analyses. This remapping would only be undertaken if there was a need for such detail based on postclosure PA results.

Table 3-5. Possible Remapping of DSNF in WG5, WG7, WG9 and WG10 into Groups 1–11

Waste Group	Fuel Group	Fuel Matrix	Typical Fuel in the Group	Degradation Model
WG5	2	Pu/U alloy	FERMI Core 1 and 2 standard fuel assembly fuel	U-<8 wt% Mo/water model
	7	U-metal	N-reactor fuel	Instantaneous degradation model
	9	Al-based	Foreign Research Reactor fuel	Aluminum alloy model
	10	Miscellaneous fuel	Miscellaneous fuel	Instantaneous degradation model
	11	U-Zr-Hx	Training Research Isotopes—General Atomic fuel	UO_2-type degradation model
WG7	4	MOX and Pu-oxide	FFTF (FFTF-DFA/TFA) oxide fuel	Commercial model
	6	Th/U oxide	Shippingport LWBR fuel	Ceramic model
	8	U-oxide	Three Mile Island fuel Shippingport PWR fuel	UO_2-type degradation model
WG9	3	Pu/U carbide	FFTF (FFTF-TFA-AC-3) carbide fuel	Instantaneous degradation model
	5	Th/U carbide	Fort St. Vrain fuel	Instantaneous degradation model
WG10	1	Naval fuel	Surface Ship/Submarine Assemblies	UO_2-type degradation model

NOTE: FFTF = Fast Flux Test (Reactor) Faciity
LWBR = light water breeder reactor
MOX = mixed oxide (fuel)
UNF = used nuclear fuel

As discussed above, those 11 TSPA DSNF groups resulted from successive down-selections of the initial 34 intermediate condensed DSNF groups in support of OCRWM's postclosure safety case into 16 groups for the TSPA (DOE 1998b), followed by a reduction to 13 groups for PA analyses (DOE 2002). In addition to the aforementioned degradation models discussed for 11 TSPA DSNF groups, a dissolution model was used for each of the 16 groups for the TSPA to represent the fuel's radionuclide release rate to the repository's unsaturated zone and eventual transport to the receptor. Details of the rationale for the use of such dissolution models can be found in DOE (1998b). The level of detail is enhanced for the dissolution models assigned to the DSNF of WG5, WG7, WG9 and WG10 via the tentative remapping into the TSPA Groups 1–11 (Table 3-5). A second analysis of the degradation/dissolution details of the DSNF in WG5, WG7, WG9, and WG10 could be achieved by a similar remapping of the waste forms in these groups to those 16 TSPA DSNF groups.

One-to-one correspondences exist between Groups 1, 3, 4, 6, 7, 10, and 11 of Table 3-3 and their counterparts in the 16 initial TSPA partitions. Two of the 16 groups—Canyon Stabilization and Na-Bonded Fuels—that were considered have been eliminated because they would be processed into other waste forms. Four of the 16 groups have been consolidated. U-Zr fuels and U-Mo fuels have been merged into Group 2, and U/Th carbide high-integrity and U/Th carbide low-integrity have been included in Group 5. Some of the DSNF have been rearranged in the remaining groups. Those rearrangements resulted in Group 8 containing both U-oxide intact fuel and U-oxide failed/decladded fuel (also referred to as Group 8a and 8b, as shown in Table 3-4). Many of the changes were driven by the state or composition of the fuel cladding. As a result, in the context of a PA, in which zero credit is given to the fuel cladding in terms of degradation, the mapping proposed above between the DSNF of WG5, WG7, WG9, and WG10 and Groups 1–11 in the TSPA-SR/LA of FY1999 appears to contain a sufficient level of detail.

The various DSNF groupings proposed in support of PA and disposal concepts have been reviewed and analyzed. While as a crude first approximation DSNF can utilize either UO_2-type UNF or instantaneous degradation models, it was shown that some of the recently introduced groupings from the WFDOE (SNL 2014) can be mapped to a wider variety of degradation/dissolution models than was previously established for the 11 DSNF groups considered in the early work of the YM SAR. A finer remapping into the original 16 groups considered is not expected to provide additional useful information in terms of degradation at the PA level, although future work may elucidate fuel degradation/dissolution models at the level of the 34 condensed DSNF groups.

3.3.2.2 Calcine Waste and Associated Degradation Behavior

SNF was reprocessed to recover enriched uranium and other radionuclides at the Idaho Nuclear Technology and Engineering Center (INTEC), located at INL in southeastern Idaho. Reprocessing operations ran from 1953 to 1994 and produced highly radioactive aqueous wastes that were temporarily stored in underground tanks. Fluidized-bed calcination was then used at INTEC to solidify the aqueous acidic metal nitrate radioactive wastes. In the calcination process, the liquid wastes are sprayed using air-atomizing nozzles into a fluidized bed of heated spherical calcine particles, evaporating water and nitric acid in the wastes, and leaving behind solid-phase metal oxides and fluorides known as calcine.

Calcination operations ran from 1963 to 2000 and produced approximately 4,400 m^3 of calcine that is stored in a total of 6 Calcine Solids Storage Facilities (CSSF). A CSSF consists of several stainless-steel storage bins that are housed within concrete vaults and are commonly referred to as “bin sets.” Each CSSF has between three and twelve bins containing the calcine (Staiger and Swenson 2011). Different fuel configurations and the use of different fuel-cladding materials led to the generation of several chemically distinct liquid wastes during reprocessing and consequently led to several different calcine compositions. For example, “aluminum” and “zirconium” wastes are so named because each was generated from the reprocessing of aluminum- and zirconium-clad fuels respectively. SBW is a term used to describe wastes that contain relatively high concentrations of sodium salts. The compositions of four primary types of calcine waste stored at INTEC are provided in Table 3-6.

Table 3-6. Typical Compositions of the Four Types of Calcine

Element/ Chemical Species	Units	Type of Calcine			
		Aluminum[a]	Zirconium[a]	Fluorinel/SBW Blend[a]	Aluminum Nitrate/SBW Blend[a]
Al	wt%	47	8.1	7.5	38
B	wt%	0.1	1.0	1.0	0.1
Cd	wt%	—[b]	—	5.0	0.2
Ca	wt%	—	28	27	3.2
Cl	wt%	—	—	0.1	0.4
Cr	wt%	0.1	0.3	0.1	0.1
F	wt%	--	25	17	1.7
Fe	wt%	0.8	0.1	0.3	0.6
Hg	wt%	1.9	—	—	—
NO_3	wt%	2.5	0.8	6.0	5.9[c]
O	wt%	42	16	17	38
K	wt%	0.2	0.1	0.7	1.8[c]
Na	wt%	1.3	0.4	2.9	8.4[c]
SO_4	wt%	1.8	2.0	3.5	0.3
Sn	wt%	—	0.3	0.2	—
Zr	wt%	0.1	17	11	1.3

NOTE: [a] Column totals are not 100% because of rounding values and the exclusion of trace components.

[b] A dash within a cell indicates an insignificant quantity.

[c] The aluminum nitrate/SBW blend nitrate value is a high-temperature (600°C) calcination value. Nitrate values were higher and alkali (sodium and potassium) values were lower when SBW was calcined at 500°C.

SBW = sodium-bearing waste

Source: Staiger and Swenson 2011.

Initially DOE intended to immobilize the calcine waste in a vitrified (glass) waste form before shipping it to a geologic repository. INTEC proposed to implement its vitrification program in 2020 and complete it in 2035 (INEEL 1998, pp. A-39 to A-42). For this reason, it was assigned the properties of HLW glass in terms of its dissolution rate in the YM TSPA. More recently, in the 2010 ROD 75 FR 137 (DOE 2010), DOE-selected HIP technology to treat the calcine and create a new waste form that is suitable for disposal. The HIP process uses calcine retrieved from the CSSF and heat-treated at temperatures up to 600°C to remove moisture and NO_x. After heating, the calcine is mixed with silica, titanium and calcium sulfate (or elemental sulfur), and the mixture is placed in a stainless steel can that is then sealed with a lid with a vent tube. The can is evacuated, the vent is sealed, and the can is placed in the HIP process vessel.

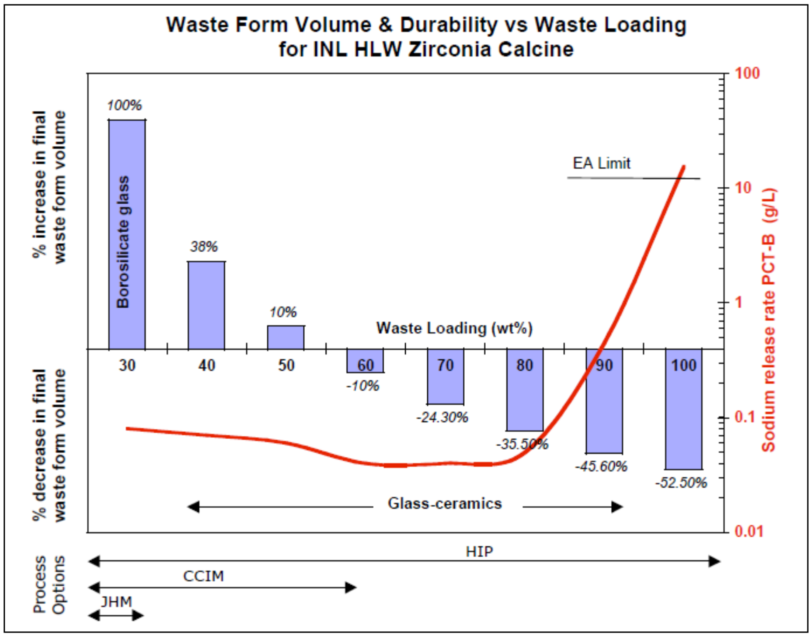
The vessel is pressurized with argon gas to between 7,200 and 15,000 psi and is heated to between 1,050°C and 1,200°C.

At these processing conditions, the calcine is converted to a glass ceramic consisting of a mixture of titanates, sulfides, glass/quartz, and nepheline (CDP 2012). It is expected that this glass ceramic has properties consistent with HLW borosilicate glass. ROD 75 FR 137 (DOE 2010) also retains an option to HIP the calcine without the addition of the silica, titanium, and calcium sulfate. It is expected that this option would provide additional volume reduction of up to approximately 50%. However, this alternative calcine waste form would release RCRA waste constituents and therefore would require disposal at a facility that accepts RCRA wastes. Yet a third option under consideration is the direct disposal of calcine waste without additional treatment. Similar to the additive-free HIP calcine waste, it is expected that this waste form would release RCRA waste constituents and would require disposal at a facility that accepts RCRA wastes.

3.3.2.3 Degradation Model for HIP Calcine Waste with Additives

A literature survey revealed very little research has been done to establish the long-term dissolution rates of HIP calcine waste under repository conditions. However, Begg et al. (2005) studied HIP simulated zirconia calcine samples at various loadings of glass additives to create a set of simulated glass-ceramic waste materials that are intended to represent HIP zirconia calcine waste forms. The glass-ceramic samples were prepared with the simulated zirconia calcine at various loadings from 60 wt% to 90 wt% with proportionate amounts of glass additives. In addition, a densified zirconia calcine was prepared at 100% loading (no additives). These simulated waste forms were then subjected to the Product Consistency Test (PCT-B) (American Society for Testing and Materials (ASTM) C 1285–95), a leach test designed to determine the chemical durability of nuclear waste glasses. The PCT-B test results show high chemical durability with waste loadings of up to 80% as indicated by the retention of numerous elements within the simulated waste forms including B, Na, Cs, Mo, Sr, Gd, Al, Ca, Cr, F, Fe, Mg, Si, and Zr. Figure 3-17 shows that Na release rates are well below the environmental assessment (EA) glass release limit in samples for which the simulated zirconia calcine loadings are below 80 wt %. It is important to note that the HIP and fully densified 100% zirconia calcine sample exceeds the EA glass release rate limit for Na.

With the very limited amount of data available on calcine degradation, it is difficult to assign a dissolution rate to HIP calcine waste. However, Knecht and Berreth (1989) assert that the overall durability of the resulting glass ceramic is expected to be similar to a HLW glass. Further, the work by Begg et al. (2005) suggests HIP calcine waste with loading below 80 wt% may perform as well as the HLW glass waste. In the best case, the recommended glass dissolution rates above can be used to model the performance of HIP calcine waste. Conservatively, instantaneous dissolution may be assumed. The behavior of HIP calcine is very likely bounded by these two rates.



NOTE: EA = environmental assessment
HLW = high-level radioactive waste
INL = Idaho national laboratory
PCT = Product Consistency Test

Source: Begg et al. 2005.

Figure 3-17. Relationship between Various Waste Form Alternatives including Process Options as a Function of Waste Loading and Chemical Durability

3.3.2.4 Degradation Model for HIP Calcine Waste without Additives

Once again, a literature survey revealed very little research has been done to establish the degradation rates and leachability of HIP calcine waste in the absence of glass additives. As noted above, Begg et al. (2005) showed that leach testing on a fully densified 100% zirconia calcine sample exceeds the EA glass release rate limit for Na. In the absence of long-term degradation rates under geologically relevant conditions, an instantaneous dissolution rate is recommended.

3.3.2.5 Degradation Model for Direct Disposal of Granular Calcine Waste

Available data on untreated granular calcine dissolution behavior, leachability, and degradation rates are also limited, and little has been done to examine long-term degradation rates under geologically relevant conditions. However, a comparison of the leach rates of glass waste forms to calcine waste indicates calcine leach rates range from 10^{-1} to 10^{-2} g/cm^2·day and are 4 to 6 orders of magnitude higher than glass leach rates (Stewart 1985). In addition, several papers summarized below provide data on short-term (days to several weeks) leaching in distilled water and dilute nitric acid.

Granular alumina calcine produced in the Waste Calcining Facility (WCF) at the INTEC was leached continuously in laboratory experiments with distilled water at 25°C and 80°C to 90°C and with dilute

(0.25 to 0.5 M) nitric acid at 25°C (Paige 1966). In this study, more than 95% of the Cs and 33% of the Sr was leached by distilled water at 25°C from the alumina calcine in seven weeks; most of the leaching occurred during the first two or three days. Only 0.01% of the Al leached in a similar period, and the Ce and Ru were leached effectively at the same rate as the Al. During six weeks of leaching with dilute HNO_3 (0.25 to 0.5 M) at 25°C, the alumina calcine disintegrated, and more than 99% of the alumina dissolved.

More recently, Staples et al. (1979) examined the leaching characteristics of both alumina and zirconia calcine wastes. They concluded that leaching characteristics of both alumina and zirconia calcines by distilled water are similar. Cesium and strontium were selectively leached at significant rates, although cesium leached much more completely from the alumina calcine than from the zirconia calcine. After 2,000 hours, about 95% of the cesium and 33% of the strontium leached from the alumina calcine. In this same time period, nearly 60% of the cesium and 33% of the strontium leached from the zirconia calcine. Cesium and strontium are probably contained in both calcines as nitrate salts and also as fluoride salts in zirconia calcine, all of which are at least slightly soluble in water. Radionuclides of cerium, ruthenium, and plutonium in both calcines were much more resistant to leaching and leached at rates similar to or less than those of the matrix elements. For example, after 1,300 hours of continuous leaching, 0.1% of the total plutonium in the zirconia calcine had been removed and the rate of removal became extremely slow.

Chipman (1990) reported the leaching characteristics of Fluorinel/SBW calcines produced at INTEC. The samples tested included two nonradioactive pilot plant calcines as well as a radioactive Fluorinel-SBW calcine sample. The leaching methods employed were the Environmental Protection Agency's Extraction Procedure (EP) Toxicity Test and the Materials Characterization Center-1 (MCC-1) Static Leach Test at 25°C.

The MCC-1 leach test results on the nonradioactive pilot plant calcines show that total mass loss and component mass loss are affected by solution temperature, initial concentration of calcine in water, and time. Total mass loss increases rapidly and reaches a maximum after about three to seven days and then decreases as some species that are initially leached into solution precipitate as time continues. In the test using the lowest initial concentration of calcine in water (0.001 g calcine/ml water), the total mass loss reached a maximum of about 45% after a seven-day period. Further, MCC-1 testing revealed that NO_3 and Cl were totally leached from the calcine within one day of water contact, and about 90% of the Na and K leached from the calcine within one day of water contact at 25°C. Only a few tenths of a percent of Zr, Cd, and F species are leached from the calcine after 28 days. Partial re-precipitation of a phase containing Al, B, Ca, Cr, and SO_4 was also observed. Additionally, the EP Toxicity Tests on both pilot calcines showed that the limit of toxicity was exceeded by a factor of about 10 to 70 for Cr and about 170 to 850 for Cd.

The MCC-1 static leach testing on the radioactive Fluorinel/SBW (4.7:1 blend of HLW and liquid SBW) revealed a similar behavior in total mass loss with respect to time as the pilot-plant calcines. The total mass loss increases rapidly and reaches a maximum of about 50 wt% after one day. At intermediate times out to seven days, the total mass loss decreases and then slowly increases to about 45 wt% at the conclusion of the 28-day tests. Similar to the simulated calcines, leaching followed by re-precipitation of some components was also observed. Analysis of the leachate shows that about 93 wt% of the Cs, which accounts for about one-half of the total β^{-} activity for this age of calcine used, leaches from the calcine after one day. The quantity leached varies slightly for the remainder of the 28-day test. About 65 wt% of the ^{90}Sr leaches from the calcine after one day, and this quantity increases up to about 86 wt% after 28 days. Only a small amount of the α activity leaches (0.060% gross α) in the 28-day test.

In summary, the leach studies on alumina calcine, zirconia calcine and Fluorinel/SBW summarized above all indicate the rapid and substantial leaching of soluble species such as Cs, Tc and Sr in distilled water at 25°C while actinides including Pu, Am, and Cm are leached at slower rates. Meanwhile, leach studies on alumina calcine in nitric acid (0.25 to 0.5 M) revealed nearly all of the alumina dissolved into solution. EP toxicity tests on Fluorinel/SBW, exceed the limit of toxicity for the RCRA metals Cr and Cd. Based upon the studies summarized above and the absence of long-term degradation rates under geologically relevant conditions, an instantaneous dissolution rate is recommended.

3.3.2.6 Summary of Literature Addressing Glass Waste Form Degradation in Stage 3

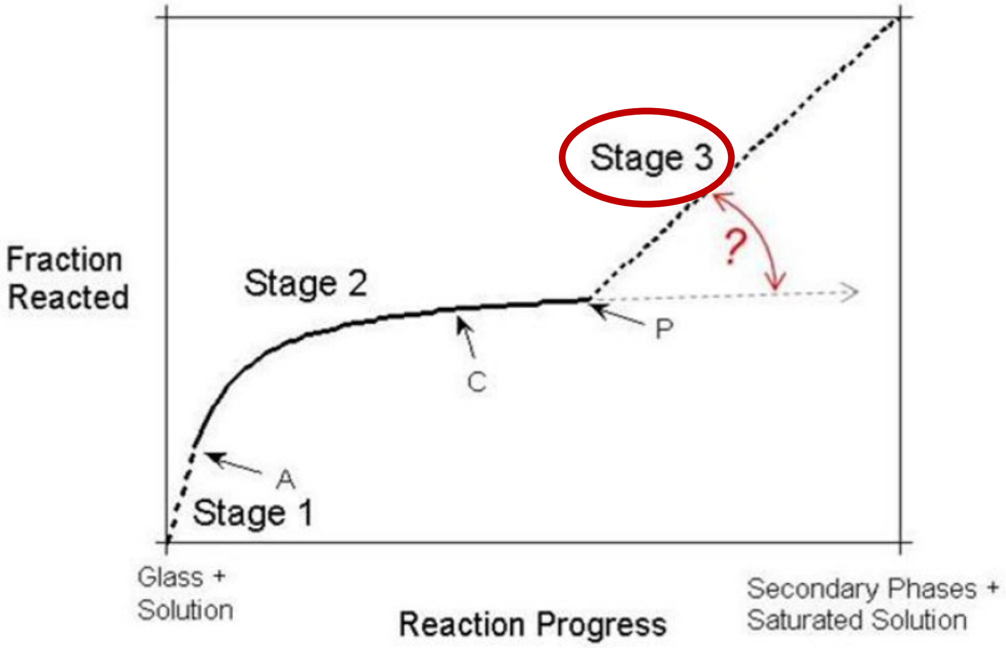
Several reports (Criscenti and Sassani 2010; Freeze et al. 2011; Criscenti et al. 2011) summarize research on glass degradation rates using models and experiments to study three major stages:

1. The initial far-from-equilibrium (glass-solution) rates, or Stage 1 rates, in which the fresh glass surface reacts with solution and the glass dissolution rate is high
2. Evolution to slower, longer term Stage 2 rates, in which alteration layers (e.g., diffusion layer, gel layer, secondary phase layer) are forming on glass surfaces and growing at different rates relative to one another, allowing the solution at the glass interface to approach equilibration and the degradation rate to approach a steady state
3. Glass degradation rates increase dramatically starting at Stage 3, which is characterized by a resurgence in glass dissolution accompanied by the precipitation of more stable secondary phases

As such, recent international efforts have focused on investigating glass degradation rates in more detail to establish an understanding of the transition to increased Stage 3 rates under uncertain conditions during the Stage 2 (slower rate) behavior of HLW glasses (Figure 3-18). The goal is to develop an understanding of the mechanisms initiating the transition to the higher rates such that models can account explicitly for these transitions and the detailed behavior can be incorporated into PA models.

