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PORFLOW Implementation of Vadose Zone Conceptual Model for Naval Reactor Component Disposal Area in the E-Area Low Level Waste Facility Performance Assessment

T. Hang

L. L. Hamm

January 2022

SRNL-STI-2019-00357, Revision 1

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REVIEWS AND APPROVALS

AUTHORS:

____

T. Hang, Advanced Modeling & Simulation, SRNL Date

____

L. L. Hamm, Advanced Modeling & Simulation, SRNL Date

TECHNICAL REVIEW:

____

T. L. Danielson, Environmental Science & Dosimetry, SRNL, Reviewed per E7 2.60 Date

____

S. E. Aleman, Environmental Science & Dosimetry, SRNL, Reviewed per E7 2.60 Date

____

J. J. Mayer, II, Earth & Biological Systems, SRNL, Reviewed per E7 2.60 Date

APPROVAL:

____

B. D. Lee, Manager Date
Earth & Biological Systems, SRNL

____

P. L. Lee, Manager Date
Advanced Modeling & Simulation, SRNL

EXECUTIVE SUMMARY

PORFLOW models have been developed to implement the proposed conceptual models for the two Naval Reactor Component Disposal Areas (NRCDAs), 643-7E and 643-26E, for the purpose of evaluating dose impacts and producing disposal limits for the E-Area Low-Level Facility (LLWF). New NRCDA conceptual models were proposed by Wohlwend and Butcher (2019) for two areas within/adjacent to the E-Area LLWF used as storage/disposal sites for reactor components from the U.S. Navy since 1987. Naval Reactor (NR) waste is comprised of highly radioactive components consisting of activated corrosion-resistant metal alloy contained within welded thick-walled steel casks, and auxiliary equipment primarily contaminated with lower levels of Activated Corrosion Products (ACPs) residing on the metal surfaces and contained within thinner-walled bolted containers.

Separate three-dimensional models have been developed for each NR Pad to capture the unique geometry/features of the waste zone and subsurface hydrostratigraphic units, and chronology of facility events for each disposal unit. Radionuclide, chemical and material properties, as well as subsurface features represented in the models, were obtained from data packages containing key performance assessment (PA) data (Smith et. al. 2019, Kaplan 2016, Nichols and Butcher 2020, and Bagwell and Bennett 2017, respectively).

Four modeling cases have been proposed to capture the uncertainty in the waste release characteristics of the two types of waste forms (i.e., time to hydraulic failure of outer container and type of metal alloy component for bolted containers versus welded casks, respectively). Surface ACP contamination on auxiliary equipment is assumed to be released instantaneously as soon as the outer container hydraulically fails. Availability of contaminants for transport from activated metal components is represented by a corrosion-controlled release model following hydraulic failure of the outer welded cask. Worst case disposal limits and dose impacts will be calculated from the four modeling cases for each pad in the ongoing E-Area LLWF PA.

Results from modeling two of the four cases described above are presented in this report for a limited set of isotopes representing a range of radionuclide decay and elemental chemical properties. The full set of radionuclides resulting from an ongoing radionuclide screening analysis (Aleman and Hamm 2020) will ultimately be run to obtain inventory limits in the PA. One-dimensional GoldSim and PORFLOW models were developed and used to test and refine the three-dimensional PORFLOW models being employed in the E-Area PA. GoldSim models were then calibrated using the final set of PORFLOW transport model runs and are described separately in Smith (2020). PORFLOW model results are presented as flux to the water table (curies per year per curie of parent buried) in a series of flux-time history profiles at the end of this report. Subsequent aquifer analyses (beyond the scope of this report) will employ these fluxes to the water table files as source terms along with others generated for the remaining list of radionuclides of interest.

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LIST OF ABBREVIATIONS

ACP	Activated Corrosion Products
AP	All-Pathways
BMPC	Bechtel Marine Propulsion Corporation
CB/TS	Core Barrel/Thermal Shield
CLSM	Controlled Low Strength Material
DOE	Department of Energy
DU	Disposal Unit
EIC	End of Institutional Control
gmole	gmole
GW	Groundwater
GWP	Groundwater Protection
IC	Institutional Control
KAPL	Knolls Atomic Power Laboratory
Kd	Soil-Water Distribution (Partition) Coefficient
LAZ	Lower Aquifer Zone
LLWF	Low-Level Waste Facility
LVZ	Lower Vadose Zone
LAWV	Low Activity Waste Vault
NR	Naval Reactor
NRCDA	Naval Reactor Component Disposal Area
NRCSA	Naval Reactor Component Storage Area
OSC1	Operational Soil Cover Before Dynamic Compaction
PA	Performance Assessment
PO	Performance Objective
POP	Period of Performance
SA	Special Analysis
SBDC	Shear Block Disposal Container
SIC	Start of Institutional Control
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
TCCZ	Tan Clay Confining Zone
UAZ	Upper Aquifer Zone
WT	Water Table

