Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

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April 28, 2020 SRNL-STI-2020-00162
Revision 0

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PORFLOW IMPLEMENTATION OF SPECIAL WASTE FORM MODELS FOR SLIT AND ENGINEERED TRENCHES IN THE E-AREA LOW LEVEL WASTE FACILITY PERFORMANCE ASSESSMENT

Summary

The implementation of special waste forms (SWFs) in the deterministic PORFLOW Slit Trench (ST) and Engineered Trench (ET) models to be used in the next revision of the E-Area Low Level Waste Facility's (ELLWFs) Performance Assessment (PA) is outlined in this report. Four SWF implementation methods will be used: effective K_d, delayed release, solubility-controlled/diffusion-controlled release, and complex SWF model updates. In addition, the implementation of models that address the presence of tall used equipment storage boxes in ST08-10 is considered a special waste form and will be described.

Background

SWFs are a category of trench waste that exceed or consume a large fraction of the allowable inventory for specific radionuclides without taking credit for the waste form or disposal container. Additional characterization and modeling, generally performed as part of a Special Analysis (SA), are needed to produce acceptable trench disposal limits. SWF modeling incorporates chemistry, corrosion rates, hydraulics, radionuclide decay and administrative controls, as needed, to produce acceptable disposal limits through hold up or controlled release of contaminants into the backfill soil within the waste zone. Radionuclide limits treated in this manner are given a unique designation in the Waste Inventory Tracking System (WITS) to distinguish them from the equivalent "generic" radionuclide limit (i.e., limits established assuming instantaneous release of radionuclide to the surrounding backfill soil) and contribute independently to the sum-of-fractions (SOF) calculation to ensure the distribution of radionuclides in a trench are always at or below a SOF of one. SWFs are typically obtained from limited waste campaigns (e.g., deactivation and decommissioning, disposition of legacy LLW items, etc.) or are generated from site processes. The majority of SWFs are disposed in STs and ETs, including formerly designated Component-in-Grout (CIG) trenches being repurposed as STs in the next PA (due to the lack of CIG waste projections from site generators). CIG special waste form segments of STs, and SWFs in other disposal units, specifically the Intermediate Level Vault and Naval Reactor Disposal Areas, are to be addressed in other disposal unit specific model documentation. The table in Appendix A is a complete listing of ST and ET SWFs and associated historical characterization and modeling references.

In all four types of SWF models, placement of SWF inventory will be conservatively assumed to occur on the date when each trench unit was first opened to waste (

Table 1), consistent with the modeling assumption for generic waste (i.e., instantaneous disposal of all inventory at the start of operations for each trench unit). Assumptions regarding SWF placement timing for future trenches has yet to be determined. Timing of closure activities will be updated to the current facility lifecycle assumptions, (i.e., dates for operational stormwater cover, interim cover, and final closure cap).

Table 1 Date that SWF inventories will be placed in PORFLOW models for each existing ET and ST containing a SWF.

Trench	Open Date
ET01	2/13/2001
ST01	12/21/1995
ST02	9/20/2001
ST03	10/20/2003
ST04	2/26/2004
ST05	5/27/2004
ST07	6/26/2006
ST08	2/6/2007
ST09	3/17/2011
ST14	3/29/2011

The four proposed SWF model implementation methods are described in the following sections.

Effective K_d

The effective K_d implementation is applied to seven specific waste forms that have been disposed and/or are approved for future disposal in STs and ETs in the ELLWF. The waste forms are listed in Table 2 and the K_d values are taken directly from the 2016 Geochemical Data Package (Kaplan, 2016). These SWFs are strictly for I-129 generated from water treatment processes [i.e., F-Area groundwater treatment unit (F-WTU), H-Area groundwater treatment unit (H-WTU), or Effluent Treatment Facility (ETF)]. The effective K_d implementation assumes that the SWF is distributed uniformly throughout the waste zone except where a unique or sporadic disposal pattern requires a bounding type analysis (e.g., SWF placed at the downgradient end of a trench closest to the groundwater point of assessment).