Nuclear waste glass degradation evolves the solution composition naturally to alkaline conditions. However, because some systems may remain far from pH conditions set by the HLW glass itself, a comprehensive rate law over the full range of pH values is desired. Strachan (2017) started with a rate equation (e.g., Pierce et al. 2008; Cassingham et al. 2015) that depends directly on amorphous silica as the "equilibrium phase" and accounts for Stage 1 dissolution ($Q \sim 0$) under acidic, neutral, and alkaline conditions. Strachan (2017) refit the data of Gislason and Oelkers (2003) with a two-term, acid-based version of this rate law and found that it could be used to represent the data for basalt glass dissolution without adding a term involving Al^{3+}.

$$rate_G = k_0 \times 10^{\eta \cdot pH} \times \left[\exp\left(\frac{-E_a}{RT} \right) \right] \times \left[1 - \frac{Q}{K} \right] + k_{long}$$



Source: Modified from Ebert 2017.

Figure 3-18. HLW Glass Rate Law and Schematic Plot of Evolution

Frugier et al. (2008) show that as glass dissolves, a gel layer is formed between the pristine glass and the aqueous solution. The importance of this gel layer in terms of its role in glass degradation remains uncertain. Porous media diffusion of glass constituents out through the gel into aqueous solution and of dissolved species from the solution to the pristine glass surface is suggested. This diffusive process may become the rate-limiting mechanism as the solution at the glass surface becomes closer to being dominated by the glass constituents. Secondary phases nucleate and precipitate within the gel layer suggesting that the trigger for Stage 3 degradation rates is in this layer. Research focusing on the trigger for Stage 3 evaluates (1) the pristine glass composition, (2) the gel composition, and/or (3) the conditions of degradation including temperature and solution pH (Frugier et al. 2008, 2009).

Strachan and Croak (2000) performed geochemical calculations to determine why, in some static dissolution tests, the experimentally observed formation of a zeolite, such as analcime, causes a rapid increase in the dissolution rate for some glasses, but not for others. These calculations, which were performed using the EQ3/EQ6 package, only allowed four phases to precipitate: analcime, amorphous silica, gibbsite, and calcite. A simple glass consisting of six components—SiO_2, Al_2O_3, B_2O_3, Na_2O, CaO, and Li_2O—was used. The calculations were performed assuming that H_4SiO_4 is the dominant dissolved species. It is suggested that analcime precipitation will decrease silica saturation, thereby increasing glass dissolution in Stage 3. The results of this study suggest that analcime precipitation has a strong dependence on the Al content of the glass. For glass with ratios of Si/(Si+Al) < 0.7, the amount of glass that must dissolve is only 1/100 to 1/1,000 of that for glasses with higher ratios before analcime precipitation triggers Stage 3 rates. Strachan and Neeway (2014) calculated the relationship between glass dissolution rates and the precipitation of analcime and concluded that, in the absence of a gel layer, the rate of glass dissolution and the rate of analcime precipitation are coupled. Like Strachan and Croak (2000), Strachan and Neeway (2014) also noted that analcime formed most readily from glasses that had higher Al content.

Jantzen et al. (2016, 2017) created a glass corrosion database (ALTGLASS^{TM}) that was used to determine if gel compositions which evolve are correlated with the generation of zeolites and increased (Stage 3) glass dissolution rates. Using the database, the study team estimated gel compositions based on the difference between the elemental glass starting compositions and the measured elemental leachate concentrations for glasses that had been leached for 15–20 years. The results demonstrated that hydrogel compositions with Si*/Al* ratios of <1.0 (Si* and Al* are defined as the activated Si and Al in the gel) did not generate zeolites and maintained low dissolution rates for the duration of the experiments. These hydrogels have an overall stoichiometry of allophane-hisingerite ($(Al,Fe)_2O_3\bullet1.3\text{-}2Si(OH)_4$) and precipitate clay minerals. Glasses that formed hydrogel compositions with Si*/Al* ratios >1 precipitated zeolites and were accompanied by a resumption in the glass dissolution rate. These hydrogels have a stoichiometry close to that of imogolite ($Al_2O_3\bullet Si(OH)_4$) with ferrihydrite ($Fe_2O_3\bullet0.5H_2O$). Interaction of these hydrogels with excess alkali from the glass and OH^- in the leachates causes the formation of zeolites. In summary, according to this study, the critical factors required for zeolite formation are a hydrogel Si*/Al* ratio >1 and a pH >10. It is also suggested that the high pH values of the leachate solutions are directly proportional to the alkali content of the glass.

Gin et al. (2015) conducted experiments on the International Simple Glass (ISG) at 90ºC in a solution initially saturated with respect to amorphous $^{29}SiO_2$ (i.e., ~Stage 2 conditions). At pH 9, the corrosion rate continuously drops, and the glass slowly transforms into a uniform, homogenous, amorphous alteration layer. At pH 11.5, the alteration process differs; the glass completely dissolves and secondary phases precipitate. At pH 11.5, the glass dissolution rate is maintained close to that in Stage 1 by the hydrolysis of the silicate network promoted by OH^- and by the precipitation of zeolites and other less stable phases. Fournier et al. (2017) followed this work by introducing zeolite seeds into the ISG leaching experiments. They concluded that high pH values combined with high Al concentrations in solution lead to zeolite precipitation, and that the sudden decrease in Al concentrations caused by zeolite formation leads to an increase in glass dissolution rate. In agreement with Gin et al. (2015), the study results demonstrated that the effect of zeolite precipitation decreases with decreasing pH and T and was no longer detectable in unseeded leaching experiments conducted at pH 9. These experiments show that the glass composition alone is insufficient to determine if the transition to Stage 3 will occur and that different pH conditions can lead to different long-term outcomes.

Fournier et al. (2018) further investigated the effect of zeolite precipitation on the dissolution kinetics of the ISG using the GRAAL (Glass Reactivity with Allowance for the Alteration Layer) model. The GRAAL model relies on the reactivity (i.e., formation and dissolution) of a transport-limiting layer called the passivating reactive interphase (PRI) (Frugier et al. 2008).

The equations used in the GRAAL model by Fournier et al. (2018) to study ISG dissolution include expressions for (1) zeolite nucleation and growth, (2) first-order rate laws to constrain the Si/Al and Ca/Al ratios of the gel layer to the stoichiometry $SiAl_{0.3}Ca_{0.15}O_{2.6}$, and (3) first-order rate laws derived from transition state theory to describe the precipitation of secondary phases including both zeolites and C-S-H. Fournier et al. (2018) argue that to match experiments, the Si/Al ratio of the PRI should be in the 0.1–0.7 range. They also point out that using the solubility of the endmember $SiAl_{0.3}Ca_{0.15}O_{2.6}$ in the rate expression accounts for the roles of Al and Ca on Si precipitation at pH > 10.

Gin (1995) first suggested that Al is involved in the rate-limiting reaction and defined a mixed Al-Si activity product, but McGrail et al. (1997, 2001) found this proposed ion activity product to be inconsistent with the existing data and modeling of glass dissolution. Others have also proposed a role of Al^{3+} in the rate-limiting reaction (Bourcier 1994; Hamilton et al. 2000; Abraitis et al. 2000; Hamilton et al. 2001; Oelkers and Gislason 2001; McGrail et al. 2001; Gislason and Oelkers 2003; Criscenti et al. 2005, 2006). The rate laws of Oelkers and Gislason (2001) and Gislason and Oelkers (2003) suggest that at constant $[H_4SiO_4]$, the rates should increase with decreasing Al^{3+}.

Because the gel layer between the glass and the aqueous solution appears to play a key role in nuclear waste glass dissolution, many researchers have focused on understanding this gel layer in detail. One of the key issues under investigation is whether the gel layer is (1) a residual glass layer formed by the incongruent dissolution of the glass (i.e., preferential leaching of mobile cations leaving behind the framework glass structure), or (2) the result of congruent dissolution of the glass followed by precipitation of an amorphous silica-rich layer. Another issue under debate is the role of the gel layer in glass degradation. Does the gel layer passivate the glass surface slowing glass dissolution because now glass and aqueous solution components must diffuse through this protective layer, or does the gel layer enhance glass degradation by providing nucleation sites for secondary minerals, or both?

Hellmann et al. (2015) and Putnis (2015) both focus on how advanced atomic-resolution analytical techniques show that the structural and chemical interface between pristine glass and the altered zone is always extremely sharp, with gradients in the nanometer to subnanometer range. This observation supports the hypothesis that the alteration layer is a consequence of congruent dissolution followed by precipitation of an amorphous silica layer. The techniques used to observe this sharp interface include scanning transmission electron microscopy with a high-angle annular dark-field detector (STEM-HAADF), energy-filtered TEM (EFTEM) mapping, electron energy-loss spectroscopy (EELS), and atom probe tomography (Hellmann et al. 2015). Putnis (2015) points out that these results are consistent with experimental results that found that stable isotope tracers introduced in the aqueous solution (e.g., Geisler et al. 2010; Dohmen et al. 2013) were discovered in the alteration layer. Geisler et al. (2015) continued to conduct experiments using oxygen and silicon isotope tracers to study the degradation of ternary Na-borosilicate glasses and concluded that the experimental data fit with a model of congruent dissolution of the glass followed by the precipitation and growth of an amorphous silica layer. Geisler et al. (2019) conducted real-time *in-situ* experiments of reaction and transport phenomena during silicate glass corrosion by fluid-cell Raman spectroscopy. The formation of a water-rich zone (several micrometers thick) between the alteration/gel layers and the glass was found. This zone was detected, as were pH gradients at the glass surface and within the alteration layers. Using a deuterated solution, the researchers observed that water transport through the gel is not rate limiting.

Murphy et al. (2013) conducted experiments on both Advanced Fuel Cycle Initiative glass and a simplified version of this glass in ASTM type I water at 90°C and then used a suite of nuclear magnetic resonance (NMR) techniques to investigate the composition of the gel layer. Both glasses developed alteration layers composed primarily of $^{[IV]}$Si species. Aluminum was also retained in the alteration layers, with a change in coordination from $^{[IV]}$Al to $^{[VI]}$Al, which correlates with a loss of charge-balancing cations. ^{1}H-^{11}B cross polarized magic angle spinning NMR observations indicated a retention of boron in the hydrated glass layer (defined as between the bulk glass and gel/alteration layer), a result that has not been characterized by previous work. The ratio of $^{[III]}$B/$^{[IV]}$B was found to be ~0.95 in the pristine glass. Secondary phases in the alteration layers (termed precursor phases) were identified as crystalline sodium metasilicates.

Pierce et al. (2010) studied the dissolution kinetics of five glasses along the $NaAlSiO_4$-$NaBSiO_4$ join to evaluate how the structural variations associated with boron-aluminum substitution affect the rate of dissolution. Analysis of unreacted glass samples by ^{27}Al and ^{29}Si magic angle spinning NMR suggested that most Al and Si atoms occupy a tetrahedral coordination, whereas B-atoms occupy both tetrahedral and trigonal coordination. The $^{[III]}$B is fractionated between $^{[III]}$B(ring) and $^{[IV]}$B(nonring) moieties with the $^{[III]}$B(ring)/$^{[III]}$B(nonring) ratio increasing with an increase in B/Al ratio. The fraction of $^{[IV]}$B also increases with B/Al ratio, and there appears to be mixing between the $^{[IV]}$Al and $^{[III]}$B sites, assuming avoidance between tetrahedral trivalent cations.

Within the Materials Recovery and Waste Form Development (MRWFD) Campaign within DOE-NE, the mechanistic behavior that initiates Stage 3 degradation rates for glass are being incorporated into a performance assessment model. When this MRWFD glass model becomes available, SFWST will incorporate this into GDSA so it can be used to represent glass long-term degradation behavior. This approach involves ongoing cross-campaign integration activities.

3.4 Additional Waste Form Characteristics Refinement Studies

Starting in FY2018, the OWL team has pursued three studies to evaluate/redefine waste form characteristics and/or performance models. The first study evaluates characteristic isotopic ratios for various waste forms included in postclosure performance studies to delineate isotope ratio tags that quantitatively identify each particular waste form. This evaluation arose due to questions regarding the relative contributions of radionuclides from disparate waste forms in GDSA results, particularly, radionuclide contributions of DSNF versus DHLW glass. In the second study, the team is evaluating the conceptual and mechanistic bases for applying the glass waste degradation rate models to evaluate the degradation of the HIP calcine waste form (this application is discussed above). The HIP calcine may likely be a multiphase glass ceramic mixture, with the ceramic phases having different degradation performance from the glass portion. The distribution of radionuclides among those phases may also be a factor in the release rates. The third study is an ongoing investigation of the performance behavior of TRISO particle fuels. The study includes development of a stochastic model for the degradation of those fuels that account for simultaneous corrosion of the SiC layer and radionuclide diffusion through it.

3.4.1 Study Determining Feasibility of Using Characteristic Isotopic Ratios

3.4.1.1 Delineating Characteristic Isotopic Ratios for Various Waste Forms

The OWL team has continued a study to define characteristic isotopic ratios for various waste forms included in postclosure performance studies. Questions regarding the relative contributions of radionuclides from disparate waste forms in the previous generic GDSA results for salt and granite systems (Sevougian et al. 2016) led to initiation of this evaluation. Particularly, the question arose as to whether it was possible to develop a direct method to deconvolve the radionuclide contributions of DSNF versus DHLW glass at various locations in a generic repository system represented in the GDSA.

Depending on the design of the generic repository evaluated, it may be easy to assess individual waste form contributions proximal to the source terms if the various waste forms are segregated into sections of the repository. However, given the complexity of some geologic systems, isotopic ratios (two or more) that effectively tag their source waste form distinctly would facilitate such assessments at distal points. Using such ratios to define mixing lines may allow quantitative estimates of relative waste form contributions to be "mined" from existing GDSA results, as long as the particular isotopes are tracked. This method would be similar to geochemical techniques using natural isotopic ratios to assess mixing in natural systems. For future analyses, fictive particles singular to individual waste forms could be added to each waste form inventory and used as tracking mechanisms; both unretarded and retarded fictive particles could be utilized.

In addition to the design of a generic repository, the repository inventory plays a role in how easily waste form contributions can be delineated. Given that the GDSA for both a generic salt and a generic granite (Sevougian et al. 2016) repository contain both DSNF and HLW glass, these GDSA results would provide initial idealized test to check the efficacy of the approach. Useful isotopes for defining characteristic isotopic ratios of the waste forms of interest should have at least the following characteristics:

- They should be heavy molecular weight isotopes so fractionation processes are not an issue.
- They should have distinct signatures between the waste forms of interest (larger differences should provide more sensitivity).
- They should have signatures that are not overwhelmed by the natural system background signatures, if those are included in the GDSA evaluations.

Isotopes of the actinides provide a direct means for meeting the first and third above characteristics, with the level of distinction for each waste form inventory assessed preliminarily below.

A first-order assessment of the isotopes most likely to distinguish HLW glass from DSNF has been derived from Rechard and Stockman (2014, Figure 19) where it can be seen that

- Isotopes ^{230}Th, ^{233}U are about 30- to 100-fold the mass per package for DSNF than for HLW glass.
- Isotopes ^{234}U, ^{235}U, (^{238}U) are about 5- to 10-fold the mass per package for DSNF than for HLW glass.

- Isotope ^{99}Tc is about 1/10 the mass per package for DSNF than for HLW glass.

The results shown in Rechard and Stockman (2014) simply provide an initial starting point primarily because those waste form inventories represent averages of

- Various projected HLW glasses from a number of sites
- All DSNF compositions (not including naval SNF or Na-bonded fuel components)

In order to quantitatively extract mixing data from a specific set of GDSA results, the waste forms and their inventory data used in that GDSA evaluation are the data that delineate any discriminating isotopic ratios. Isotopes other than those above (e.g., ^{229}Th, some Pu isotopes) may also be useful for some particular waste forms in the inventory. Note that, as more waste forms are included into a GDSA analysis, more distinguishing characteristics (isotopic ratios) would likely be required to define quantitatively the mixing lines with enough independent constraints.

The next step in this analysis was to evaluate characteristic isotopic ratios based on the GDSA inventory specifics to see if there are ratios that discriminate among the waste forms, which may be useful for evaluating GDSA results away from the repository. Two uranium isotope ratios were assessed, ^{238}U/^{236}U and ^{234}U/^{233}U. For ^{238}U/^{236}U about 2.5 orders-of-magnitude (OoM) variation is observed for waste forms including Hanford and SRS HLW glasses, INL calcine, and a number of the DSNF, whereas for ^{234}U/^{233}U there is about 3 OoM variation. Preliminary examination of ^{242}Pu/^{239}Pu indicates ~2 OoM variation, but with clustering around two values indicating that this ratio may not be as discriminating as the uranium isotopic ratios, but it is possibly useful. Lastly the ^{135}Cs/^{129}I was examined, and it was found that this ratio is fairly similar for most of these waste forms (~0.5 OoM variation). This activity will continue the evaluation of the various waste form inventories to define a set of ratios that allow quantitative evaluation of mixing of waste form contributions at various locations in the GDSA results.

3.4.1.2 Using Isotope Ratios To Determine the Contribution of Waste Forms to Dose

Ultimately, the question under study is the feasibility of defining isotope ratios that uniquely identify waste form source terms in a repository and then using those tracer ratios to evaluate quantitatively how much each waste form contributes to the isotopic composition and its dose at any other location in the system, including at the accessible environment.

If many waste forms are disposed, then the combined release and transport processes convolve the contributions to the mobile radionuclide content from all these waste forms through time and space. In order to deconvolve the contribution from each waste form quantitatively, unique distinguishing tracers for each waste are being defined. Hence, the OWL team evaluated the use of isotopic ratios from the inventory of previous analyses to roughly estimate the dose contribution (Section 3.4.1.1). Given the limited radionuclides included in those inventories, it was not possible to fully deconvolve the contributions. In future PA work, including unique fictitious tracers with defined concentrations in each waste form and with chemical characteristics defined identically to other radionuclides in that inventory should allow for defining the needed ratios to deconvolve each waste form contribution to dose at any location in the disposal system. However, including numbers of fictitious radionuclides can be computationally burdensome and needs to be done before performing the calculations. So this method does not permit evaluating previous analyses.

The feasibility of the method is being demonstrated using the generic GDSA clay/argillite repository. The generic clay repository has six waste forms that degrade as HLW glass—four DHLW forms (from Hanford, SRS, INL HIP calcine), FRG glass and vitrified Cs and Sr capsules from Hanford, and instantaneously degrading DSNF (N-reactor)—segregated into eight categories based on heat generation.

Several approaches to demonstrate isotopic ratio feasibility focus on ^{129}I because only ^{129}I transports substantially away from the generic GDSA clay/argillite repository source term. First, fictitious tracers with the decay and chemical (not solubility-limited and no sorption) characteristics of ^{129}I will be added to the inventory with the fictitious tracers added to each waste form with defined contents to allow definition of the unique ratios for deconvolving the contribution of each waste form. Second, variation of waste degradation rates, sorption, and solubility characteristics are to be studied. In each case, the ratios will be assessed at three locations in the sandstone and limestone layers above and below, respectively, the GDSA repository horizon in the clay/argillite.