1.0 Introduction

Reactor components from the U.S. Navy have been disposed in two areas within the E-Area Low-Level Waste Facility (LLWF) at the Savannah River Site (SRS). These areas are the currently operating at-grade gravel disposal pad, 643-26E, located inside the original 100-acre E-Area LLWF, and the operationally closed at-grade gravel disposal pad, 643-7E, located in the old burial ground adjacent to the E-Area LLWF as shown in Figure 1. These units are formally designated as Naval Reactor Component Disposal Areas (NRCDAs). The new disposal unit (DU) designations have been employed in Figure 1, along with updated footprints (Hamm 2019).

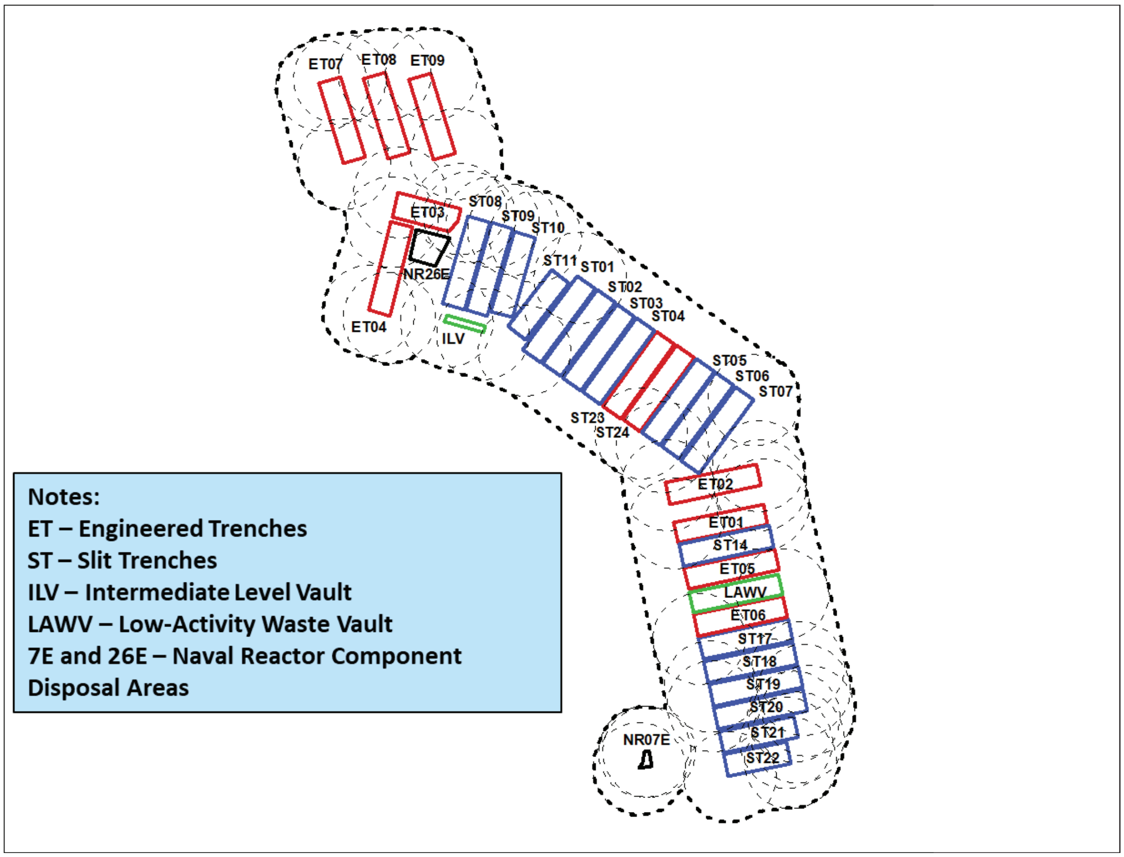


Figure 1. 643-26E NRCDA (labeled NR26E) and 643-7E NRCDA (labeled NR07E) and adjacent units in the E-Area LLWF

Naval Reactor (NR) waste is comprised of: (1) highly radioactive reactor components consisting of activated corrosion-resistant metal alloy stored within thick carbon-steel welded casks, and (2) auxiliary equipment contaminated on the surface with Activated Corrosion Products (ACP) (referred to as "crud" by the U.S. Navy) at low levels and stored within thinner-walled bolted steel containers. The 643-7E disposal pad contains 41 casks and other containers and is closed to future receipts. In 2005, soil was mounded around and over these containers for shielding. For 643-26E, the current estimates are for a total of 33 heavily shielded-welded casks, and 400+ thinner-walled bolted containers by 2065. A detailed description of the NRCDAs and typical NR waste components together with a proposed conceptual model is provided by Wohlwend and Butcher (2018). Note that the casks are welded shut, while the bolted containers are hydraulically gasket-sealed and are assumed to potentially hydraulically leak much sooner than the casks.