Each trench type (i.e., STs and ETs) has been assigned a unique set of waste zone chemical and hydraulic properties into which the SWF is placed. The waste zone K_d is specified based on the values given in the

2016 Geochemical Data Package (Kaplan, 2016) for clayey material. The set of hydraulic properties is selected to represent the types of waste forms and waste zone conditions over the ST or ET lifecycle. Effective, or "hybrid", hydraulic properties have been estimated for the ST waste zone based on a proportional blending of containerized and bulk wastes that have been historically received. Alternatively, ET's are assigned a set of hydraulic properties reflecting containerized waste disposals surrounded by backfill soil. Hydraulic properties before and after dynamic compaction are estimated for both STs and ETs. Descriptions and values of ST and ET hydraulic waste zone properties are provided in Nichols (2020).

The ELLWF hydrostratigraphy, updated in 2017 by Bagwell et al, was used as a basis for the development of the ST/ET conceptual models (Danielson, 2019). The STs and ETs containing these SWFs will be modeled as having the depth to the water table and a clayey thickness beneath the waste zone as specified by Danielson (2019).

Table 2 Special waste forms to be modeled using the "Effective K_d" implementation.

Waste Form	WITS Designation	Existing Trench Locations	Potential Future Locations	Still Being Generated?	K_d (mL/g)
ETF GT-73	I129I	ST02-ST04, ET01	NA	No	10000
F-WTU CG-8	I129G	ST02, ET01	NA	No	50
F-WTU Dowex 21K	I129D	ST02, ET01	NA	No	6800
F-WTU Filtercake	I129J	ST01-05, ST07, ET01	NA	No	56.9
H-WTU CG-8	I129H	ST02, ST04, ET01	NA	No	380
H-WTU Dowex 21K	I129E	ET01	NA	No	15600
H-WTU Filtercake	I129F	ST01	NA	No	650

Delayed Release Implementation

The delayed release implementation of SWFs is similar to the effective K_d implementation except in this case, the specific radionuclide is kept immobile until dynamic compaction at the beginning of the post-closure period (i.e., the year 2165). In this SWF category, credit is being taken for the integrity of the disposal container in radionuclide holdup. Two waste forms fall into this category: Naval Reactor pumps and ETF carbon vessels. These waste forms and their locations and K_d's are shown in Table 3. Once again, the waste is assumed to be uniformly distributed in the waste zone except where a unique or sporadic disposal pattern requires a bounding type analysis (e.g., SWF placed at the downgradient end of a trench closest to the groundwater point of assessment). In PORFLOW, during the operational and

institutional control periods, the waste zone K_d will be specified as 1e20, which will render the radionuclide immobile to represent an intact container condition. Upon dynamic compaction, the radionuclide is supplied with the K_d listed in
Table 3 that is obtained from the 2016 Geochemical Data Package (Kaplan, 2016).

The STs and ETs containing these SWFs will be assigned the waste zone chemical and hydraulic properties obtained from Kaplan (2016) and Nichols (2020) and the hydrostratigraphy will be represented as specified by Danielson (2019).

Table 3 Special waste forms to be modeled using the "Delayed Release" implementation.

Waste Form	WITS Designation	Existing Trench Locations	Potential Future Locations	Still Being Generated?	K_d (mL/g)
Naval Reactors Pump	C14N	ST01-05, ST07, ST14	ST01-11, ST14-21	Yes	30
Effluent Treatment Facility Carbon Column	H3C	ST03, ST07	ET01, ET02, ST01-11, ST14-21	Yes	0
Effluent Treatment Facilities Carbon Columns	I129C	ST03, ST07	ET01, ET02, ST01-11, ST14-21	Yes	7400

Solubility-Controlled and Diffusion-Controlled Release

Solubility-controlled release models require a specially defined source term in PORFLOW simulations. M-Area glass, one of the two SWFs in this category, was generated by the vitrification of waste sludge from the production of depleted uranium targets. The Paducah cask, the other SWF, was a depleted uranium shielded cask containing various radioactive sources from SRS reactors. For both SWFs, the same source term that was used in the 2008 PA will be used for each of the radionuclides of interest. These source term files specify the concentration through time that is released. The waste zone K_d is specified based on the values given in the 2016 Geochemical Data Package (Kaplan, 2016) for clayey material. Each waste form has already been placed and no future disposal is expected. Therefore, the waste form will be placed in the location of the generic ST model setup that is most representative of the known location within the trench.