3.4.2 Study Evaluating Applicability of Glass Waste Degradation Rate Models to HIP Calcine Waste Forms

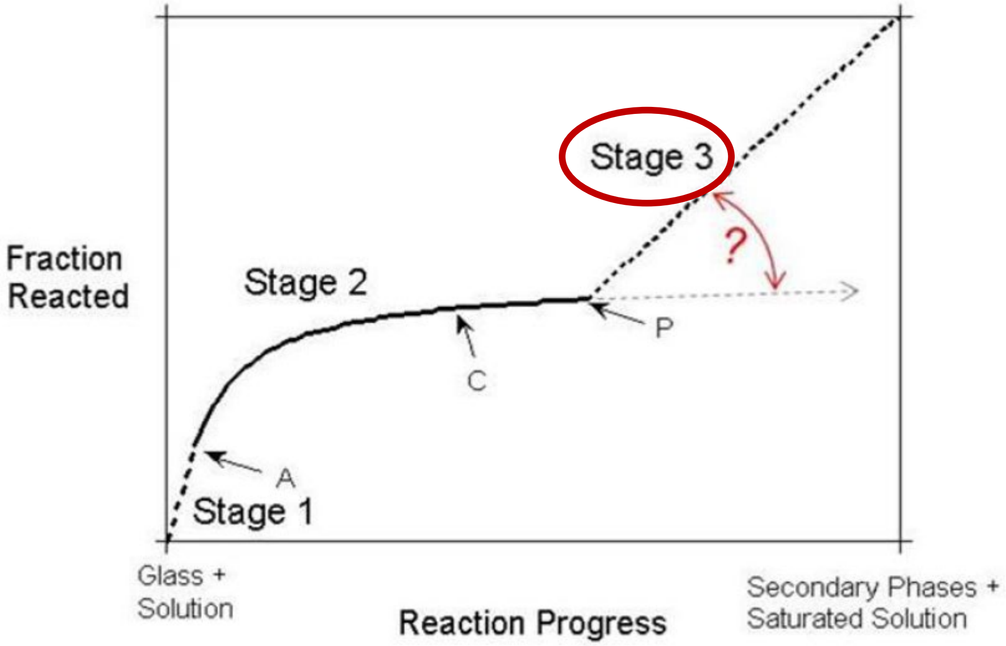
The FY2018 analysis of HIP calcine waste degradation (1) considers the technical basis for the rate law to be used for geologic disposal, namely the HLW glass rate law by analogue (Section 3.3.2.3), (2) identifies knowledge gaps, and (3) outlines how these knowledge gaps might be bounded for future PAs.

Current plans call for INL calcine waste to be mixed with silica, titanium, calcium, sulfur, and other additives, then go through a HIP process to produce an assemblage of radionuclide-containing titanates, sulfides, glass/quartz, and nepheline. The resulting waste form might be expected to be at least as stable as HLW glass because short-term HIP calcine dissolution rates measured from Na release appear to be lower than HLW glass rates, except at very high waste loadings (Begg et al. 2005). However, no long-term HIP calcine dissolution rates exist; the comparison of Begg et al. (2005) is based on seven-day, 90°C leach results. Moreover, the mechanistic understanding that allows HLW glass dissolution to be projected over the life of a repository is not directly applicable for HIP calcine. Lastly, HIP calcine is a mineral-glass mixture, which obscures the simple analogy of HIP calcine and HLW glass degradation.

Because of the mineralogical complexity of HIP calcine, using the HLW glass rate law for HIP calcine would involve a more mechanistic justification for the HLW glass-HIP calcine analogy than simply the similarity in seven-day, Na release rates. To this end, the current fundamental basis of the HLW glass rate law is outlined below, and the HIP calcine data that should be considered for use with the HLW glass rate law in a repository setting are identified.

If radionuclide release from HIP calcine and HLW glass is similar, then the HIP calcine waste form degradation will reflect a three-stage process that was discussed previously in Section 3.3.2.6 and illustrated in Figure 3-18. For convenience, Figure 3-18 is reproduced below as Figure 3-19. The three-stage process consists of (1) rapid initial degradation of the glass phase, (2) slower/minimal degradation once dissolved glass components accumulate and approach saturation with a metastable hydrated silica-or titanium-rich surface alteration layer, and (3) renewed rapid release upon transformation of the metastable alteration layer into more stable phases. The onset of Stage 3 HLW glass dissolution is a challenge to predict and remains the current focus of study (e.g. Ebert 2017).

$$rate_G = k_0 \times 10^{\eta \cdot pH} \times \left[\exp\left(\frac{-E_a}{RT} \right) \right] \times \left[1 - \frac{Q}{K} \right] + k_{long}$$



NOTE: This figure is the same as Figure 3-18. It is reproduced here for convenience.

Source: Modified from Ebert 2017.

Figure 3-19. HLW Glass Rate Law and Schematic Plot of Evolution (repeat intentional)

The rate law at the top of Figure 3-19 is used to describe the functional form of the HLW glass dissolution rate shown below it. The terms in the rate law are the following:

- k_o = intrinsic glass dissolution rate (mass area^{-1} time^{-1})
- $10^{\eta.pH}$ = empirical function to calculate pH dependence of rate (unitless)
- $\exp[-E_a/RT]$ = activation energy expression to calculate effect of temperature on rate
- $1 - Q/K$ = affinity expression to track free energy dependence of dissolution
- k_{long} = lower limit glass dissolution rate (mass area^{-1} time^{-1})

Stage 1 dissolution occurs far from equilibrium where $Q/K \sim 0$. Stage 1 rates tend to reach a minima at near neutral pH and increase with increasing or decreasing pH (e.g., Knauss et al. 1990). Stage 2 dissolution rates decrease because of back reaction between the dissolving glass surface and dissolved silica, i.e., $0 < Q/K < 1$. A nearly constant residual rate, k_{long}, prevails very near equilibrium ($[1 - Q/K] \sim 0$). Stage 3 dissolution occurs after the alteration phases present at the dissolving glass surface condense to form a more stable assemblage with a lower K. This decreases the Q/K term thereby increasing the overall rate. Again, the chemical details of the HLW glass Stage 2-to-Stage 3 transition remain unclear.

Features peculiar to HIP calcine are the following: (1) it is multiphasic, being minerals + glass versus glass only, (2) it has a higher Ti and S content, and (3) specifics of its composition are not publicly available (e.g., Bateman et al. 2013). Lack of a publicly available HIP calcine recipe prevents quantitative assessment of long-term stability in a repository, though analyses of previous recipes give some useful information about why the various additives are used and their effect on waste form leaching (e.g., Staples 1988; Raman 1998).

Degradation of multiphasic HIP calcine can probably be conservatively bounded by setting the overall rate equal to the degradation rate of the faster-dissolving HIP calcine glass phase. For example, silica glasses tend to dissolve roughly ten times or more faster than their crystalline equivalents. However, a thermodynamic analysis of the solubility of the crystalline phases in the HIP calcine glass matrix must be done to assure lower solubility than the glass itself. The fraction of reacting glass surface area to overall surface area might be approximated from the mass fraction of the two.

A Ti-rich surface alteration layer may form on HIP calcine, not the Si-rich surface alteration layer that dominates Stage 2 dissolution of HLW glass. Ti-rich gel layers form when titanate minerals dissolve, but the extent to which the Ti gel layers control overall dissolution of the titanate minerals, or the HIP calcine glass, is unclear.

HIP calcine dissolution may be sensitive to the redox state of repository fluids, unlike HLW glass dissolution. Redox-sensitive elements like sulfur are largely absent from HLW glass; so the redox state of repository fluids should play no direct role in HLW glass dissolution. Redox-sensitive components can become the focus of biologic activity and degrade faster. Oxidation of reduced components like sulfur might decrease ambient pH and indirectly accelerate HIP calcine dissolution.

Lastly, the surface area of the HIP calcine must be constrained. Note that the HLW glass rate law described in Figure 3-19 is normalized to HLW glass surface area. In practice, the HLW glass rate law uses the product of the nominal surface area of HLW glass monoliths and a crack surface area factor; the latter accounts for increased solid surface area from cracking. Presumably, the HIP calcine dissolution rate would be calculated similarly, with surface areas defined for the rate controlling phase and possibly for each dissolving phase, again also accounting for the smaller fraction of glass.

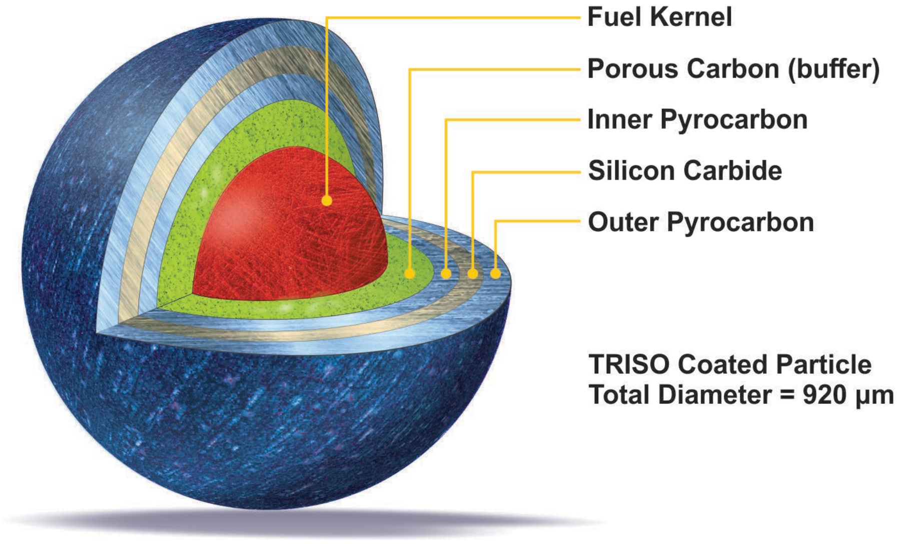
3.4.3 Study Investigating Constraints on Performance Models of TRISO Particle Spent Fuels

The objective of this investigation is (1) to develop a general and stochastic model for radionuclide releases from TRISO particle spent fuel under geological repository conditions with the available data, (2) to identify gaps in the current data and analyses available, and (3) to synthesize a general model to estimate radionuclide releases over time for generic repository concepts.

3.4.3.1 Background: TRISO Fuel Description

TRISO particle fuel, consists of numerous coated fuel particles, slightly less than 1 mm in diameter, that are embedded in blocks or spheres of graphite. The particles consist of a micro spherical kernel of UO_x about 500–600 µm in diameter, and four coating layers as shown schematically in a cut-away view in Figure 3-20. The purpose of each layer is given in Nabielek et al. (2010) and summarized below in Table 3-7. Given in order away from the UO_x fuel kernel, these layers are (1) a buffer layer of porous pyrolytic carbon, (2) an inner dense pyrolytic carbon (IPyC) layer, (3) a SiC layer, and (4) an outer dense pyrolytic carbon (OPyC) layer.

Two studies (Fachinger et al. 2006; Van den Akker and Ahn 2013) have evaluated the potential releases from TRISO spent fuel in geologic repository environments. Fachinger et al. (2006) conducted experiments to measure hydrologic properties (i.e., porous media diffusivities) and corrosion rates for the various materials of the TRISO fuel pebbles/particles in a number of fluid compositions at relevant temperatures. The measurements were made on separated materials rather than intact pebbles or particles. The diffusive transport behavior was measured for the graphite matrix (i.e., from the pebble) using isotopes of hydrogen, chlorine, strontium, and cesium. Corrosion rates were measured for the graphite matrix, the SiC (nonirradiated and irradiated), and the pyrocarbon (Fachinger et al. 2006). Fachinger et al. (2006) also measured leaching rates of ThO_2, UO_2, and (Th-U) MOX fuel kernels in various fluids over a range of redox conditions.



NOTE: pyrocarbon = pyrolytic carbon
TRISO = tristructural-isotropic

Figure 3-20. Schematic Drawing of a TRISO Fuel Particle with Four Protective Layers

Table 3-7. Characteristics of TRISO Fuel with a UO_x Core of Radius 250–300 μm

Layer	Nominal Thickness (μm)	Purpose/Function
Porous pyrolytic carbon buffer	60 – 95	- allows kernel to swell - stops recoiling fission products from reaching SiC layer - provides void volume for gases
IPyC	30 – 40	- barrier to gaseous fission products - slows down metallic fission product transport
SiC	25 – 35	- main fission product barrier - structural support to contain gas pressure
OPyC	40 – 45	- protects SiC layer from chemical and mechanical damage - adds to support to contain gas pressure

NOTE: IPyC = inner dense pyrolytic carbon
OPyC = outer dense pyrolytic carbon
SiC = silicon carbide

Source: Minato et al. 1994; Moormann et al. 2001; Nabielek et al. 2010; Fachinger 2006.

The conclusions of Fachinger et al. (2006) include the following: (1) the graphite matrix of the pebble serves as a porous medium that reduces water contact with the TRISO particles, (2) porous media diffusion is the primary transport mechanism through the graphite matrix of the pebble, (3) pyrocarbon and SiC layers have corrosion lifetimes from thousands to hundreds of thousands of years depending on conditions (temperature, fluid composition, radiation dose), and (4) fuel kernels may have relatively long corrosion lifetimes (≥100,000 years) depending on conditions. This study also recommended further work evaluating (1) the porous media behavior of the graphite matrix and how it changes due to graphite corrosion, (2) the effect of internal pressure build-up on the layer lifetime, (3) mass transport through the graphite matrix, and (4) development of an integrated model of the total set of processes.

In the second study, Van den Akker and Ahn (2103) constructed a PA of hexagonal graphite fuel elements (with TRISO particles in graphite compacts) degrading within an unsaturated (oxidizing) geologic repository system. The primary waste form barrier in that work was the graphite matrix of the fuel element (or the graphite matrix of the compact in a second scenario), which slowly oxidatively corrodes to release radionuclides uniformly over tens of millions of years. That study evaluated stochastic failure (rupture) of the SiC layer of the TRISO particle due to combined effects of SiC corrosion and internal pressure build-up from helium generation. The analyses included statistical variability of the SiC strength and concluded that, if protection by the OPyC layer is ignored, then lifetimes on the order of thousands to hundreds of thousands of years were expected. Although Van den Akker and Ahn (2013) estimated that protection by the OPyC layer could extend SiC-layer lifetime to millions of years, they made the simplifying assumption that the particle lifetime was short compared to graphite matrix corrosion (of either the fuel element or the compact). Hence for their model, they assumed the TRISO particles had released all radionuclides and distributed those radionuclides uniformly throughout their spherical approximations (of either the entire fuel element or just of a single graphite compact) of corroding graphite. The corrosion of the graphite sphere was then used to assess radionuclide releases from the TRISO fuel directly to the host rock.

As recommended by Fachinger et al. (2006), the OWL team has begun the construction of a quantitative integrated model on the scale of a fuel compact. The integrated model includes major features, events, and processes to evaluate stochastically the release of radionuclides under varying repository conditions through time. This report presents the analyses of the primary coupled process considerations for the SiC layer of the TRISO particles. The analyses assess the relevance of these processes at repository conditions. Future work will consider uncertainties in material properties for the porous media transport processes. This effort will include assessment of whether or not the SiC-layer porosity would render the layer effectively impermeable until after corrosion breach, as well as assessment of parametric uncertainties in the material properties of the other layers to the extent data are available.

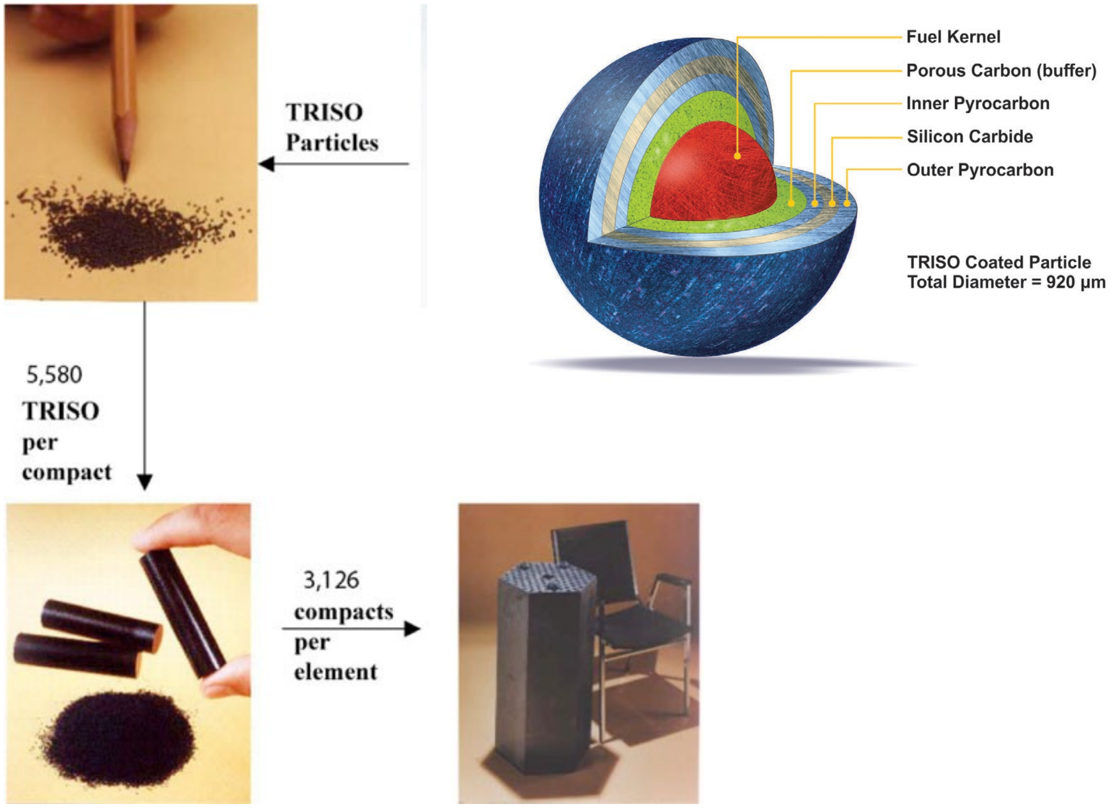
3.4.3.2 Release Mechanisms for Intact TRISO Fuel in a Geological Repository

For the release analysis, it is assumed that all the layers remain intact upon removal from the reactor, and the fuel has cooled to a temperature that is far below the maximum reactor operating temperature of 1,200°C, but above the ambient repository temperature due to continuing radioactive decay. Even for initially intact layers, there are three mechanisms that may lead to release of radionuclides: (1) helium pressure buildup that could rupture the main barrier, which is the SiC layer, (2) diffusive transport through the layers, and (3) corrosion of the layers in brine. These processes are not totally independent. Corrosion reduces layer thickness, which may result in higher radionuclide gradients and hence may increase diffusive transport. The reduced layer thickness may also reduce the effective tensile strength to retain pressure within the particle and avoid layer rupture. The purpose of this work is to assess these release processes for intact fuel under repository conditions.

As shown in Figure 3-21 and discussed by Van den Akker and Ahn (2013), about 5,580 TRISO particles are embedded in graphite compacts (graphite cylinders 4.928-cm long and 1.245 cm in diameter). Figure 3-21 also shows the hexagonal fuel elements in the lower right corner. The fuel elements are hexagonal graphite blocks with 324 holes, 216 of which are filled with compacts (and some containing alignment dowels) and 108 holes of which are used for coolant flow. There is a total of 3,126 compacts per fuel element, each of which is 79.3 cm in height and 36-cm wide flat-to-flat. An alternative fuel design has the TRISO particles embedded in graphite spheres called pebbles (analogous to compacts), which are 6 cm in diameter (e.g., Fachinger et al. 2006).

Coupled Corrosion and SiC Rupture by Helium Pressure Buildup

Pressure buildup effects have been reported by Van den Akker and Ahn (2013), and their estimates of SiC tensile strength variability and pressure with time are used in the model. From their calculation, the pressure may exceed 10 MPa after 10^5 years. Whether or not the SiC layer will rupture is very much dependent on the corrosion rate. A plot of the SiC layer rupture probability with time in various fluids/brines relevant to geologic disposal concepts (Fachinger et al. 2006; Van den Akker and Ahn 2013) is being developed.