Consistent with Wohlwend and Butcher (2018) for each disposal unit (i.e., 643-7E and 643-26E) there are four separate cases being considered. A summary of those cases is provided in Table 1 and is discussed in the following chapters.

Table 1. List of the various cases considered for vadose zone PORFLOW modeling.

Disposal Unit	Waste Form	Waste Material	Release Time	Case ID
643-7E	Generic	Soil	Instantaneous at time of initial soil cover	Case 1
			Instantaneous at 750 yr post disposal	Case 2
	Special	Inconel	Corrosion limited starting at 750 yr post disposal	Case 3
		Zircaloy		Case 4
643-26E	Generic	Soil	Instantaneous at SIC[1]	Case 1
			Instantaneous at 750 yr post disposal	Case 2
	Special	Inconel	Corrosion limited starting at 750 yr post disposal	Case 3
		Zircaloy		Case 4

[1] SIC – Start of Institutional Control Results presented in this report highlighted in orange

As indicated in Table 1, vadose zone PORFLOW transport simulations for the above four cases will be run for both NRCDAs. Bolted containerized waste and welded cask waste will be handled as generic and special waste forms, respectively.

- Cases 1 and 2: Instantaneous release of radionuclide inventory from generic waste in bolted containers. Separate vadose zone analyses will be performed for two release times, SIC and 750 years following burial, to evaluate the impact of early and delayed hydraulic failure of containers. Subsequent aquifer analyses (beyond the scope of this report) will combine results to establish a "worst" case, and
- Cases 3 and 4: Corrosion-controlled release of radionuclides from special waste forms, Inconel and Zircaloy reactor components, in welded casks. Separate vadose zone analyses will be performed for Inconel and Zircaloy components, to evaluate the impact of the different corrosion rates of the two material alloys. Subsequent aquifer analyses (beyond the scope of this report) will combine results to establish a "worst" case.

Of the four cases listed in Table 1 only the PORFLOW results from two of these cases are being presented within this report (i.e., Case 1 and Case 3 highlighted in orange). For demonstration purposes only one case for generic waste and one for special waste forms was deemed necessary. For demonstration purposes, a small subset of parent radionuclides has been considered in this report. The list of parent nuclides considered is provided in Table 2 along with radionuclide decay and elemental chemical properties (Smith et al. 2019 and Kaplan 2016, respectively).

Table 2. List of parent nuclides considered for vadose zone PORFLOW modeling.

Parent Nuclide	Progeny	Half-life (yr)	Sand K_d (ml/g)	Clay K_d (ml/g)
C-14	none	5,700	1	30
I-129	none	1.57e+7	1	3
Nb-94	none	20,300	1,000	1,000
Ni-59	none	76,000	7	30
Pu-239		24,110	650	6,000
	U-235	7.07e+8	300	400
	Pa-231	32,760	3	9
	Ac-227	21.772	1,100	8,500
Tc-99	none	211,100	0.6	1.8

As Table 2 illustrates, a wide range of radiological and sorption aspects are being considered when looking at the list of nuclides chosen (i.e., including a short chain as well).

Production runs, that are beyond the scope of this report, will be performed for all four cases listed in Table 1 and will also be evaluating a larger list of parent nuclides consistent with groundwater (GW) screening criteria.

2.0 Naval Reactor Component Disposals at SRS

Above-grade storage of NR waste forms on the 643-7E pad began in 1987. Waste was received from the Bettis Atomic Power Laboratory, Knolls Atomic Power Laboratory (KAPL) and various Naval shipyards. In 1997, the Department of Energy (DOE) approved *disposal* of NR waste forms on the new 643-26E pad. In 2004 the existing casks and containers stored on the 643-7E NR pad were evaluated for in-place disposal and the storage pad reclassified as a disposal area (Wilhite and Flach 2004). 643-7E and 643-26E locations in/adjacent to the E-Area LLWF are shown in Figure 1.

Historically, sealed shipping casks and containers of components and auxiliary equipment have been shipped by NR programs to SRS by rail and placed on the NRCDA pads. The containers/casks are to remain on these pads for a period of years until covered by soil or, possibly, controlled low strength material (CLSM, a flowable soil-cement material used as backfill). For the closed 643-7E NR pad, a soil cover was applied in 2004 to provide shielding due to the proximity of adjacent E-Area operations. For the currently operating pad, 643-26E, this cover is assumed to be applied at the time of interim closure of E-Area estimated to be the year 2065. Following a minimum 100-year interim closure period where the closed facility will be monitored and maintained, the final multi-layer soil-geomembrane cover will be installed over the E-Area LLWF, including the two pads. Installation of the final cover is the start of the DOE Order 435.1 prescribed 1,000-year post-closure period. Implementation of a modeling timeline corresponding with this operational/closure sequence is described in Section 2.2.