H-3 containing concrete rubble disposed in ST01 from the demolition of building 232-F (the old tritium facility) is the only SWF that is in the diffusion-controlled release category. The presence of concrete rubble changes the hydraulic properties of the waste zone, effectively lowering the saturated hydraulic conductivity and the porosity. The rate of leaching of H-3 from chunks of rubble is diffusion dominated and dependent upon the size distribution of the concrete chunks (i.e., small chunks release tritium at a faster rate than large chunks). A previous SA (Flach, 2005) employed a methodology to account for the size distribution and diffusion of H-3 from the concrete rubble. No changes to the 2005 SA's methodology will be introduced in the next revision of the PA, but all properties, the infiltration rates, and the hydrostratigraphy will be updated prior to re-running the models.

ST01, ST02, and ST05 will be assigned the waste zone chemical and hydraulic properties obtained from Kaplan (2016) and Nichols (2020), and the depth to the water table and the clayey thickness beneath the waste zone will be modeled as specified for each trench unit by Danielson (2019).

Table 4 Special waste forms to be modeled using the "Solubility-Controlled Release" implementation.

Waste Form	WITS Designation	Existing Trench Locations	Potential Future Locations	Still Being Generated?	K_d (mL/g)
M-Area Glass	U234G	ST02	NA	No	400
M-Area Glass	U235G	ST02	NA	No	400
M-Area Glass	U236G	ST02	NA	No	400
M-Area Glass	U238G	ST02	NA	No	400
Paducah Cask	U235P	ST05	NA	No	400
232-F Concrete	H3F	ST01	NA	No	0

Complex Special Waste Form Model Updates

Two complex special waste forms will be modeled in the next revision of the ELLWF PA: the Heavy Water Components Test Reactor (HWCTR) and the Reactor Process Heat Exchangers (HXs). The implementation will make use of models deployed for each waste form in SAs performed in 2010 (HWCTR: Hamm et al, 2010) and 2012 (HXs: Hamm et al, 2012). Each of the models that were carried out in these SAs will be re-run with adjustments made to the infiltration rates (i.e., accounting for the newly designed final closure cap) and to all input parameters that are impacted by infiltration rates such as the source and sink terms in the HXs flow model that account for lateral flow around the cylindrical shape of the heat exchangers. Likewise, the timeline of events will be adjusted to more accurately reflect the currently intended placement of the interim and final closure caps (i.e., marking time periods when infiltration rate changes) which has changed since the 2008 PA and the subsequent SAs. The most up-to-date hydraulic properties (Nichols, 2019) and geochemical properties (Kaplan, 2016) will be used and as built dimensions of the trench segments will be implemented on the existing 2D meshes. Table 6 provides an updated table of K_d's to be used in the HWCTR model, which is structured the same as Table 4-8 in Hamm et al, 2010 for comparison. Because no grout is used for the HXs, the waste zone K_d's are set to 0 mL/g for both H-3 and C-14 in the waste form and the standard clayey K_d's are used as waste is released from the waste form. Note that both models make use of a corrosion release model, but no updates will be made to the corrosion rates because these were not directly impacted by infiltration or any other properties that will be changed.

The ELLWF hydrostratigraphy was updated in 2017 by Bagwell et al, which was used as a basis for the development of the ST/ET conceptual models (Danielson, 2019). ST09, where the HXs are located, is to be modeled having a depth to the water table of 75 feet (from ground surface) and a clayey thickness beneath the waste zone of 11 feet. The 2012 SA depth to the water table was 66 feet (from ground surface, 46 feet from the bottom of the waste zone) and had no clayey layer beneath the waste. In the interest of preventing the need to re-mesh, and because it is a conservative assumption, the depth to the water table will not be changed. However, the clayey layer will be incorporated through the use of PORFLOW "LOCAte" commands. ST14, which is where HWCTR is buried, had a depth to the water table of 55 feet (from ground surface, 35 feet from the bottom of the waste zone) in the 2010 SA and no clayey layer beneath the waste. This depth to the water table matches the hydrostratigraphic grouping containing ST14 for the next revision of the ELLWF PA, but an addition of 15 feet of clay beneath the waste will be added using PORFLOW "LOCAte" commands.