Note: TRISO = tristructural-isotropic

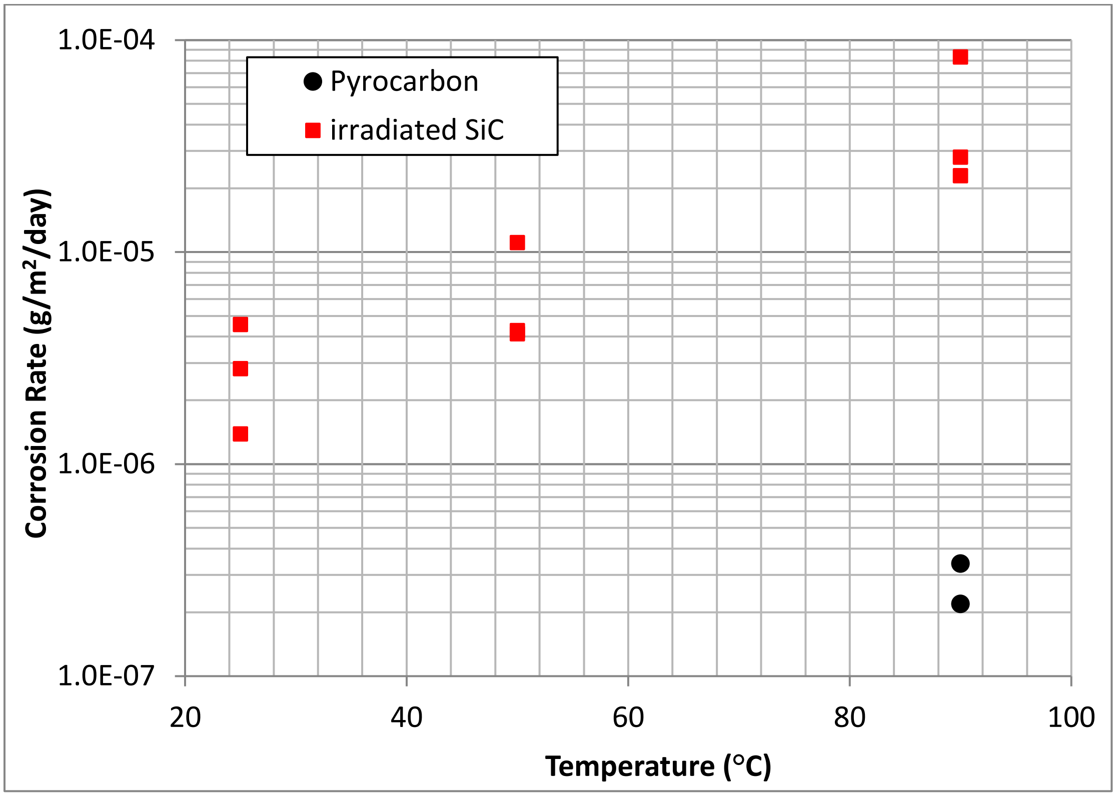
Source: Photographic images from Sterbentz et al. 2004 and values from Van den Akker and Ahn 2013.

Figure 3-21. Assembling of TRISO Particles into Compacts and Then Elements

The corrosion rate of irradiated SiC and pyrolytic carbon in different brines has been reported by Fachinger et al. (2006). Their data are plotted in Figure 3-22. The cumulative probability for SiC layer failure is 100% according to Van den Akker and Ahn (2013) at about 7,000 years or 1.4×10^5 years for SiC corrosion rates of 4.09×10^{-5} g/m^2/day and 2.03×10^{-6} g/m^2/day, respectively. From Figure 3-22, these corrosion rates are in the range of laboratory measured rates for temperatures at or below 90°C. Van den Akker and Ahn (2013) also noted that if the protective aspect of the OPyC layer is considered, the SiC layer may have lifetime of up to 2×10^6 years, which is substantial for performance time frames of a geologic repository.

Release by Diffusion through a Multilayered Particle

SiC layer rupture by pressure buildup is a physical process that is independent of the radionuclide. However, the diffusion rate is dependent on the radionuclide, the medium, and the temperature. For geological repository timescales, a subset of the radionuclides of interest for long-term performance are given in Table 3-8.



NOTE: Data Points at the same temperature corresponding to different brine compositions.
SiC = silicon carbide

Source: Data from Fachinger et al. 2006.

Figure 3-22. Corrosion Rate Variation of Pyrolytic Carbon and Irradiated SiC as a Function of Temperature

Table 3-8. Example Radionuclides of Interest for a Geological Repository

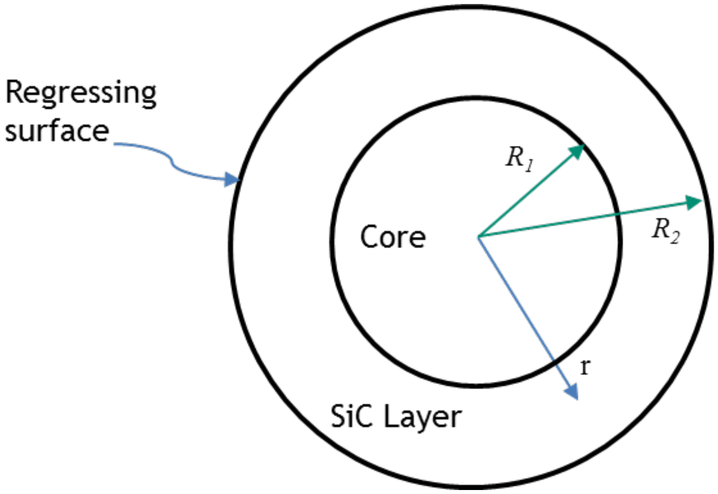
Radionuclide	Half-life (years)	Decay Product
^{129}I	1.57×10^{7}	^{129}Xe
^{36}Cl	3.01×10^{5}	^{36}Ar
^{226}Ra	1.60×10^{3}	^{222}Rn → ^{218}Po → ^{214}Pb → ^{214}Bi → ^{214}Po → ^{210}Pb → ^{210}Bi → ^{210}Po → ^{206}Pb
^{79}Se	2.95×10^{5}	^{79}Br
^{99}Tc	2.13×10^{5}	^{99}Ru

NOTE: Actinides are relevant in oxidizing systems.

Diffusion data at high temperatures in SiC have been collected by Malherbe (2013), but no diffusion data in SiC were found for any of the radionuclides given in Table 3-8 at repository temperatures. Data for diffusion of ^{36}Cl, ^{90}Sr, and ^{134}Cs through graphite in different brines range from 1.2×10^{-13} m^2/s to 6.3×10^{-13} m^2/s (Fachinger et al. 2006). For noncorroding layers, the problem of determining radionuclide releases by diffusion through consecutive layers has been reported by Gelbard (2003). The challenge is that the diffusivities of radionuclides in Table 3-8 through SiC and pyrolytic carbon need to be estimated. Such basic principles calculations have been reported for radionuclides by De Bellefon and Wirth (2011), Ko et al. (2016), Minato et al. (1994), Rabone et al. (2014), and Rabone and Lopez-Honorato (2015), and this information will be considered in future work. This work will establish the minimum diffusivities in SiC for which diffusional releases are significant. Thus, accurate diffusivities may not be needed if the diffusivities can be shown to be bounded to be below the minimum diffusivity to be important relative to corrosion.

Coupled Corrosion and Diffusion

The coupled process of corrosion and diffusion has been developed as part of this work. Consider a spherical pellet core surrounded by a single spherical (comprised of SiC) layer with inner and outer radii R_1 and R_2 as given in Figure 3-23. The core is comprised of (1) the fuel kernel, (2) the porous pyrolytic carbon buffer layer, and (3) the IPyC layer. Note that these core components are not discretized (i.e., are lumped together) here as the radionuclides have diffusivities through these regions that are much, much greater than the radionuclide diffusivities through the SiC layer.



NOTE: SiC = silicon carbide

Figure 3-23. Schematic Diagram of Corroding Outer Layer through which Radionuclides Are Diffusing from Inner Core

Within the SiC layer (the primary barrier to release considered here), the radionuclide concentration may be described by the diffusion equation in spherical coordinates with a term to account for radioactive decay and is given by

$$\frac{\partial C}{\partial t} = \frac{\mathcal{D}}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) - \lambda C \qquad (Eq. 1)$$

where

$\mathcal{D}$ = radionuclide diffusivity in the SiC layer (m^2/s),

C = radionuclide concentration in the SiC layer (kg/m^3),

λ = radioactivity decay constant (s^{-1}),

r = radial distance (m), and

t = time (s).

The boundary conditions for coupled diffusion and corrosion are

$$C = 0, \text{at } r = R_2(t) \text{ and } t > 0, \qquad (Eq. 2)$$

$$C = C_1, \text{at } r = R_1 \text{ and } t > 0, \quad \text{and} \qquad (Eq. 3)$$

$$C = C_0(r), \text{at } R_1 \le r \le R_2 \text{ and } t = 0. \qquad (Eq. 4)$$

The system of Eqs. 1–4 is solved with $R_2(t)$ determined from the corrosion data given by Fachinger et al. (2006).

The mass of radionuclide in the core and SiC layer is given by

$$M(t) = \frac{4}{3}\pi R_1^3 C_1 e^{-\lambda t} + \int_{R_1}^{R_2} 4\pi r^2 C e^{-\lambda t}\, dr. \qquad (Eq. 5)$$

If all the radionuclide mass is originally in the core, then the mass fraction of radionuclide retained in the core plus SiC layer system is given by

$$F(t) = \frac{\frac{4}{3}\pi R_1^3 C_1(t) + \int_{R_1}^{R_2} 4\pi r^2 C\, dr}{\frac{4}{3}\pi R_1^3 C_1(0)}. \qquad (Eq. 6)$$

The ideally performing barrier equates to $F(t)$ approaching unity, which indicates all the radionuclide has been retained.

For corrosion of the SiC layer, the constant corrosion rate is given by k, and the mass of the layer is given by m, and so then by mass balance (Peterson and Dunzik-Gougar 2011; Van den Akker and Ahn 2013)

$$\frac{dm}{dt} = -Ak \qquad (Eq. 7)$$

where

m = layer mass (kg),

k = corrosion rate (kg/m^2/s),

A = outer surface area of corroding layer (m^2), and

t = time (s).

For later use, let

L = layer thickness (m), and

ρ = material density of layer (kg/m^3).

For a spherical particle as given in Figure 3-22 in which the inner radius is constant, the layer thickness is given as

$$L \equiv R_2(t) - R_1 = L_{initial} - \frac{kt}{\rho}, \qquad \left(t \leq \frac{\rho L_{initial}}{k}\right), \qquad (Eq. 8)$$

where $L_{initial}$ is the initial layer thickness at $t = 0$. In Eq. 8, the condition in parentheses is required so that corrosion is not considered beyond the time that the layer thickness is zero. To get a physical feel for the time to completely corrode the SiC layer, consider

ρ = 3100 kg/m^3,
$k = 10^{-5}$ g/m^2/day $= 1.16 \times 10^{-13}$ kg/m^2/s, and
$L_{initial} = 35 \times 10^{-6}$ m.

From Eq. 8,

$$t = \frac{\rho L_{initial}}{k} = \frac{(3100)(35 \times 10^{-6})}{1.16 \times 10^{-13}} = 9.4 \times 10^{11} \text{ s} = 30{,}000 \text{ years}. \qquad (Eq. 9)$$

Clearly if the SiC layer is to remain intact for 10^6 years, the corrosion data indicate the SiC may not last for such a long period. However, this estimate neglects the OPyC layer that may protect the SiC layer from exposure to brine. For the OPyC layer,

ρ = 2,300 kg/m^3,

$k = 3 \times 10^{-7}$ g/m^2/day = 3.47×10^{-15} kg/m^2/s, and

$L_{initial} = 45 \times 10^{-6}$ m.

$$t = \frac{\rho L_{initial}}{k} = \frac{(2300)(45 \times 10^{-6})}{3.47 \times 10^{-15}} = 3.0 \times 10^{13} \text{ s} = 9.5 \times 10^{5} \text{ years.} \qquad (Eq. 10)$$

Thus, the OPyC layer may provide adequate protection for the SiC for nearly 10^6 years.

There are three timescales for the coupled processes of corrosion and diffusion of a radionuclide released from the SiC layer as given in Table 3-9. The corrosion timescale is derived from Eq. 9. To determine the diffusion timescale, the diffusivity is needed, but such data in SiC were not found. Nonetheless, the diffusivity in SiC is expected to be much smaller than that in graphite. For the diffusion and corrosion timescales to be comparable, the diffusivity in SiC is about an order of magnitude smaller than measured for other radionuclides through graphite. If the diffusivity through SiC is two or three orders of magnitude lower than through graphite, then the diffusion timescale is more than 10^6 years and diffusion is unimportant. Because the diffusion timescale depends on the layer thickness squared, small reductions in the layer thickness by corrosion can have a very significant reduction in the diffusion timescale, making this process more important.

Table 3-9. Timescales for Coupled Corrosion and Diffusion of a Decaying Radionuclide

Process	Timescale	Nominal Value
Corrosion of SiC layer	$\tau_{cor} = \frac{\rho L_{initial}}{k}$	3×10^4 years
Diffusion through SiC layer	$\tau_{dif} = \frac{L^2}{\mathcal{D}}$	3×10^4 years for $L = 35\ \mu\text{m}$ $\mathcal{D} = 4 \times 10^{-14}\ \text{m}^2/\text{s}$
Radioactive Decay	$\tau_{dec} = 1/\lambda$	2.3×10^3 to 2.3×10^7 years

Because of the multiple timescales of the various processes, with the diffusion and decay timescales being radionuclide-dependent, there are several possibilities to simplify the analysis as given in Table 3-10. If the radionuclide decay timescale is much shorter than either the diffusion or corrosion timescales, most of the radionuclide will have decayed before being released. Of course, for long-lived radionuclides, direct evaluation of release via diffusion and corrosion is being performed. If the corrosion timescale is much longer than the diffusion timescale, then geometry changes need not be directly coupled. In this case, the solution given by Gelbard (2003) may be used with the outer radius being time dependent. If the diffusion timescale is much longer than the corrosion timescale, diffusion is unimportant and release will primarily occur upon corrosion of the layer.

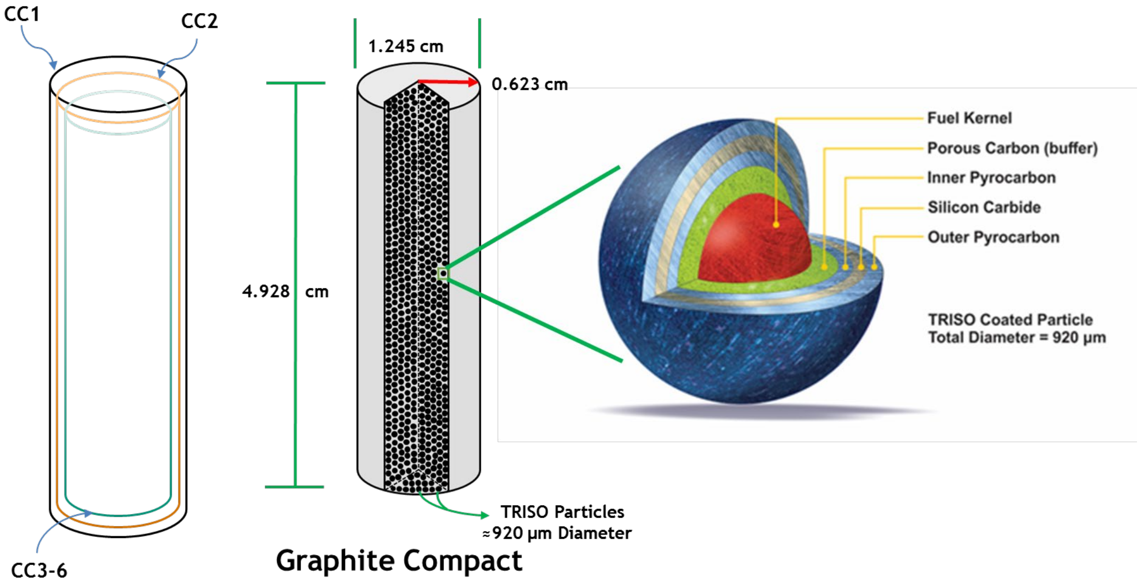
Table 3-10. Simplifying Conditions Depending on Relative Timescales

Timescale Conditions	Nominal Value
$\tau_{dec} \ll \tau_{dif}$ $\tau_{dec} \ll \tau_{cor}$	no significant radionuclide release
$\tau_{dif} \ll \tau_{cor}$	quasi-steady diffusion with variable geometry
$\tau_{dif} \gg \tau_{cor}$	neglect diffusion and consider release only upon corrosion of layer

Computer codes for multilayer diffusion and for coupled corrosion and diffusion through a layer have been written and are being tested (Gelbard and Sassani 2018). These analyses will be completed to determine the range of diffusivities in SiC for which gaps exists in the data or in basic-principles calculation. Additionally, the physical characteristics and the potential degradation mechanisms of the encapsulating graphite matrix and fuel element are being evaluated for integration into a stochastic model of the entire TRISO particle fuel element. The formulation has been completed in detail and implemented in a parametric evaluation of the relative dominance of diffusivity versus corrosion rates of SiC for release of radionuclides beyond the SiC layer (Gelbard and Sassani 2018; Sassani and Gelbard 2019).

In this work, the OWL team analyzed the combined simultaneous effects of (1) bulk (e.g., solid-state) diffusion of a radionuclide through the SiC barrier, (2) SiC barrier corrosion, and (3) radioactive decay for TRISO particles. The analysis is general for a single corroding barrier with specified radionuclide bulk diffusivity and decay rate. From the timescales for bulk diffusion, corrosion, and decay, estimates were obtained on how each process would affect the radionuclide release. Because the team did not find the bulk diffusivities in SiC of interest at repository temperatures, a broad range of diffusivities was used in the analysis. Release may occur predominantly via diffusion before the SiC barrier has corroded if the bulk diffusivity is higher than about 10^{-20} m^2/s. For bulk diffusivity less than 10^{-21} m^2/s significant diffusional release should not occur prior to SiC corrosion removal.

At this point, the SiC is not considered likely as a porous media pathway (i.e., with fast diffusion) until after corrosion. This conclusion is based on the low porosity and disconnected nature of the pores (e.g., Slavin and Quinn 1986). In the next stages of this work, the OWL team will evaluate the uncertainty range of potential radionuclide release via aqueous diffusive pathways in a coupled performance degradation/release model for the graphite compact that integrates quantitatively porous media behavior of the TRISO particle layers and the surrounding compact matrix graphite. The conceptual representation of the graphite compact as shown in Figure 3-24 will allow for stochastic representation and sampling of TRISO particle failure times (distributed randomly throughout six concentric cylinders within the compact) with effectively instantaneous release from the compact (due to the high diffusivities, only years of transport time; Fachinger et al. 2006) to represent radionuclide releases from the compacts. The primary uncertainty appears to be the corrosion lifetime of the SiC layer, with additional lifetime if either the OPyC layer (Van den Akker and Ahn 2013) or the corrosion products (Hagan and Opila 2015) are protective and lesser lifetime if localized corrosion mechanisms occur. Assessing these conceptual processes for corrosion of SiC and quantifying them are the next steps for this investigation. Initial analyses are described in the next subsection.



NOTE: TRISO = tristructural-isotropic

Figure 3-24. Conceptual Model of Graphite Compact Containing TRISO Particles Distribution in Six Concentric Cylinders Internally (CC1 – CC6)

Mineralogic Corrosion Products and Formation of Protective Layers on SiC

Corrosion of SiC at high temperatures (i.e. above 1,000 °C) has been extensively studied (e.g., Ervin 1958; Ogbuji and Opila 1995; Jacobson et al. 1997), as has oxidation of silicon at high-temperatures (Deal and Grove 1965). Such studies are applicable directly to reactor operating conditions. However, SiC corrosion at repository-relevant temperatures, on the order of ~90°C down to ~25°C in aqueous conditions has not received comparable attention, but some data on bulk corrosion are available (Fachinger et al. 2006).