NR components have consisted of core barrels, adapter flanges, closure heads, pumps, shear blocks and other similar equipment from the Navy. Due to the variety of NR waste components and levels of contamination, there is no standard NR waste container. Detailed configurational descriptions of the NR waste components are not available because of the classified nature of this information. According to unclassified information supplied by the NR program, a representative type of activated metal component is the KAPL core barrel/thermal shield (CB/TS) in a heavily shielded, welded cask (Yu et al. 2002). The KAPL CB/TS has been used in PA modeling as a conceptual type of waste form representing the various types of activated metal components (WSRC 1997, 2000 and 2008, and Yu et al. 2002) as the majority of the inventory projected for the 643-26E NRCDA will be contained in this type of component. The key safety feature of this cask is its 1.25-inch continuous weld, representative of the minimum weld thickness for all welded casks received from NR Programs. A representative type of an ACP-contaminated component is the shear block contained in a thinner-walled box with a bolted-in-place gasket seal. No hydraulic credit is taken for radionuclide holdup from this type of container as described in Sections 2.1.3 and 2.1.4 below.

Corrosion of the outer container and inner waste forms is a key consideration in the release of contaminants from buried NR waste. Key safety features of the two NR waste types and corresponding corrosion considerations are discussed below.

2.1 Key NR Waste Form Safety Features and Corrosion Considerations

2.1.1 Welded Cask

Highly radioactive components consisting of activated corrosion-resistant metal alloy are stored within thick carbon-steel welded casks. As described above, a representative type of activated metal component is the KAPL core barrel/thermal shield. The KAPL CB/TS welded cask is illustrated in Figure 2. As seen in Figure 2, the robust design and construction of NR welded casks ensures they will remain structurally intact and support the overlying closure cap well past the end of the 1,000-year post-closure period.

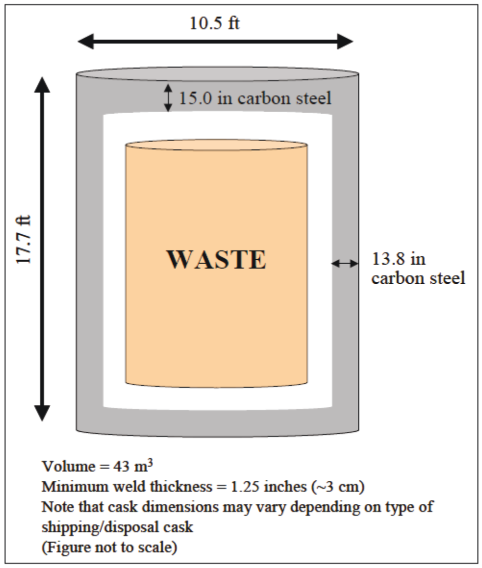


Figure 2. Schematic of KAPL CB/TS Welded Cask

Generally, carbon steel corrosion rates in air are at or below the low end of corrosion rates in soil for atmospheric conditions representative of SRS (Wohlwend and Butcher 2018). Therefore, assuming immediate NR waste burial under a soil cover (i.e., ignoring the open-air period) and initiating corrosion of the welded cask at the beginning of operations is conservative. Also, considering soil instead of CLSM as the interim cover material is conservative due to the impact of slightly acidic soil moisture on corrosion of carbon steel. Finally, corrosion from inside the cask to the outside is expected to be insignificant due to the negligible amount of water present in the casks before being welded shut. Taking these disposal conditions into consideration, corrosion is estimated to penetrate the welds after 750 years of disposal allowing water to enter the disposal casks via small holes in the welds (i.e., hydraulic failure).

A more detailed account of welded cask corrosion considerations in setting up the model is described in Wohlwend and Butcher (2018).

2.1.2 Activated Metal Components

Release of radionuclides from NR activated metal components depends on the corrosion rate of the specific metal alloy. According to Yu et al. (2002), the activated waste components in the KAPL CB/TS are made of either Inconel or Zircaloy, which are corrosion resistant metal alloys. Corrosion rates for these alloys are different. The corrosion rate for Inconel is conservatively estimated at 2.5 x 10^{-5} cm/yr, and for Zircaloy, 2.5 x 10^{-6} cm/yr. The corrosion rates are based on data from the Hanford site (Hanford 1993). Assuming that corrosion occurs on both sides of a metal plate, effective corrosion rates for Inconel and Zircaloy are estimated at 5 x 10^{-5} cm/yr and 5 x 10^{-6} cm/yr, respectively. Because of uncertainty in the composition of components and impacts of daughter ingrowth, a worst case rate of release from the waste form is to be derived from the following two cases: 1) all radionuclides reside within Inconel and therefore have a corrosion rate of 5×10^{-5} cm/yr; and 2) all radionuclides reside within Zircaloy and therefore have a corrosion rate of 5×10^{-6} cm/yr. Minimum disposal limits (or maximum dose impacts of closure inventory) selected from these two cases will make up a worst case set of inventory limits.