Table 5 Special waste form radionuclides released from the complex special waste forms HWCTR and the reactor process HXs.

Waste Form	Radionuclide	Existing Trench Locations	K_d (mL/g)
HWCTR	Ag-108m	ST14	See Table 6
HWCTR	C-14	ST14	See Table 6
HWCTR	Co-60	ST14	See Table 6
HWCTR	Fe-55	ST14	See Table 6
HWCTR	Mo-93	ST14	See Table 6
HWCTR	Nb-93m	ST14	See Table 6
HWCTR	Nb-94	ST14	See Table 6
HWCTR	Ni-59	ST14	See Table 6
HWCTR	Ni-63	ST14	See Table 6
HWCTR	Tc-99	ST14	See Table 6
HX	C-14	ST09	0
HX	H-3	ST09	0

Table 6 Reproduction of Table 4-8 from SRNL-STI-2010-00574 with updated chemical properties as listed in Kaplan, 2016. Note that the K_dConGone is set to the smaller of stage III concrete and clay as a conservative estimate, which is consistent with the SA methodology.

Material	Pore Water pH	K_d Ag-108m (mL/g)	K_d C-14 (mL/g)	K_d Co-60 (mL/g)	K_d Fe-55 (mL/g)	K_d Mo-93 (mL/g)	K_d Nb-93m (mL/g)	K_d Nb-94 (mL/g)	K_d Ni-59 (mL/g)	K_d Ni-63 (mL/g)	K_d Tc-99 (mL/g)
KdSand	**High**	32	5	128	300	1400	1400	1400	22.4	22.4	0.06
KdClay	**High**	96	150	320	600	1400	1400	1400	96	96	0.18
KdSand	**Low**	10	1	40	200	1000	1000	1000	7	7	0.6
KdClay	**Low**	30	30	100	400	1000	1000	1000	30	30	1.8
KdConYng		4000	2000	4000	6000	3	1000	1000	65	65	0.8
KdConMid		4000	5000	4000	6000	3	1000	1000	400	400	0.8
KdConOld		400	50	400	600	3	500	500	400	400	0.5
KdConGone		30	30	100	400	3	500	500	30	30	0.5

KdMet		0	0	0	0	0	0	0	0	0	0
KdGrv		0	0	0	0	0	0	0	0	0	0
KdCks		0	0	0	0	0	0	0	0	0	0

Tall Boxes

Tall used equipment storage boxes, or "Tall boxes", that have been disposed of, or are approved for disposal, in ST08-10 will be treated as a special waste form model. Tall box burial is limited to the southern-third (i.e., 220 feet) of ST08 and ST09 and the southern 180 feet of ST10. ST08-10 are part of the hydrostratigraphic grouping that is considered to have a depth to the water table of 75 feet and 11 feet of clay thickness beneath the waste zone (Danielson, 2019). Tall box models will be implemented in three dimensions and will incorporate a portion of a ST segment that is 35 feet deep (i.e., the maximum depth of the tall boxes), where the waste zone is 31 feet and four feet of backfill material is placed on top. Both intact and subsided cases will be modeled using a similar procedure to that found in Flach (2010).

Some of the tall boxes contain lead requiring a one-foot encapsulation layer of grout surrounding the waste component. While the grout encapsulation layer is intact it provides a barrier to infiltration and changes the chemistry of the waste zone. Both grouted and non-grouted tall-box waste forms will be compacted at the end of institutional control from 31 feet down to 4.8 feet, which is consistent with Flach (2010) and the ratio of compaction for the standard 16-foot B-25 boxed waste form that is compacted to 2.5 feet. The grout encasement will be degraded to ILV Backfill soil properties at compaction.