The chemical mechanisms for corrosion at high temperatures are more straightforward than for repository conditions as kinetic constraints are much smaller and equilibrium processes apply effectively directly. Ervin (1958) reports high temperature experimental results for SiC corrosion when heated in air, oxygen, and carbon dioxide atmospheres. That study evaluated eight SiC oxidation reactions that included SiO_2, CO_2, SiO, CO, and/or C as reaction products. Each of the eight reactions evaluated are thermodynamically favored (i.e., having negative free energy of reaction) at both 25°C and 1,627°C, and in roughly the same order of relative reaction stability. More specifically, the reaction forming SiO_2 and CO_2 as the products is the most stable of the eight at both conditions. This situation provides a thermodynamic basis for the observations at high-temperature of the formation of a silica layer on the SiC surface (Ervin 1958; Deal and Grove 1965; Ogbuji and Opila 1995; Jacobson et al. 1997), though the major gas species formed depends in part on the bulk composition of the gas. From a conceptual standpoint, essentially the same (or similar) simple reactions are expected to dominate from a thermodynamic perspective at repository conditions; however, at these lower temperatures, kinetic barriers are more likely to affect shorter term behavior of even this simple system.

In these high-temperature experiments, the kinetic limitations to the chemical reactions were minimal, and the limiting process for conversion of SiC to SiO_2 and gaseous products was theorized to be the rate of oxygen diffusion through the layer of SiO_2 formed on SiC, i.e., a protective layer isolating the SiC surface from the fluid (Deal and Grove 1965; Jacobson et al. 1997). This process results in a parabolic growth rate in which the diffusion barrier thickness grows as the square root of time. The analysis by Deal and Grove (1965) for silicon oxidation has the barrier growth rate and corrosion rate initially varying linearly with time, and then the corrosion rate transitions to being proportional to the square root of time. Additionally, Ogbuji and Opila (1995) show that the SiO_2 layer thickness growth varies with the square root of time, which supports a diffusion-limiting oxide growth rate model at high temperatures as well.

If such a SiO_2 layer would form on SiC at repository conditions, this situation could provide a rate-limiting process (e.g., oxidant diffusion through the SiO_2 layer) that would be slower (i.e., protective) than the far-from-equilibrium corrosion rate of SiC in aqueous solution, e.g., as measured by Fachinger et al. (2006). However, no reports have been found as yet that clearly identify and validate the chemical mechanism to explain SiC corrosion data at conditions directly relevant to repository conditions. According to Fachinger et al. (2006), the mass of SiC corroded is proportional to time, and hence they report a constant corrosion rate, but have not identified the corrosion mechanisms or corrosion products explicitly.

4. Summary

This report represents completion of milestone deliverable M2SF-19SN010309013 “Online Waste Library (OWL) and Waste Forms Characteristics Annual Report” that provides the annual status/update on FY2019 activities for the work package SF-19SN01030901 and is due on August 2, 2019. This annual report includes updates to the OWL development (content and structure), descriptions of the OWL management development and version control processes, and evaluations of waste form characteristics and waste form performance models.

This annual report includes updates to the OWL development, and descriptions of the management processes for the OWL, evaluations of waste form characteristics and of waste form performance models. Updates to the OWL include an updated user’s guide (Appendix B), additions to the OWL database content for wastes and waste forms (Section 3.2.1), with data entry focused on the Na-bonded spent fuel and updated data for SRS glass waste (HLW glass waste form) production, and the results of the beta testing and the implemented changes (Section 3.2.3). Section 3.2.4.2 provides descriptions of the management/control processes for the OWL development, version control, and archiving. These processes have been implemented as part of the full production release of OWL (i.e., OWL Version 1.0), which has been developed on, and will be hosted and managed on, Sandia National Laboratories (SNL) systems. The version control/update processes will be implemented for updates to the OWL in the future. Additionally, another process covering methods for interfacing with the DOE SNF Database (DOE 2007) at Idaho National Laboratory on the numerous entries for DOE-managed SNF (DSNF) has been pushed forward by defining data exchanges and is planned to be implemented sometime in FY2020. Once fully implemented, this integration effort will serve as a template for interfacing with additional databases throughout the DOE complex.

OWL Development—From the beginning, the plan for OWL has been to allow the database to evolve over time in terms of both content and capability. One of OWL’s primary functions is to provide access to information on DOE-managed wastes that are likely to be disposed of in a mined geologic repository. As a complement to this function, OWL is being expanded to include information on the vessels capable of disposing of that DOE-managed waste, with the ancillary aspects of storing and transporting those wastes/waste forms.

Note that certain “vessels” are considered a part of the waste form if that vessel cannot be separated easily from the waste form. As such, those vessels are already included in the descriptions in the waste form information of OWL and would not, in general, be added in this expanded OWL Vessel information. A good example is the glass pour canister that is essential for making the glass waste form. The glass pour canister contains the glass waste form, but is not easily removed, and is not intended to contain other waste forms or waste types. There are also exceptions such as when the vessel itself has an alternative use for a different waste/waste form—either existing or officially planned—that does not permanently bind it to the waste/waste form in that alternative. For example, glass canisters have no existing or planned alternative uses that would justify inclusion in OWL as a vessel (i.e., no planned or alternative use involving some other waste/waste form that would be contained therein). In summary, within OWL, the generic term “vessel” will be used to describe a can, canister, container, cask, overpack, waste package, etc. that can serve as a single layer in a nested system designed to surround and contain the waste form for potential disposal, storage, or transportation uses.

The DOE has a database that contains information regarding the SNF that DOE manages, namely, the SFDB. The intent for OWL is not to replicate the SFDB and the information in it, but rather to take advantage of that existing data set to incorporate it efficiently into OWL so it is available for use in postclosure PA. Although the DSNF inventory for N-reactor has been entered directly into the OWL database for use directly in GDSA analyses (primarily because this represents the major mass of DSNF, it is not efficient, nor desirable, to re-enter the other 700+ entries of DSNF in the INL's SFDB, a Nuclear Quality Assurance-1 (NQA-1) quality assurance database (DOE 2007). As such, the OWL team is currently working with INL staff (primarily Layne Pincock and Brett Carlson) to develop a plan for the OWL to synchronize periodically with the SFDB.

Because of the nature of the SFDB content, care is being taken to select a subset of information fields to be supplied to the OWL that is sufficient for performance analyses of the back end of the fuel cycle (primarily disposal). The current work in this area is delineating exactly what the desired data fields from the SFDB are for use in the OWL. For example, numbers of DSNF elements, masses, and dimensions are all parameters that are desired for constraining numbers and types of canisters for storage or disposal. But there are many additional fields that would perhaps be useful beyond those. Location information would be limited to the DOE facility of storage (e.g., Hanford, INL) to help ensure the OWL can be made publicly available with no restrictions. Currently, the draft schedule calls for such synchronizations to occur twice annually with about two to three months lead time prior to OWL version updates to allow time to deal with any unforeseen issues with the file handling. This schedule will be finalized during initial implementation of this interface, currently planned for some time in FY2020.

Sassani et al. (2017) reported OWL database updates in three areas. First, additional data for waste types (and their potential waste forms) and source documentation had been added to the OWL to flesh out its content covering DHLW and DSNF. Second, in conjunction with further data entry, a process of checking the data entry into the OWL against the source documentation was launched to search for and rectify any errors in data entry. This checking was performed by technical individuals independent of the data-entry process, who documented any issues noted and resolved the issues with the data-entry staff. Third, because the OWL was modified throughout the year in terms of its interface and features, another process to assess the usability of the OWL was completed. This process is referred to here as the external OWL beta test and involved technical staff from within the DOE-NE and DOE-EM, as well as at other national laboratories, using the OWL and providing feedback on its utility and content. That feedback resulted in changes implemented in the OWL for improved usability.

Inventory—The recent inventory data entry focused on the Na-bonded spent fuel that was produced from DOE's experimental fast-neutron breeder reactor program. The data for the associated spent fuel wastes, electrometallurgical treatment (EMT) produced wastes/waste forms, and other planned waste forms that are being, or are planned to be, produced are being incorporated into OWL. These wastes represent a large number of waste types and waste forms in OWL because they have been classified based on the reactor of origin and the type of fuel (driver versus blanket) from each nuclear reactor. Additionally, the data on SRS glass waste (i.e., HLW glass logs formed at the SRS) has been updated with the most recent production data.

Sassani et al. (2017) updated the preliminary FY2016 inventory by adding the additional possible waste forms (DOE 2014) that were not previously included in GDSA representations, for which GDSA evaluation of thermal or radionuclide inventory aspects may be somewhat expanded compared to the previous analyses. Specifically, this effort included the following:

- The 340 Hanford Cs and Sr vitrified glass canisters (Wilson 2016, Table 2-6)
- The 34 glass canisters of Hanford FRG glass, which is material that has been designated as remote-handled TRU wastes (Bounini and Anderson 2000), though it may be disposed in a deep geologic repository with other heat producing waste
- The planned waste form for calcine waste, which is a HIP waste form (glass ceramic) can with ~10 HIP cans loaded/stacked into naval canisters for a total of ~320 canisters (~5.5-ft diameter × ~15-ft height naval canisters/waste packages containing ~10 HIP cans each; SNL 2014)

Although most of these updates are relatively small from the standpoint of inventory mass, they may have some implications for analyses of thermal effects because some of these added wastes tend to have higher average thermal loads per canister than the inventory previously evaluated in GDSA. Additionally, some of these waste forms represent larger waste packages, which may expand handling and emplacement considerations (e.g., planned calcine HIP waste form waste packages).

As detailed above, Sassani et al. (2016) provided the initial development status including (1) developing the preliminary inventory for engineering/design/safety analyses (updated with additions herein as described above), (2) assessing the major differences of this included inventory relative to that in other analyzed repository systems and the potential impacts to disposal concepts (unchanged), and (3) the initial design and development of the prototype online waste library (OWL) to manage the information of all those wastes and their waste forms (updated as discussed above). In addition, Sassani et al. (2016) reported on potential candidate waste types/forms identified, which may be added to the OWL in the future to the full list from the WFDOE (SNL 2014, Table C-1).

Sassani et al. (2016) discussed the Wilson (2016) preliminary inventory for initial GDSA analyses. That inventory includes both DHLW and DSNF waste canister counts and thermal information (Wilson 2016, Tables 2-1 and 2-3 to 2-6). The Wilson (2016) report describes each waste form in terms of both average radionuclide content and overage thermal output evolution. The tabulation includes canister counts and ranges of thermal characteristics for each DHLW and DSNF waste form considered (Wilson 2016). The various types of DSNF are listed in Appendix A of Sassani et al. (2016, 2017) for the ~2,485 DSNF canisters (Wilson 2016, Table 2-1). The DHLW canister counts are given in Wilson (2016) in Tables 2-3 through 2-6, respectively, for SRS glass (7,824 canisters), Hanford glass (11,800 canisters), INL HIP calcine (4,391 canisters), and Hanford vitrified Cs and Sr capsules (340 canisters; also SNL 2014).

Waste Form Performance for GDSA—The models for degradation of both UO_2 and HLW glass (Sassani et al. 2016) are currently being used within the GDSA for PA modeling of postclosure system evolution. The waste forms in the current GDSA generic repository analyses have been mapped into those models as either performing similarly or being bounded by a particular model degradation behavior. For example, the HIP calcine waste form degradation rate is assumed to be the same as the HLW glass degradation. For waste forms that have relatively short waste form lifetimes (generally ~10,000 years or less), the instantaneous degradation rate is used. Note that in all cases the waste form degradation is the initial, kinetic step, and the dissolved radionuclides are evaluated against solubility limits based in part on the geologic environment.

Within the materials recovery and waste form development (MRWFD) campaign within DOE NE, the mechanistic behavior that initiates stage 3 degradation rates for glass are being incorporated into a performance assessment model. When this MRWFD glass model becomes available, SFWST will incorporate this into GDSA so it can be used to represent glass long-term degradation behavior. This approach involves ongoing cross-campaign integration activities.

The current assumptions for degradation rates of the DSNF in the included inventory are based on the work in the YM SAR (DOE 2008), which assumed virtually all the DSNF degraded instantaneously except for the naval SNF, which degrades as UO_2 SNF. This assumption was based primarily on both that the primary mass of DSNF is N-reactor metallic uranium fuel, which would degrade effectively instantly in any system, and the small amounts of the other DSNF relative to the mass of commercial SNF represented in the YM SAR. The OWL team has been reviewing the bases for the PA groupings from the YM SAR and some prior analyses to see if there may be some of the DSNF waste forms that have a basis for better performance in postclosure. In addition, the assumption of glass degradation being assigned to the HIP calcine waste form is being reevaluated as well. The results of these efforts will provide input to potential adjustments to the GDSA models, if appropriate.

The various DSNF groupings proposed in support of PA and disposal concepts have been reviewed and analyzed. While as a crude first approximation DSNF can utilize either UO_2-type UNF or instantaneous degradation models, it was shown that some of the recently introduced groupings from the WFDOE (SNL 2014) can be mapped to a wider variety of degradation/dissolution models than previously established for the 11 DSNF groups considered in the early work of the YM SAR. A finer remapping of into the original 16 groups considered is not expected to provide additional useful information in terms of degradation at the PA level, although future work may elucidate fuel degradation/dissolution models at the level of the 34 condensed DSNF groups.

Studies of the degradation performance of HIP calcine (with additives) provide information that allows assigning glass degradation rates to the glass ceramic calcine waste form as a reasonable approach. The use of instantaneous degradation rates for the HIP calcine waste form would represent a conservative bounding approach. For untreated calcine, or HIP calcine without additives, instantaneous degradation rates should be used in GDSA PA analyses. Additional analyses are evaluating the bases for application of the glass degradation model to HIP calcine, which may be more realistically represented by a combined model of glass degradation and ceramic phase degradation within that matrix.

Additional Waste Form Characteristics/Performance Evaluations—Starting in FY2018, the OWL team has pursued three studies to evaluate/redefine waste form characteristics and/or performance models. The first study involves evaluating characteristic isotopic ratios for various waste forms included in postclosure performance studies to delineate isotope ratio tags that quantitatively identify each particular waste form. This evaluation arose due to questions regarding the relative contributions of radionuclides from disparate waste forms in GDSA results, particularly, radionuclide contributions of DSNF versus DHLW glass. The second study examines the basis for using the glass waste degradation rate models to simulate degradation of the HIP calcine waste form. The HIP calcine may likely be a ceramic matrix material, with multiple ceramic phases with/without a glass phase. The ceramic phases are likely to have different degradation performance (likely much longer lifetimes) from the glass portion. The distribution of radionuclides among those various phases may also be a factor in the radionuclide release rates. For the third study, the team has an ongoing investigation of the performance behavior of TRISO particle fuels. These particles appear to have substantial waste form lifetimes (~100,000 years) based primarily on the corrosion behavior of the SiC layer. The study includes developing a stochastic model for the degradation of those fuels that accounts for simultaneous corrosion of the SiC layer and radionuclide diffusion through it. The detailed model of the TRISO particles themselves will be merged with models of the degradation behavior(s) of the graphite matrix (either prismatic compacts or spherical "pebbles") containing the particles and the hexagonal graphite elements holding the compacts.

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APPENDIX A—OWL MODEL ARCHITECTURE FOR VESSEL DATA SETS

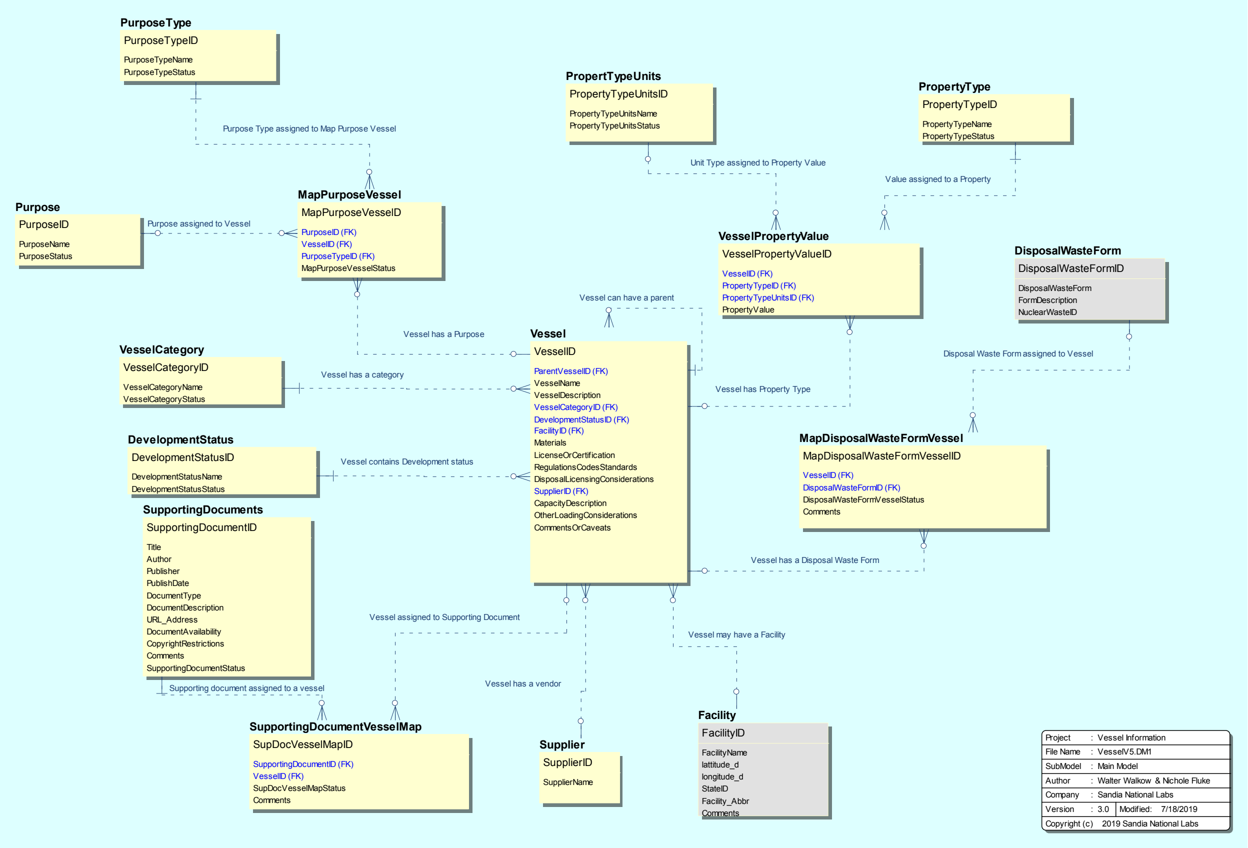

Figure A-1. OWL Model Architecture for Vessel Data Sets

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APPENDIX B—EXCERPT OF *OWL USER'S GUIDE*

The homepage of OWL has a link to the *OWL User's Guide*, the majority of which is excerpted below starting with the subhead "Navigation". Rather than use the numbering for subheads and figures that would normally be appropriate for Appendix B, the subheads will not be numbered and the figure numbering will start with "1" to maintain consistency with the *OWL User's Guide*.

Navigation

Clicking on an item to open it, such as a link to a document, opens the item in a new window. To close the item, simply close the window. To go back to the previous webpage, click on the window containing that page. Many webpages allow the user to navigate back to the Home Page, to the DOE-Managed Wastes webpage, or to the User Guide via links in the upper left corner of the webpage, as shown in Figure 1.