The total rate of release (combining Inconel and Zircaloy) of a given radionuclide from activated metal at time t (yrs) can be calculated from:

$$R_i(t) = I_{Ai}(t)(f_I \lambda_I + f_Z \lambda_Z)$$

where

$I_{Ai}(t)$:	Total activated metal inventory at time t for the i^{th} radionuclide (Ci)
f_I:	Fraction of I_A in Inconel
f_Z:	Fraction of I_A in Zircaloy (1-f_I)
C_I:	Corrosion rate for Inconel metal alloy (1/yr)
C_Z:	Corrosion rate for Zircaloy metal alloy (1/yr)
R_i:	Total release rate of species i (Ci/yr)

In the application of this equation for the NRCDA rate, we are employing the two endpoints (i.e., $f_I = 1$ or 0 and, conversely, $f_Z = 0$ or 1). The parameters in the release rate equation are given in Table 3 (Yu et al. 2002). Note that the above release rate equation does not directly account for the impact of daughter ingrowth for radionuclides within a decay chain. For parent nuclides with progeny the time dependent metal inventories are computed externally, and the metal releases rates associated with all short chain progeny are then provided as source terms to subsequent PORFLOW vadose zone transport runs. Further discussion on the rate of release from activated metal components is found in subsection 3.2.5.2.

NR programs has indicated only negligible amounts of water are present inside the typical KAPL CB/TS cask (Hsu 1997). Due to the construction of the thick carbon-steel casks with full-penetration weld closures, the PORFLOW model assumes no corrosion of the metal alloys occurs while the cask remains sealed. The alloy corrosion begins with hydraulic failure of welds on KAPL CB/TS cask, letting water into the casks. Therefore, radionuclides are only released from the activated metal after 750 years. The metal alloy corrosion completes in 16,079 years for Inconel and 104,349 years Zircaloy.

Table 3. Corrosion Rates of the Naval Reactor Waste Components

Metal Alloy	Corrosion Rate, λ (1/yr)
Inconel	6.2194E-05
Zircaloy	9.5832E-06

2.1.3 Bolted Container

Auxiliary equipment contaminated with ACP at low levels is stored within thinner-walled bolted containers. Because of the variety of bolted containers received from NR Programs, the large Shear Block disposal container (SBDC) was selected as the representative type of bolted container for the PORFLOW model (BMPC-KAPL 2009a and 2009b). Both large and small versions of SBDC's ($8ft^3$ and $4ft^3$ internal volume, respectively) are being shipped to E-Area by the Navy with approximate external dimensions shown in Figure 3. The SBDC was selected because it represents the largest category of bolted containers currently disposed or projected to be shipped to E-Area. Also, assuming this waste configuration conservatively concentrates the inventory from larger bolted containers into the smaller SBDC volume located closer to the water table.

Because of their robust design and generally dense payload (e.g., shear blocks, hold down barrels, closure heads, recirculating pumps, etc.) bolted containers are considered non-crushable during the 1,000-year period of performance. Dynamic compaction is prohibited from occurring over the two NRCDA's at final closure.

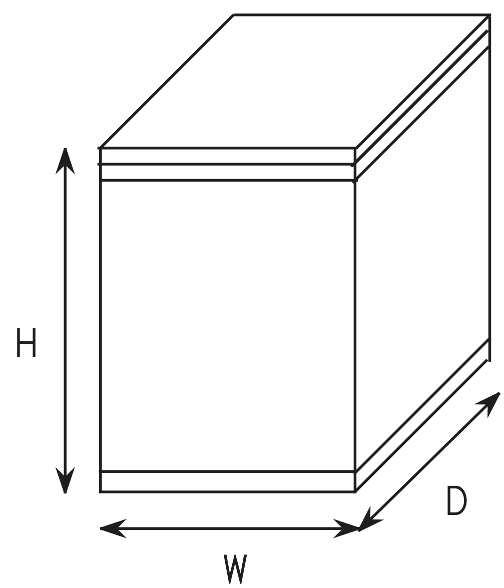
Lids for bolted containers are sealed by a gasket and bolted in place. Because of uncertainty in the long-term durability of gaskets in a disposal environment two cases are assumed to capture the range of potential behavior. These cases are described in the next section.