A single tall-box VZ model will be used to represent both grouted and non-grouted waste forms. The hydraulic properties of the intact grout layer will not be explicitly modeled, but the chemistry of the waste zone will be set to the smaller of the concrete K_d or clay K_d during the operational and institutional control periods. During the post-closure period, following dynamic compaction, the radionuclides in the waste zone will be set to clay K_d values reflecting the breakup of the grout encapsulation layer.

Automation of Model Implementation

To ensure proper linking of datasets and error-free construction of PORFLOW input files the automation scheme that is used for generic waste forms will be updated. The implementation of the SWF models fits nicely into the scheme for generic waste forms and only requires updates to the PORFLOW Transport input file pre-processor. For SWFs falling under the effective K_d, delayed release, or solubility-controlled release classification, the WITS designation of the radionuclide [e.g., H3C (SWF) vs. H-3 (generic)] is used to trigger the algorithm to appropriately select either the SWF K_d and/or the appropriate source term file and write the proper syntax of the PORFLOW 'SOURce' command.

For the SWFs that are to be re-run with updated parameters (i.e., HWCTR, HXs, 232-F concrete rubble), the existing input files will be parsed based on the PORFLOW input file syntax to locate the parameters that need to be updated and the most up-to-date values will be selected from the hydraulic and/or geochemical data packages.

Tall boxes models will require a new mesh and can use the same automation scheme as is used for generic waste forms.

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Kaplan, 2016. D. I. Kaplan, *Geochemical Data Package for Performance Assessment Calculations Related to the Savannah River Site,* WSRC-TR-2009-00473, Revision 1, July 22, 2016.

Nichols, 2019. R. L. Nichols, *Hydraulic Properties Data Package for the E-Area Soils, Cementitious Materials, and Waste Zones – Update*, SRNL-STI-2019-00355, Revision 0, January 2020.

Appendix A Indexing of important references for each special waste form.

SWF	WITS ID	Waste Characterization References	SA and/or UDQE References
Reactor Heat Exchangers	C14X, H3X	WSRC-TR-2009-00473	SRNL-STI-2012-00321
ETF GT-73	I129I	WSRC-TR-2002-00091 WSRC-TR-99-00270	WSRC-TR-2001-00021
F-WTU CG-8	I129G	WSRC-TR-2000-00308	WSRC-TR-2001-00021
F-WTU Dowex 21K	I129D	WSRC-TR-2002-00091 WSRC-TR-99-00270	WSRC-TR-2001-00021
F-WTU Filtercake	I129J	WSRC-TR-2001-00253	WSRC-TR-2001-00021
H-WTU CG-8	I129H	WSRC-TR-2002-00091 WSRC-TR-2000-00308	WSRC-TR-2001-00021
H-WTU Dowex 21K	I129E	WSRC-TR-2002-00091 WSRC-TR-2000-00308	WSRC-TR-2001-00021
H-WTU Filtercake	I129F	WSRC-TR-2001-00253	WSRC-TR-2001-00021
Naval Reactors Pump	C14N	WSRC-TR-2009-00473	WSRC-STI-2007-00306
Effluent Treatment Facility Carbon Column	H3C	WSRC-TR-2009-00473	WSRC-TR-2003-00255 WSRC-RP-99-00596
Effluent Treatment Facilities Carbon Columns	I129C	WSRC-TR-99-00270	WSRC-TR-2003-00255 WSRC-RP-99-00596 WSRC-RP-99-01070
M-Area Glass	U234G, U-235G, U236G, U238G	WSRC-TR-2009-00473	WSRC-TR-2002-00337
Paducah Cask	U235P	WSRC-TR-2009-00473	WSRC-TR-2003-00521
232-F Concrete	H3F	WSRC-TR-2009-00473	WSRC-TR-2005-00093
HWCTR	Ag108MH, C14H, Co60H, Fe55H, Mo93H, Nb93MH, Nb94H, Ni59H, Ni63H, Tc99H	WSRC-TR-2009-00473	SRNL-STI-2010-00574

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