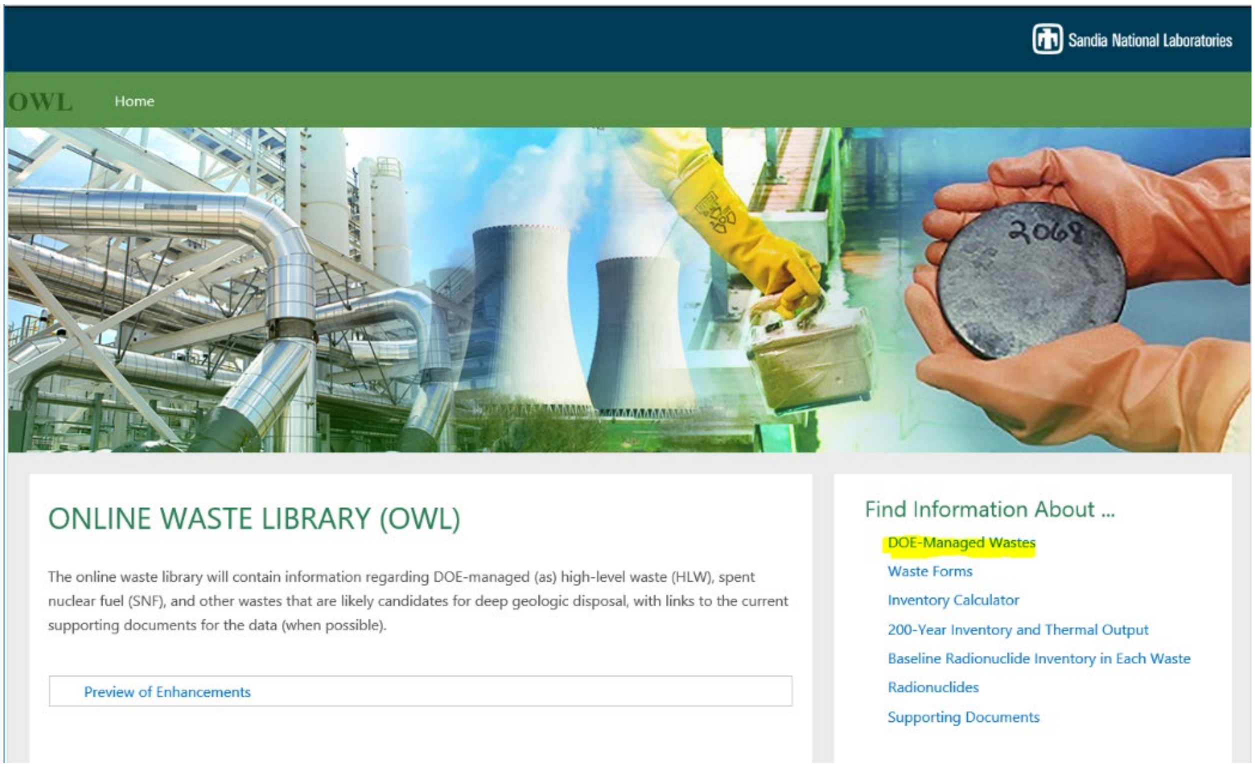
Figure 1. Navigation Links on OWL Webpages

Printing and Saving

To print or save a webpage, the user should click on "Actions" in the upper left corner of the webpage to be printed or saved. From the drop-down menu that appears, the user would then select "Print" to print the webpage or "Export" to save it in a different format (e.g., pdf, Excel, Word).

See the wastes included in OWL

To see the wastes included in OWL, the user should click on "DOE-Managed Wastes" from the home page, as shown in Figure 2. This will bring up a new webpage listing all the wastes and summarizing information about them. The user can then click on the name of the waste to open yet another webpage with more detailed information about that waste, such as its quantity, its inventory, its source, its disposal waste form(s), and a list of supporting documents.



ONLINE WASTE LIBRARY (OWL)

The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Figure 2. How to See the Wastes Included in the OWL

See which wastes are at a particular site

To see which wastes included in OWL are at a particular DOE site, the user should click on “DOE-Managed Waste” as shown in Figure 2, then select the name of the desired facility from the selection pane on the left side of the page. An example is shown in Figure 3. In this example, Hanford is selected and, thus, only those wastes currently stored at Hanford are shown.

Waste (click on Name for details)	BaseLine Inventory Date	Waste Classification	Waste Description
Calcine Waste	Jan 01, 2016	High Level Waste	This waste is a solid granular material derived from liquid wastes produced by reprocessing SNF.
Cesium and Strontium Capsules	Jan 01, 2016	High Level Waste	This waste consists of 1335 CsCl capsules and 601 SrF2 capsules, each about 21 inches tall and 3 inches in diameter. They are currently managed as high-level waste and stored in pools at the Waste Encapsulation and Storage Facility at Hanford
German Glass Waste	Jan 01, 1987	Transuranic (TRU) Waste	This waste consists of 34 canisters of glass prepared by Pacific Northwest Laboratory to provide heat and radiation sources for repository testing by the Federal Republic of Germany in the Asse salt mine. This waste has been classfied as RH-TRU but does not meet the requirements of the WIPP Waste Acceptance Criteria and so cannot be disposed of at the WIPP. Two of the 34 canisters are thought to contain depleted uranium and natural thorium, but no cesium or strontium. The 34 canisters are currently stored in 6 CASTOR casks and 2 GNS casks.
Hanford Tank Waste (CH-TRU)	Jan 01, 2008	Transuranic (TRU) Waste	This waste is material that can be contact handled (CH) and is a subset of the 54.6 million gallons of liquid waste stored at Hanford. It may be transuranic (TRU) waste but has not officially been determined to be so by the DOE.
Hanford Tank Waste (HLW)	Jan 01, 2008	High Level Waste	This waste is a subset of the 54.6 million gallons of liquid waste stored at Hanford

Figure 3. Example of Selecting a Facility

See the DOE-managed wastes by classification (high-level waste, spent nuclear fuel, or transuranic waste)

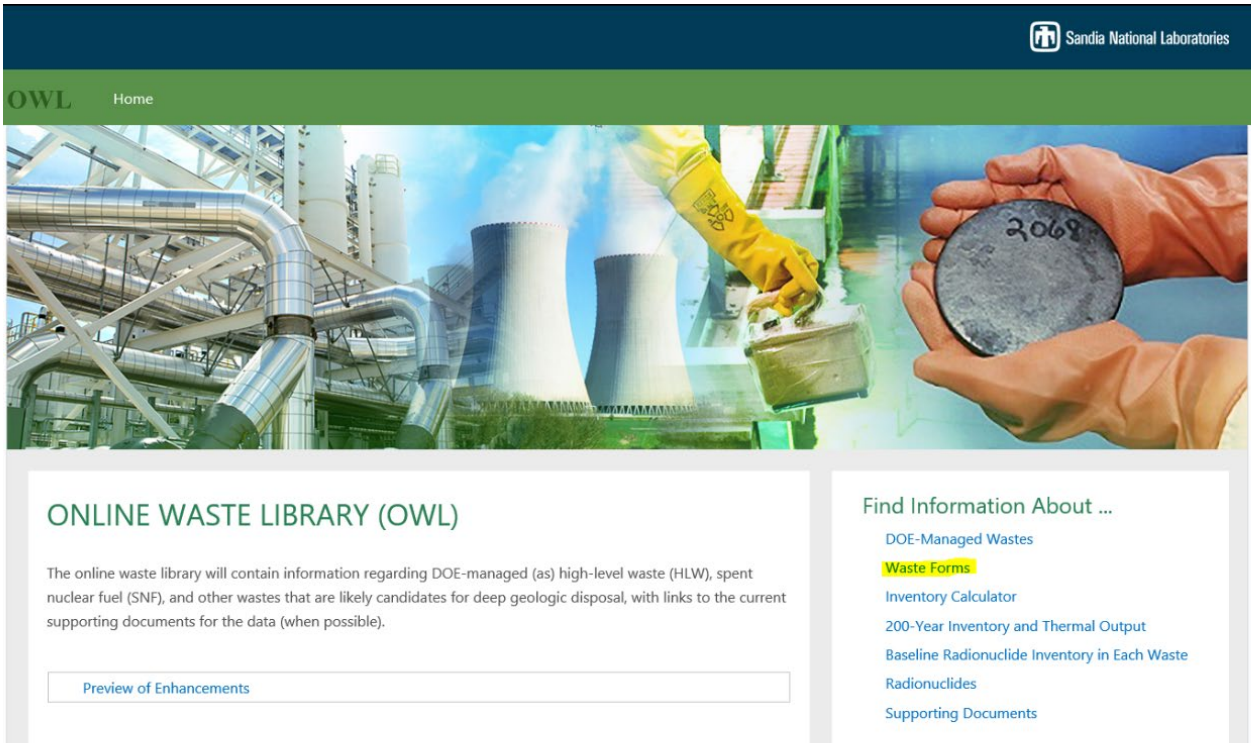
To see the DOE-managed wastes by their classification (high-level waste, spent nuclear fuel, or high-level waste), the uses should click on "DOE-Managed Wastes" as shown in Figure 2, then select the desired waste classification from the selection pane on the left side of the page. In the example shown in Figure 4 below, "Spent Nuclear Fuel" is selected, thus, only waste that is classified as spent fuel is shown.

Waste (click on Name for details)	BaseLine Inventory Date	Waste Classification	Waste Description
N-Reactor Spent Fuel	May 31, 1998	Spent Nuclear Fuel	This waste consists of 2,096 metric tons of N-Reactor spent fuel that is currently stored in about 388 multi-canister overpacks in the Canister Storage Building at Hanford.

Figure 4. Example of Selecting a Waste Classification

See what the DOE has planned or proposed with respect to the disposal waste forms for the wastes

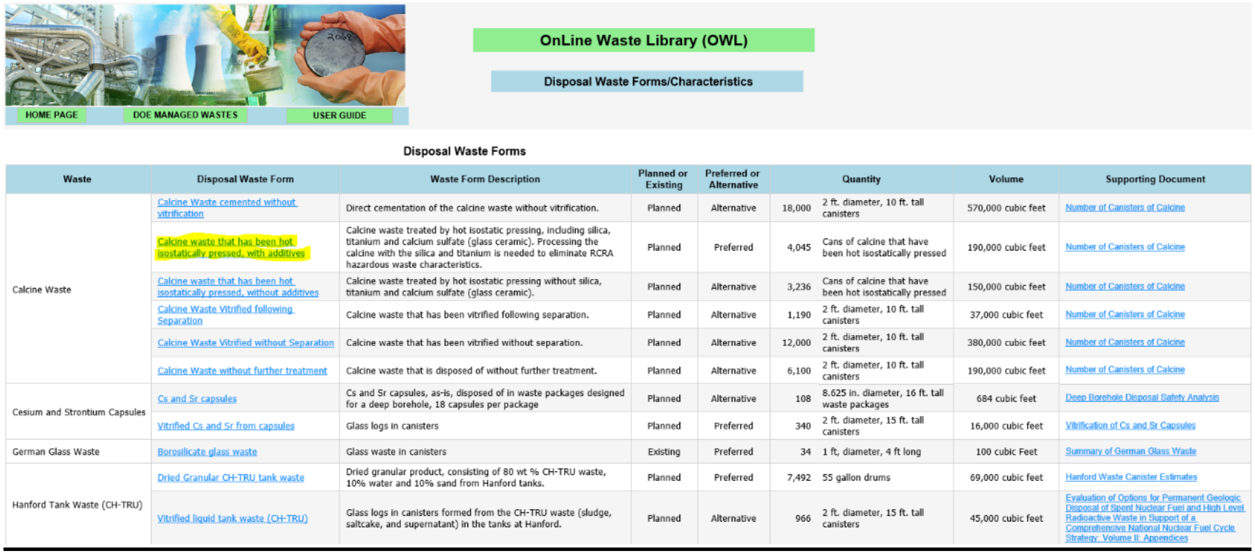
To see what the DOE has planned or proposed with respect to the disposal waste forms for the various wastes, the user should click on "Waste Forms" from the home page, as shown in Figure 5, then select the waste form of interest, as shown in Figure 6. In the example shown in Figure 6, "Calcine waste that has been hot isostatically pressed, with additives" was selected. Further information regarding the selected waste form will then appear.



ONLINE WASTE LIBRARY (OWL)

The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Figure 5. Example of How to View Waste Forms



OnLine Waste Library (OWL)

Disposal Waste Forms/Characteristics

Disposal Waste Forms

Waste	Disposal Waste Form	Waste Form Description	Planned or Existing	Preferred or Alternative	Quantity		Volume	Supporting Document
Calcine Waste	Calcine Waste cemented without vitrification	Direct cementation of the calcine waste without vitrification.	Planned	Alternative	18,000	2 ft. diameter, 10 ft. tall canisters	570,000 cubic feet	Number of Canisters of Calcine
	Calcine waste that has been hot isostatically pressed, with additives	Calcine waste treated by hot isostatic pressing, including silica, titanium and calcium sulfate (glass ceramic). Processing the calcine with the silica and titanium is needed to eliminate RCRA hazardous waste characteristics.	Planned	Preferred	4,045	Cans of calcine that have been hot isostatically pressed	190,000 cubic feet	Number of Canisters of Calcine
	Calcine waste that has been hot isostatically pressed, without additives	Calcine waste treated by hot isostatic pressing without silica, titanium and calcium sulfate (glass ceramic).	Planned	Alternative	3,236	Cans of calcine that have been hot isostatically pressed	150,000 cubic feet	Number of Canisters of Calcine
	Calcine Waste Vitrified following Separation	Calcine waste that has been vitrified following separation.	Planned	Alternative	1,190	2 ft. diameter, 10 ft. tall canisters	37,000 cubic feet	Number of Canisters of Calcine
	Calcine Waste Vitrified without Separation	Calcine waste that has been vitrified without separation.	Planned	Alternative	12,000	2 ft. diameter, 10 ft. tall canisters	380,000 cubic feet	Number of Canisters of Calcine
	Calcine Waste without further treatment	Calcine waste that is disposed of without further treatment.	Planned	Alternative	6,100	2 ft. diameter, 10 ft. tall canisters	190,000 cubic feet	Number of Canisters of Calcine
Cesium and Strontium Capsules	Cs and Sr capsules	Cs and Sr capsules, as-is, disposed of in waste packages designed for a deep borehole, 18 capsules per package	Planned	Alternative	108	8.625 in. diameter, 16 ft. tall waste packages	684 cubic feet	Deep Borehole Disposal Safety Analysis
	Vitrified Cs and Sr from capsules	Glass logs in canisters	Planned	Preferred	340	2 ft. diameter, 15 ft. tall canisters	16,000 cubic feet	Vitrification of Cs and Sr Capsules
German Glass Waste	Borosilicate glass waste	Glass waste in canisters	Existing	Preferred	34	1 ft, diameter, 4 ft long	100 cubic Feet	Summary of German Glass Waste
Hanford Tank Waste (CH-TRU)	Dried Granular CH-TRU tank waste	Dried granular product, consisting of 80 wt % CH-TRU waste, 10% water and 10% sand from Hanford tanks.	Planned	Preferred	7,492	55 gallon drums	69,000 cubic feet	Hanford Waste Canister Estimates
	Vitrified liquid tank waste (CH-TRU)	Glass logs in canisters formed from the CH-TRU waste (sludge, saltcake, and supernatant) in the tanks at Hanford.	Planned	Alternative	966	2 ft. diameter, 15 ft. tall canisters	45,000 cubic feet	Evaluation of Options for Permanent Geologic Disposal of Spent Nuclear Fuel and High Level Radioactive Waste in Support of a Comprehensive National Nuclear Fuel Cycle Strategy: Volume II: Appendices

Figure 6. Example of How to Select a Waste Form

See the radionuclide inventory of a particular waste

There are three different ways for the user to see the radionuclide inventory of a particular waste. One way is for the user to click on “DOE-Managed Wastes” from the home page (Figure 2), then click on the name of the waste (Figure 7), then click on the plus sign (+) next to “5. Radionuclide Inventory” (Figure 8). This will display the inventory (in Curies) for the waste. In the examples below (Figure 7 and Figure 8), Cesium and Strontium Capsules is the waste selected.

OnLine Waste Library (OWL)

DOE-Manageed Wastes

To filter Wastes, click on item's text below

Select a Facility Name

- ALL
- Hanford
- Idaho National Engineering Environmental Lab
- Savannah River

Select a Waste Classification

- ALL
- High Level Waste
- Spent Nuclear Fuel
- Transuranic (TRU) Waste

Waste (click on Name for details) ⬍	BaseLine Inventory Date	Waste Classification ⬍	Waste Description
Calcine Waste	Jan 01, 2016	High Level Waste	This waste is a solid granular material derived from liquid wastes produced by reprocessing SNF.
Cesium and Strontium Capsules	Jan 01, 2016	High Level Waste	This waste consists of 1335 CsCl capsules and 601 SrF2 capsules, each about 21 inches tall and 3 inches in diameter. They are currently managed as high-level waste and stored in pools at the Waste Encapsulation and Storage Facility at Hanford
German Glass Waste	Jan 01, 1987	Transuranic (TRU) Waste	This waste consists of 34 canisters of glass prepared by Pacific Northwest Laboratory to provide heat and radiation sources for repository testing by the Federal Republic of Germany in the Asse salt mine. This waste has been classfied as RH-TRU but does not meet the requirements of the WIPP Waste Acceptance Criteria and so cannot be disposed of at the WIPP. Two of the 34 canisters are thought to contain depleted uranium and natural thorium, but no cesium or strontium. The 34 canisters are currently stored in 6 CASTOR casks and 2 GNS casks.

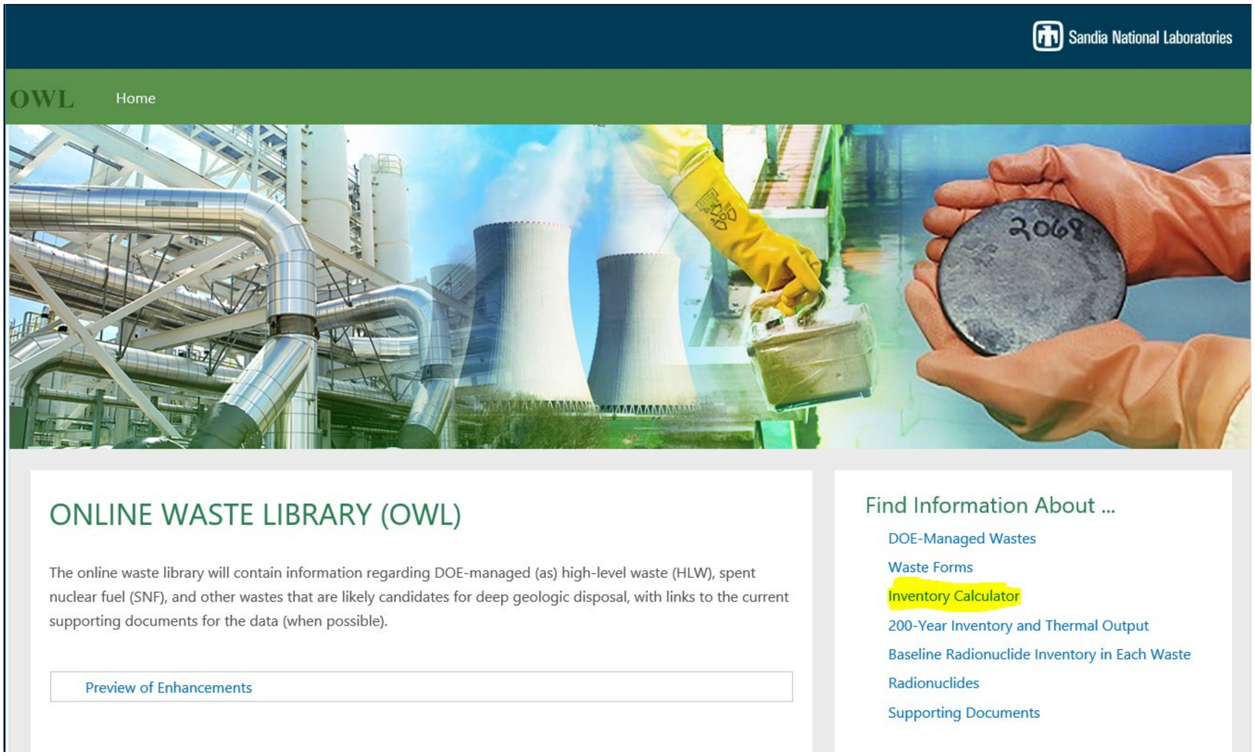
Figure 7. Example of Selecting a Waste

Cesium and Strontium Capsules

Waste Classification	Waste Description	Storage Facility	Produced By	Is Mixed Waste?	Baseline Inventory Date	
High Level Waste	This waste consists of 1335 CsCl capsules and 601 SrF2 capsules, each about 21 inches tall and 3 inches in diameter. They are currently managed as high-level waste and stored in pools at the Waste Encapsulation and Storage Facility at Hanford	Hanford	Government	Yes	1/1/2016	Projected Inventory (200 Years)

Figure 8. Example of Viewing the Radionuclide Inventory

The second way to see the inventory of a particular waste is to click on “Inventory Calculator” from the home page (Figure 9). This will display the inventory (in Curies and grams) of every radionuclide in every waste, along with the thermal output of heat-generating radionuclides in every waste, both as of the baseline date for the waste and at some specified time in the future (year). From the Radionuclide Inventory Calculator page, the list of wastes can be filtered by waste classification, waste, and radionuclide; and the year for which the inventory will be calculated can be selected by the user. In the examples below (Figure 9 and Figure 10), the inventory for the Cesium and Strontium Capsules is calculated for 2050.