2.1.4 Activated Corrosion Products Contaminated Equipment

Gasketed containers are expected to deter water infiltration for a period of years. However, time to hydraulic failure of the bolted seal is uncertain. To account for this uncertainty, the proposed release model is to be based on two extreme cases:

- Assume all bolted containers hydraulically fail immediately when soil is initially mounded (or CLSM backfilled) around and over the containers on the pad at operational closure (early failure). At that time, ACP contamination is assumed to be instantaneously released into the surrounding soil.
- Assume bolted containers are not breached for 750 years, roughly coinciding with the failure of the more robust welded casks (late failure). Thus, SBDC inventories are retained and released at the start of KAPL CB/TS corrosion and radionuclide release allowing for some plume overlap to occur. Additionally, waiting 750 years allows time for daughter in-growth before release.

Case 1 represents the base-line scenario, while Case 2 provides a sensitivity analysis case for evaluation of the impact of ACP contaminant release timing. A worst case set of limits is established by selecting the minimum disposal limits (or maximum dose impacts of closure inventory) from these two cases.



	Large Container (1)	Small Container (2)
W	24”	19.5”
D	21”	19.5”
H	49”	35”

(1) BMPC-KAPL, 2009b; (2) BMPC-KAPL, 2009a

Figure 3. Schematic of a Bolted Container

2.2 NRCDA Timelines

Modeling timelines have been established corresponding with key facility events for the two disposal pads. The time window for meeting Groundwater Protection requirements (i.e., EPA Maximum Contaminant Levels) starts with placement of the first container on each pad and runs to the end of the 1,000-year DOE Order 435.1 post-closure period. The All-Pathways (AP) groundwater performance objective is evaluated from the end of the 100-year Institutional Control (IC) period through the end of the 1,000-year post-closure period. Modeling will be carried out at least 10,000 years past the End of Institutional Control (EIC) to capture groundwater peaks.

Modeling timelines for all E-Area DU's are calculated in relation to the start of E-Area LLWF operations in 1994. An important modeling assumption is that to be conservative each disposal pad receives its final inventory (i.e., inventory at closure) on the date that the first container is placed on each pad. For 643-7E, this date is estimated to be 1/1/1987 and for 643-26E is 9/28/1997. Thus, all subsequent events are assumed to involve the total ACP or activated metal inventory on the pad.

Groundwater modeling is started at the time when hydraulic failure of the container is assumed, and initial radionuclide release occurs. Hydraulic failures of bolted containers and welded casks will in fact be distributed over time. However, to simplify the analysis all casks and containers are conservatively assumed to fail simultaneously at the times discussed in Section 2.1. Likewise, release of radionuclides from hydraulically failed casks and containers is assumed to occur at the times discussed in this same section depending on whether activated metal or activated corrosion products are present. Radionuclide decay of waste and corrosion of the outer container are assumed to start from the date the pad receives waste.

These timelines of facility events and corresponding groundwater modeling assumptions are provided for 643-7E NRCDA in Table 4 and for the 643-26E NRCDA in Table 5. Facility and groundwater modeling events are given in calendar time that is then converted into absolute and relative modeling timelines.

Table 4. 643-7E NRCDA Timeline

Calendar Date	Absolute Date	Relative Time	Facility Event	Modeling Assumption
Past (certain or estimated) and future (predicted) dates of facility events relevant to GW modeling timeline.	Absolute time is calendar time converted to a numerical value.	Relative time based on years between event and start of E-Area LLWF operations in 1994.	Past (certain) and future (predicted) facility events relevant to GW modeling timeline. Red – pertaining to welded casks; Blue – pertaining to bolted containers; Black – pertaining to both	Time Windows: 1) GWP Limits based on peak release during single 1,186-year time window (i.e., Year -7.740 to 1,171). 2) AP Limits based on peak release during single 1,000-year time window (i.e., Year 171 to 1,171). Red – pertaining to welded casks; Blue – pertaining to bolted containers; Black – pertaining to both
1/1/1987	1987.003	-7.740	First container placed in 643-7E NR container storage area (NRCSA) NOTE: NRCSA subsequently repurposed as a disposal facility, NRCDA, on 6/29/2004 (Wilhite and Flach 2004). Disposal of the 41 casks and containers was assumed to retroactively start on date of first waste placement.	Assume all containers placed on pad for disposal at this time. Start of decay for inventory in all 41 containers stored on the 643-7E NRCSA. Start of corrosion of outer cask or container assuming a soil cover. Start of 1,186-year GWP compliance period. NOTE: No corrosion of activated metal components inside cask until hydraulic failure in 750 years (Cases 3 & 4). No release of radionuclides from bolted containers until placement of soil cover in 2005 (Case 1) or at time of welded cask hydraulic failure in 750 years (Case 2).
9/28/1994	1994.742	0.000	Start of E-Area LLWF Operations with first containers received in LAWV.	No 643-7E NRCDA modeling changes.
9/27/2005	2005.740	10.997	Soil mounded over 41 containers on 643-7E NRCDA. Case 1: Assumed early hydraulic failure of seals on all bolted containers (Base Case).	Case 1: Start of GW flow and transport simulation for bolted containers on 643-7E. Radio-nuclide inventory in bolted containers immediately released to surrounding soil (Base Case).
9/28/2065	2065.742	71.000	End of E-Area LLWF Operations and start of IC. No further interim closure actions planned for the 643-7E NRCDA.	No 643-7E NRCDA modeling changes.
9/28/2165	2165.742	171.000	EIC. Installation of final closure cap.	Start of 1,000-year AP compliance period.