ONLINE WASTE LIBRARY (OWL)

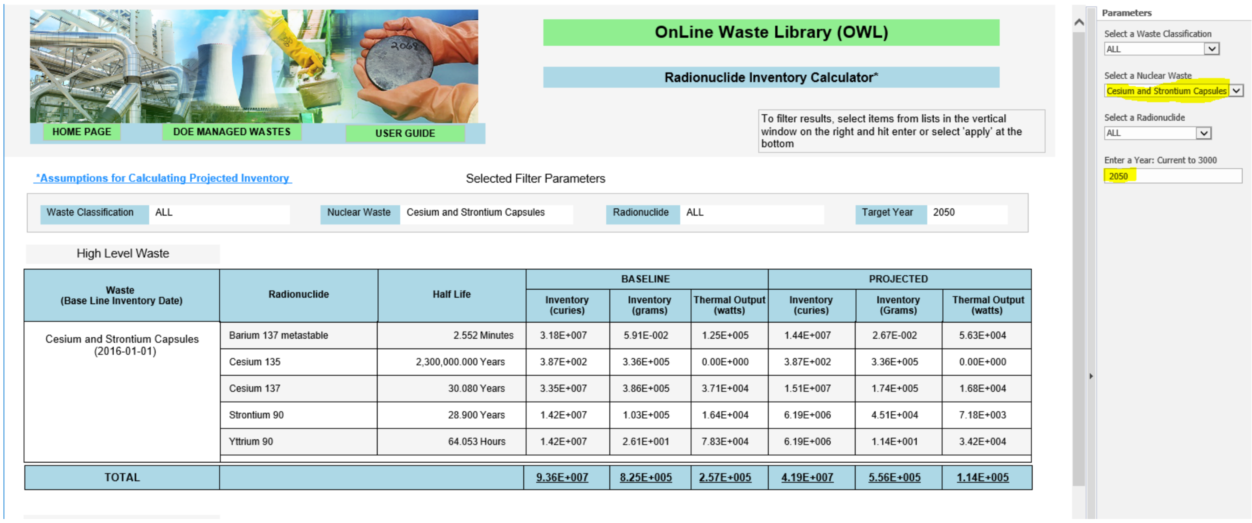
The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Preview of Enhancements

Find Information About ...

- DOE-Managed Wastes
- Waste Forms
- Inventory Calculator
- 200-Year Inventory and Thermal Output
- Baseline Radionuclide Inventory in Each Waste
- Radionuclides
- Supporting Documents

Figure 9. Example of Selecting "Inventory Calculator" from the Home Page



OnLine Waste Library (OWL)

Radionuclide Inventory Calculator*

To filter results, select items from lists in the vertical window on the right and hit enter or select 'apply' at the bottom

*Assumptions for Calculating Projected Inventory

Selected Filter Parameters

Waste Classification: ALL
Nuclear Waste: Cesium and Strontium Capsules
Radionuclide: ALL
Target Year: 2050

High Level Waste

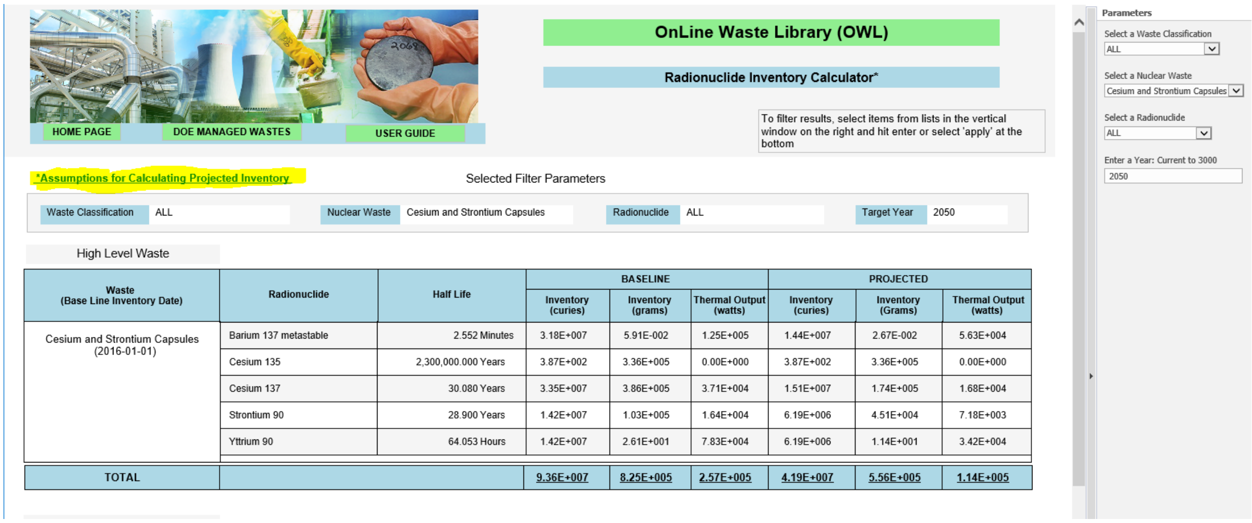
Waste (Base Line Inventory Date)	Radionuclide	Half Life	BASELINE			PROJECTED		
			Inventory (curies)	Inventory (grams)	Thermal Output (watts)	Inventory (curies)	Inventory (Grams)	Thermal Output (watts)
Cesium and Strontium Capsules (2016-01-01)	Barium 137 metastable	2.552 Minutes	3.18E+007	5.91E-002	1.25E+005	1.44E+007	2.67E-002	5.63E+004
	Cesium 135	2,300,000.000 Years	3.87E+002	3.36E+005	0.00E+000	3.87E+002	3.36E+005	0.00E+000
	Cesium 137	30.080 Years	3.35E+007	3.86E+005	3.71E+004	1.51E+007	1.74E+005	1.68E+004
	Strontium 90	28.900 Years	1.42E+007	1.03E+005	1.64E+004	6.19E+006	4.51E+004	7.18E+003
	Yttrium 90	64.053 Hours	1.42E+007	2.61E+001	7.83E+004	6.19E+006	1.14E+001	3.42E+004
TOTAL			9.36E+007	8.25E+005	2.57E+005	4.19E+007	5.56E+005	1.14E+005

Parameters

Select a Waste Classification: ALL
Select a Nuclear Waste: Cesium and Strontium Capsules
Select a Radionuclide: ALL
Enter a Year: Current to 3000: 2050

Figure 10. Example of Calculating the Inventory of Waste at a User-Selected Year

The assumptions made in calculating radionuclide inventories by clicking on "*Assumptions for Calculating Projected Inventory" on the Radionuclide Inventory Calculator webpage (Figure 11).



To filter results, select items from lists in the vertical window on the right and hit enter or select 'apply' at the bottom

*Assumptions for Calculating Projected Inventory

Selected Filter Parameters

Waste Classification: ALL
Nuclear Waste: Cesium and Strontium Capsules
Radionuclide: ALL
Target Year: 2050

High Level Waste

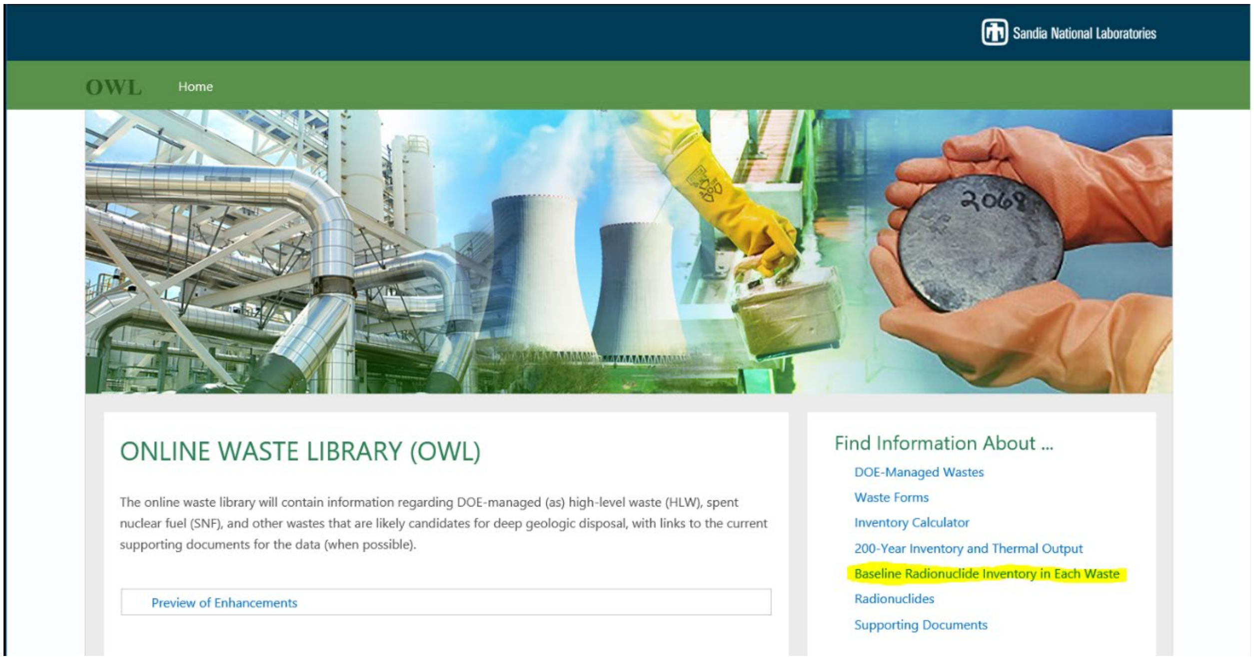
Waste (Base Line Inventory Date)	Radionuclide	Half Life	BASELINE Inventory (curies)	BASELINE Inventory (grams)	BASELINE Thermal Output (watts)	PROJECTED Inventory (curies)	PROJECTED Inventory (Grams)	PROJECTED Thermal Output (watts)
Cesium and Strontium Capsules (2016-01-01)	Barium 137 metastable	2.552 Minutes	3.18E+007	5.91E-002	1.25E+005	1.44E+007	2.67E-002	5.63E+004
	Cesium 135	2,300,000.000 Years	3.87E+002	3.36E+005	0.00E+000	3.87E+002	3.36E+005	0.00E+000
	Cesium 137	30.080 Years	3.35E+007	3.86E+005	3.71E+004	1.51E+007	1.74E+005	1.68E+004
	Strontium 90	28.900 Years	1.42E+007	1.03E+005	1.64E+004	6.19E+006	4.51E+004	7.18E+003
	Yttrium 90	64.053 Hours	1.42E+007	2.61E+001	7.83E+004	6.19E+006	1.14E+001	3.42E+004
TOTAL			9.36E+007	8.25E+005	2.57E+005	4.19E+007	5.56E+005	1.14E+005

Parameters

Select a Waste Classification: ALL
Select a Nuclear Waste: Cesium and Strontium Capsules
Select a Radionuclide: ALL
Enter a Year: Current to 3000: 2050

Figure 11. Example of How to See the Assumptions Made in Calculating the Projected Inventory

The third way to see the radionuclide inventory is to click on “Baseline Radionuclide Inventory in Each Waste” from the home page (Figure 12). This will display the inventory (in Curies) of every radionuclide in every waste as of the baseline date for that waste. The number of wastes or radionuclides that appear can be filtered by selecting a facility, a waste classification, and/or a radionuclide from the selection boxes on the left side of the page. In the example shown below (Figure 13), the facility selected is Hanford, the waste classification selected is High Level Waste, and all radionuclides are shown.



ONLINE WASTE LIBRARY (OWL)

The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Figure 12. Example of Selecting "Baseline Radionuclide Inventory in Each Waste"

Nuclear Waste	BaseLine Inventory Date	Waste Classification	Facility Name	Radionuclide	Inventory in Curies
Cesium and Strontium Capsules	Jan 01, 2016	High Level Waste	Hanford	Barium 137 metastable	3.18E+007
				Cesium 135	3.87E+002
				Cesium 137	3.35E+007
				Strontium 90	1.42E+007
				Yttrium 90	1.42E+007
Hanford Tank Waste (HLW)	Jan 01, 2008	High Level Waste	Hanford	Actinium 227	4.13E+000
				Americium 241	1.34E+005
				Americium 243	6.55E+001
				Barium 137 metastable	3.60E+007
				Carbon 14	5.40E+002
				Cadmium 113 metastable	3.82E+003
				Curium 242	1.20E+002

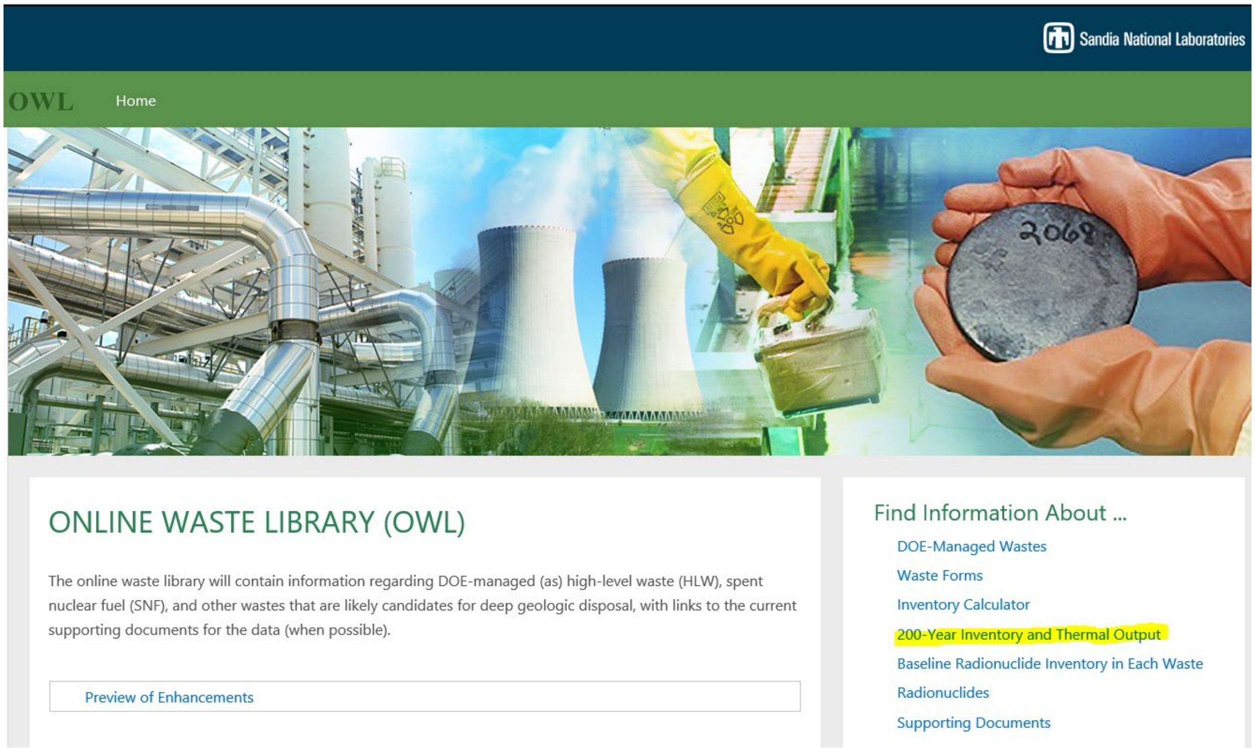
Figure 13. Example of Filtering the Baseline Radionuclide Inventory

See the radionuclide inventory of a particular waste or wastes as of a specific date (year)

To see the radionuclide inventor of a particular waste or wastes as of a specific year, the user can click on "Inventory Calculator" from the home page (Figure 9). This will display the inventory (in Curies and grams) of every radionuclide in every waste, along with the thermal output of heat-generating radionuclides in every waste, both as of the baseline date for the waste and at some specified time (date). The user can then select the desired date (year) from the selection pane on the right side of the page and click on "Apply" on the bottom of the right side of the page or hit "Enter" on the keyboard. The list of radionuclides displayed can be filtered by selecting the waste classification, a particular waste, or a radionuclide from the selection pane on the right side of the page and clicking on "Apply" on the bottom of the right side of the page or hitting "Enter" on the keyboard. In the example in Figure 10, Cesium and Strontium capsules is the selected waste and the year for which the inventory is selected is 2050.

See graph showing the total radioactivity and thermal output of a waste (or all wastes) over the next 200 years

To see graphs showing the total radioactivity and thermal output of a waste (or all wastes) over the next 200 years, the user can click on "200-Year Inventory and Thermal Output" from the home page (Figure 14) . This will display a graph of the total radioactivity of all the wastes and the thermal output of all the wastes over the next 200 years. The user can switch between Curies and GBq for the projected inventory by clicking on "Display in SI Units (Bq)" or "Display in Curies," as appropriate. The wastes included in the graphs can be filtered by selecting the waste type or radionuclide from the selection pane on the right side of the page and clicking on “Apply” on the bottom of the right side of the page or hitting “Enter” on the keyboard. In the example shown below (Figure 15), “All” waste types are selected and “All” radionuclides are selected.



ONLINE WASTE LIBRARY (OWL)

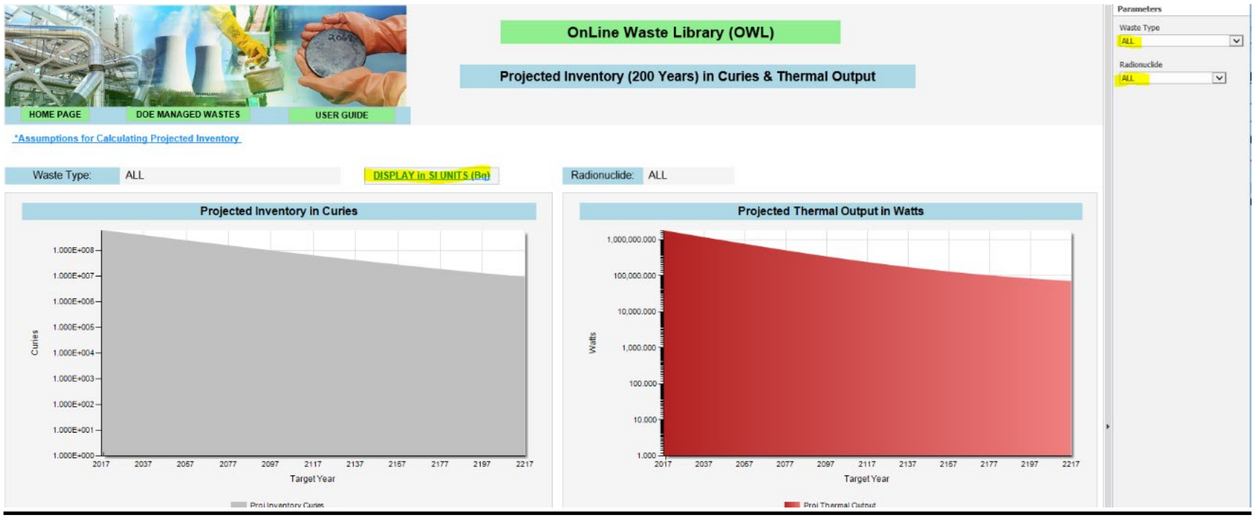
The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Preview of Enhancements

Find Information About ...