Calendar Date	Absolute Date	Relative Time	Facility Event	Modeling Assumption
1/1/2737	2737.003	742.260	Case 2: Assumed late hydraulic failure of seals on all bolted containers (Sensitivity Case). Case 3 & 4: Hydraulic failure of welds on casks.	Start of GW flow and transport simulation for casks and bolted containers (Case 2) on 643-7E NRCDA. Case 2: Radionuclide inventory in bolted containers immediately released to the surrounding soil (Sensitivity Case). Cases 3 & 4: Start of corrosion-controlled release of radionuclides from welded casks.
9/28/3165	3165.742	1171.000		End of GWP and AP POP.
9/28/12165	12165.742	10171.000		End of GW model simulation except as needed to capture peaks.

Table 5. 643-26E NRCDA Timeline

Calendar Date	Absolute Date	Relative Time	Facility Event	Modeling Assumption
Past (certain or estimated) and future (predicted) dates of facility events relevant to GW modeling timeline.	Absolute time is calendar time converted to a numerical value.	Relative time is based on years between event and start of E-Area LLWF operations in 1994 (Year 0).	Past (certain) and future (predicted) facility events relevant to GW modeling timeline. Red – pertaining to welded casks; Blue – pertaining to bolted containers; Black – pertaining to both	Time Windows 1) GWP Limits based on peak release during single 1,168-year time window (i.e., Relative Years 3 to 1,171). 2) GW All-Pathways (AP) Limits based on peak release during single 1,000-year time window (i.e., Relative Years 171 to 1,171). Red – pertaining to welded casks; Blue – pertaining to bolted containers; Black – pertaining to both
9/28/1994	1994.742	0.000	Start of E-Area LLWF Operations with first containers received in LAWV.	
9/28/1997	1997.742	3.000	First container placed on 643-26E NRCDA	Assume all containers placed on pad at this time. Start of decay for all projected inventory to be disposed in 643-26E NRCDA. Start of corrosion of outer cask or container assuming a soil cover. Start of 1,168-year GWP compliance period. NOTE: No corrosion of activated metal components inside cask and no release of radionuclides from welded casks until hydraulic failure of in 750 years (Cases 3 & 4). No release of radionuclides from bolted containers until placement of soil cover in 2065 (Case 1) or at time of welded cask hydraulic failure 750 years post disposal (Case 2).
9/28/2065	2065.742	71.000	End of E-Area LLWF Operations with no further containers placed on pad. Start of IC. Soil mounded over all containers on 643-26E NRCDA. Case 1: Assumed early hydraulic failure of bolted seals on all SBDC's (Base Case).	Case 1: Start of GW flow and transport simulation for bolted containers in the 643-26E NRCDA. Radionuclide inventory in bolted containers immediately released to surrounding soil (Base Case).
9/28/2165	2165.742	171.000	EIC. Installation of final closure cap.	Start of 1,000-year AP compliance period.

Calendar Date	Absolute Date	Relative Time	Facility Event	Modeling Assumption
9/28/2747	2747.742	753.000	Case 2: Assumed late hydraulic failure of seals on all bolted containers (Sensitivity Case). Cases 3 & 4: Predicted hydraulic failure of welds on KAPL CB/TS cask.	Start of GW flow and transport simulation for casks and bolted containers (Case 2) in the 643-26E NRCDA. Cases 3 & 4: Initial corrosion-controlled release of radionuclide inventory from activated metal components to the surrounding soil.
9/28/3165	3165.742	1171.000		End of GWP and AP POP.
9/28/12165	12165.742	10171.000		End of GW model simulation except as needed to capture peaks.

2.3 Stratigraphic Surfaces beneath E Area Low Level Waste Facility

Beneath E Area, the relationship between the water table and various stratigraphic units is locally complex and is affected by sediment properties (hydraulic conductivity), by seasonal and long-term precipitation (recharge), and by proximity to Upper Three Runs to the north of the model area. Figure 4, reproduced from Bagwell and Bennett's report (Bagwell and Bennet 2017), shows this complexity as illustrated by the multiple hydrostratigraphic units beneath E-Area. Bagwell and Bennett (2017) provide elevations for all identified subsurface units beneath the corner coordinates of each E-Area DU footprint, from which the average distance above the water table for each hydrostratigraphic surface is derived and shown in Table 6. Note that for the 643-7E NRCDA the water table is above the Tan Clay Confining Zone (TCCZ) while for 643-26E the water table dips below it and therefore the distance is shown as zero.