- DOE-Managed Wastes
- Waste Forms
- Inventory Calculator
- 200-Year Inventory and Thermal Output
- Baseline Radionuclide Inventory in Each Waste
- Radionuclides
- Supporting Documents

Figure 14. Example of Selecting Graphs of Inventory and Thermal Output for 200 Years



OnLine Waste Library (OWL)

Projected Inventory (200 Years) in Curies & Thermal Output

Waste Type: ALL

Radionuclide: ALL

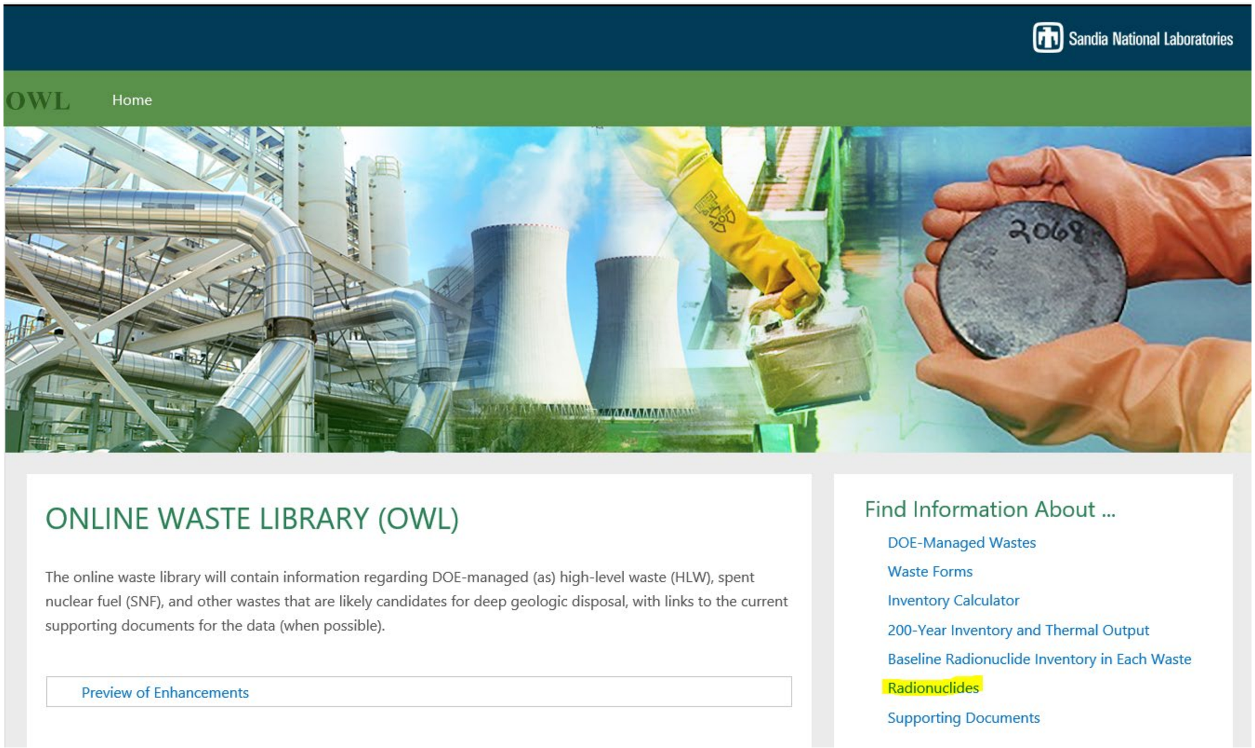
Waste Type: ALL

Radionuclide: ALL

Figure 15. Example of Selecting “All” Radionuclides and “All” Waste Type for Inventory and Thermal Output Graphs

See a list of radionuclides included in the OWL

To see a list of all the radionuclides included in the OWL, the user can click on “Radionuclides” from the home page (Figure 16). This will display a list of all radionuclides in OWL, along with the half-life of each radionuclide, a link to a graph of the inventory of that radionuclide over the next 200 years, its atomic mass, its heat generation rate (if applicable), its parent radionuclide (if needed for radioactive decay calculations), and its decay ratio (if needed for radioactive decay calculations). Radionuclides can be sorted alphabetically, by half-life, by atomic mass, and by thermal output by clicking on the up and down triangles in the header row of the table. In the example shown below (Figure 17), radionuclides are sorted by decreasing half-life.



ONLINE WASTE LIBRARY (OWL)

The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Find Information About ...

- DOE-Managed Wastes
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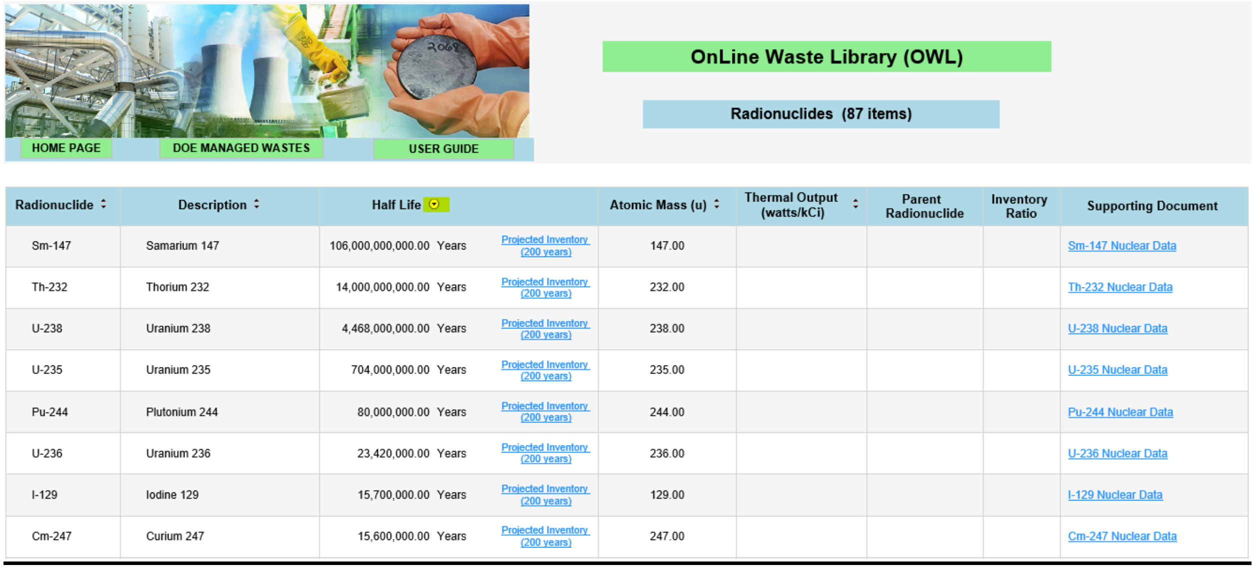
- Inventory Calculator
- 200-Year Inventory and Thermal Output
- Baseline Radionuclide Inventory in Each Waste
- Radionuclides
- Supporting Documents

Figure 16. Example of Selecting "Radionuclides" from the Home Page



OnLine Waste Library (OWL)

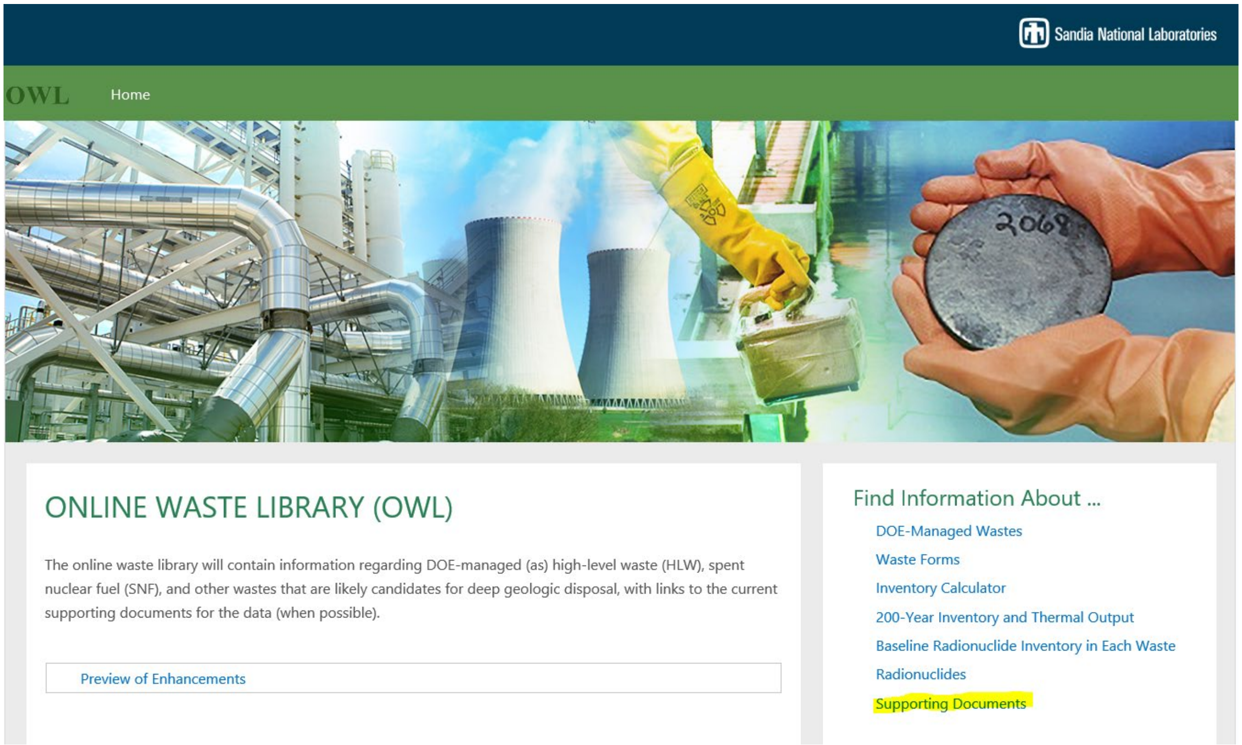
Radionuclides (87 items)

Radionuclide	Description	Half Life		Atomic Mass (u)	Thermal Output (watts/kCi)	Parent Radionuclide	Inventory Ratio	Supporting Document
Sm-147	Samarium 147	106,000,000,000.00 Years	Projected Inventory (200 years)	147.00				Sm-147 Nuclear Data
Th-232	Thorium 232	14,000,000,000.00 Years	Projected Inventory (200 years)	232.00				Th-232 Nuclear Data
U-238	Uranium 238	4,468,000,000.00 Years	Projected Inventory (200 years)	238.00				U-238 Nuclear Data
U-235	Uranium 235	704,000,000.00 Years	Projected Inventory (200 years)	235.00				U-235 Nuclear Data
Pu-244	Plutonium 244	80,000,000.00 Years	Projected Inventory (200 years)	244.00				Pu-244 Nuclear Data
U-236	Uranium 236	23,420,000.00 Years	Projected Inventory (200 years)	236.00				U-236 Nuclear Data
I-129	Iodine 129	15,700,000.00 Years	Projected Inventory (200 years)	129.00				I-129 Nuclear Data
Cm-247	Curium 247	15,600,000.00 Years	Projected Inventory (200 years)	247.00				Cm-247 Nuclear Data

Figure 17. Example of All Radionuclides Shown in Order of Decreasing Half-life

See a list of documents used to support the information in OWL

To access the documents used to support the information in the OWL, the user can click on "Supporting Documents" from the home page (Figure 18). This will display a list of all the supporting documents found in OWL, along with a description of the document, any comments (such as report number), author(s), publisher, and date of publication. Clicking on the document title will open the document in a new browser window.



ONLINE WASTE LIBRARY (OWL)

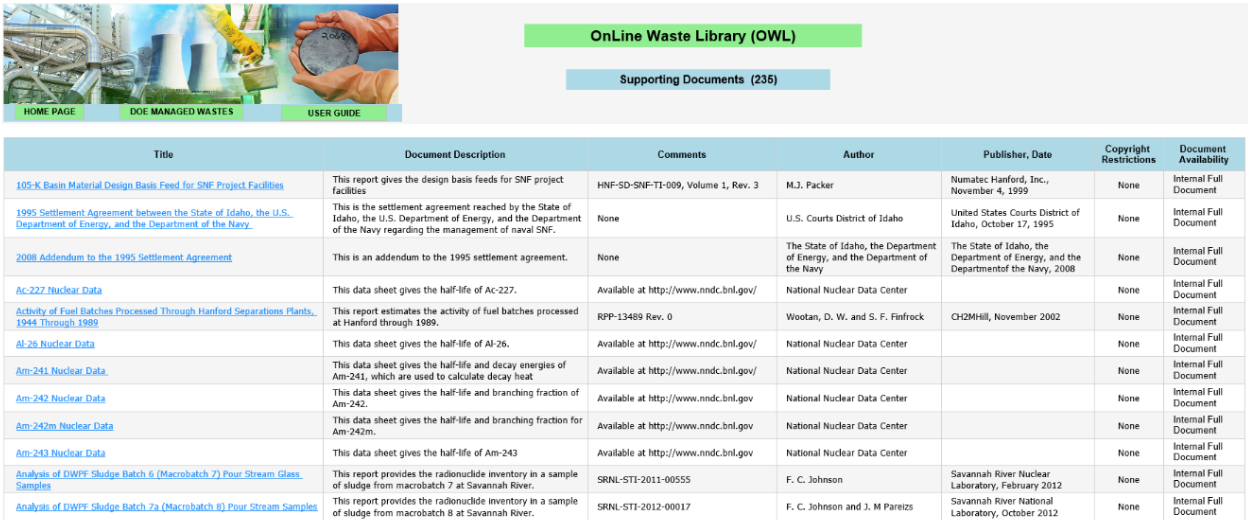
The online waste library will contain information regarding DOE-managed (as) high-level waste (HLW), spent nuclear fuel (SNF), and other wastes that are likely candidates for deep geologic disposal, with links to the current supporting documents for the data (when possible).

Preview of Enhancements

Find Information About ...

- DOE-Managed Wastes
- Waste Forms
- Inventory Calculator
- 200-Year Inventory and Thermal Output
- Baseline Radionuclide Inventory in Each Waste
- Radionuclides
- Supporting Documents

Figure 18. Example of Selecting "Supporting Documents" from the Home Page



Title	Document Description	Comments	Author	Publisher, Date	Copyright Restrictions	Document Availability
105-K Basin Material Design Basis Feed for SNF Project Facilities	This report gives the design basis feeds for SNF project facilities	HNF-SD-SNF-TI-009, Volume 1, Rev. 3	M.J. Packer	Numatec Hanford, Inc., November 4, 1999	None	Internal Full Document
1995 Settlement Agreement between the State of Idaho, the U.S. Department of Energy, and the Department of the Navy	This is the settlement agreement reached by the State of Idaho, the U.S. Department of Energy, and the Department of the Navy regarding the management of naval SNF.	None	U.S. Courts District of Idaho	United States Courts District of Idaho, October 17, 1995	None	Internal Full Document
2008 Addendum to the 1995 Settlement Agreement	This is an addendum to the 1995 settlement agreement.	None	The State of Idaho, the Department of Energy, and the Department of the Navy	The State of Idaho, the Department of Energy, and the Departmentof the Navy, 2008	None	Internal Full Document
Ac-227 Nuclear Data	This data sheet gives the half-life of Ac-227.	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Activity of Fuel Batches Processed Through Hanford Separations Plants, 1944 Through 1989	This report estimates the activity of fuel batches processed at Hanford through 1989.	RPP-13489 Rev. 0	Wootan, D. W. and S. F. Finfrock	CH2MHill, November 2002	None	Internal Full Document
Al-26 Nuclear Data	This data sheet gives the half-life of Al-26.	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Am-241 Nuclear Data	This data sheet gives the half-life and decay energies of Am-241, which are used to calculate decay heat	Available at http://www.nndc.bnl.gov/	National Nuclear Data Center		None	Internal Full Document
Am-242 Nuclear Data	This data sheet gives the half-life and branching fraction of Am-242.	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Am-242m Nuclear Data	This data sheet gives the half-life and branching fraction for Am-242m.	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Am-243 Nuclear Data	This data sheet gives the half-life of Am-243	Available at http://www.nndc.bnl.gov	National Nuclear Data Center		None	Internal Full Document
Analysis of DWPF Sludge Batch 6 (Macrobatch 7) Pour Stream Glass Samples	This report provides the radionuclide inventory in a sample of sludge from macrobatch 7 at Savannah River.	SRNL-STI-2011-00555	F. C. Johnson	Savannah River Nuclear Laboratory, February 2012	None	Internal Full Document
Analysis of DWPF Sludge Batch 7a (Macrobatch 8) Pour Stream Samples	This report provides the radionuclide inventory in a sample of sludge from macrobatch 8 at Savannah River.	SRNL-STI-2012-00017	F. C. Johnson and J. M Pareizs	Savannah River National Laboratory, October 2012	None	Internal Full Document

Figure 19. Example of Information Shown on Supporting Documents Webpage

The information available by clicking on each of the links under “Find Information About…” on the OWL home page is discussed below.

DOE-Managed Wastes

The information for each waste on this webpage includes its baseline inventory date, its classification (SNF, HLW, or TRU), a description of the waste, where it is stored, its current total volume, and its total radioactivity as of the baseline date. Clicking on the name of the waste opens a Waste Detail Report for that waste. This webpage reports whether the waste was produced by the government, whether it is a mixed waste, and its baseline inventory date, and contains links that present:

- A graphical representation of the projected inventory and thermal output of the waste over the next 200 years (Projected Inventory link)
- Waste Characteristics – thermal output, chemical constituents present, dimensions of the nuclear waste container, the number of containers of the waste, and the physical form of the waste
- Waste Source
- Disposal Waste Forms
- Disposal Waste Form Characteristics – thermal output, dimensions of the waste form, mass of the waste form
- Radionuclide Inventory – Activity (Curies) of each radionuclide reported or calculated to be present in the waste
- Radionuclide Characteristics – half-life and decay ratio (where applicable) for each radionuclide in the inventory for that waste

- Waste Supporting Documents – a list of all documents used as sources of information for that waste. Clicking on the title of a supporting document will open that document in a new window
- Waste Contacts – the name and contact information for a person who is knowledgeable about that waste.

Waste Forms

Each waste also has a "disposal waste form." For some wastes, such as N-reactor spent fuel or Savanah River glass waste, the waste is intended to be disposed of without further treatment. Hence, the current waste is also the disposal waste form. For other wastes, such as the Hanford tank wastes, the current plan is to treat the waste prior to disposal. For these wastes, the current waste is not the disposal waste form, and possible waste forms are presented. For each disposal waste form, OWL indicates whether the waste form already exists or is planned, and whether the waste form has been declared by the DOE to be the preferred waste form or if it is an alternative to that preferred waste form. All wastes and their associated waste forms are available by clicking on "Waste Forms" on the home page.

Inventory Calculator

Clicking on "Inventory Calculator" from the home page opens a page that gives the radionuclide inventory and thermal output of each waste as of its baseline date and allows the user to calculate the inventory and thermal output at a user-specified year. The selection pane for the parameters for the calculation is on the right side of the page. The user can select the waste classification (HLW, SNF, or TRU), a specific nuclear waste, a radionuclide, and a year. Clicking on the "Apply" button on the bottom of the right side of the page after selecting the desired parameters will generate the report. The selection pane on the right side of the page can be hidden by clicking on the triangle in the gray bar to the left of the selection pane. Assumptions that were made in calculating the inventory can be seen by clicking on "Assumptions for Calculating Projected Inventory" at the top of the Radionuclide Inventory Calculation page.

200-Year Inventory and Thermal Output

Clicking on "200-Year Inventory and Thermal Output" from the home page opens a page that gives a graphical representation of the inventory and thermal output of the user-selected waste and radionuclide over the next 200 years. The selection pane for the waste type and radionuclide is on the right side of the page. The user can select a particular waste (or all of the wastes) and a particular radionuclide (or all of the radionuclides). Clicking on the "Apply" button on the bottom of the right side of the page after selecting the desired parameters will generate the database report. The selection pane on the right side of the page can be hidden by clicking on the triangle in the gray bar to the left of the selection pane.

Baseline Radionuclide Inventory in Each Waste

Clicking on "Baseline Radionuclide Inventory in Each Waste" from the home page opens a page that gives the inventory of each radionuclide in each waste as of the baseline date for each waste. On the left side of the page the user can select wastes by facility or by classification, and can select "all" radionuclides or a specific radionuclide.

Radionuclides

Clicking on “Radionuclides” from the home page opens a page that gives the following information for each radionuclide in the OWL database: name, half-life, atomic mass, thermal output (if applicable), its parent (if applicable), the inventory ratio with the parent (if applicable), and a link to the supporting document for some of the information for that radionuclide.

Supporting Documents

Clicking on “Supporting Documents” from the home page opens a page that lists the following information for the supporting documents in the OWL: title of the document, a description of the document, document number (if applicable), URL address (if applicable), the author, the publisher, the date and whether there are copyright restrictions. Clicking on the title of the document will open a new webpage displaying the document or will open a dialog box that allows the user to open the document, save the document, or save the document with another name.

Waste-Specific Spreadsheets

Each waste has a spreadsheet that gives the inventory and thermal output as of the baseline date and allows the user to calculate the inventory and thermal output as of a user-specified target date. Depending on the waste, spreadsheets may also have other information, such as the volume of the waste as currently stored. These spreadsheets are displayed in pdf format to allow users to view the spreadsheet without needing access to Excel™; an Excel™ version of any spreadsheet can be obtained by sending an email to OWL@sandia.gov and requesting the desired spreadsheet(s).

Questions or Comments

Questions or comments can be sent to OWL@sandia.gov.