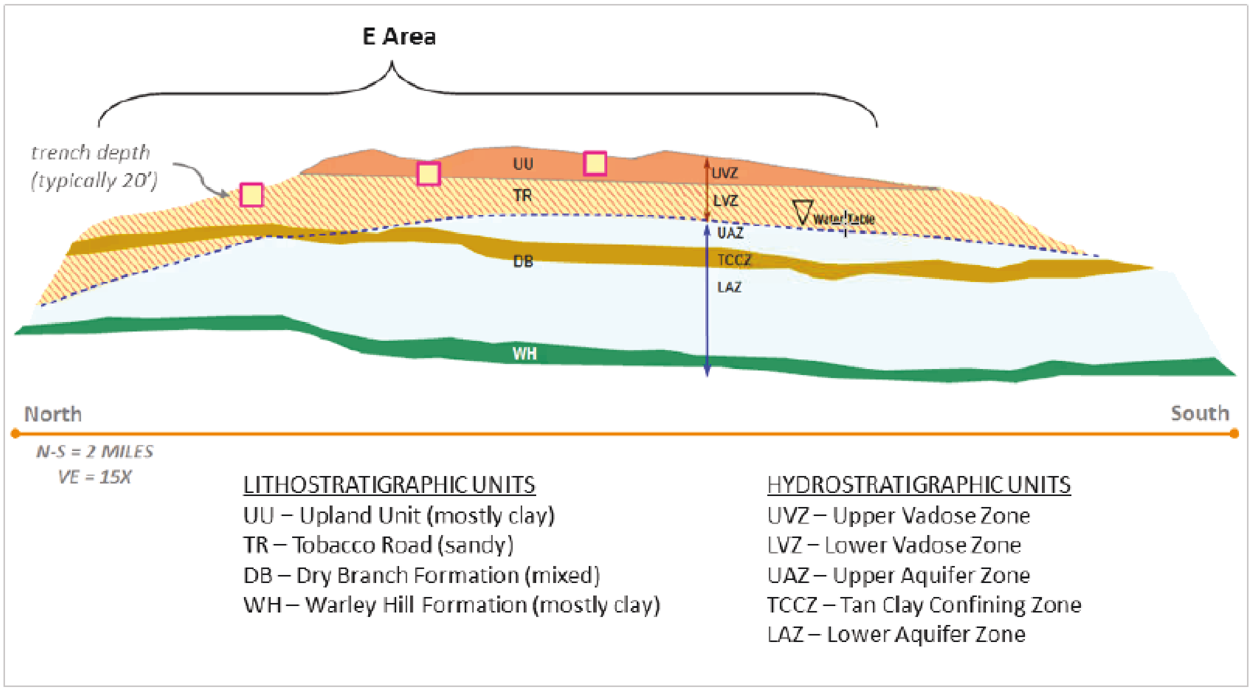


Figure 4. E Area Schematic Cross-Section showing Underlying Stratigraphic Subsurfaces

Table 6. Average Distances with respect to the WT for Subsurface Layers

	643-7E	**643-26E**
Average Depth to WT from original ground surface	63 ft	75 ft
Top of Subsurface Zones (Material Type) – Height above WT		
UVZ (UVZ)	63 ft	75 ft
LVZ (LVZ)	27 ft	57 ft
TCCZ (UVZ)	0	18 ft
LAZ (LVZ)	0	10 ft

3.0 Implementation of the Modeling

Using PORFLOW Version 6.42.9 (ACRi 2018), the 3D vadose zone flow and transport models based on the proposed NRCDA Groundwater Pathway conceptual model (Wohlwend and Butcher 2018) have been developed for use in the next PA as described below. 3D models were chosen to better accommodate the unique features of the infiltration barriers placed above these facilities.

3.1 Source Term

The above-grade NRCDA's will be covered with soil or backfilled with CLSM prior to installation of the final closure cap. Release of radionuclides from the waste zone results from hydraulic failure of containers and casks followed by instantaneous release of activated corrosion products and corrosion-controlled release from activated metal components. Radionuclides are transported by diffusion and convection processes through the vadose zone. In this work, the source term analysis focuses on the mechanisms of release of radionuclides in the vadose zone, to ultimately predict the flux at the water table for specific radionuclides of interest.

3.2 Groundwater PORFLOW Models

3.2.1 643-7E and 643-26E Footprint

The footprint coordinates for both NRCDA pads are provided by Hamm (2019). Figure 5 and Figure 6 display actual layout (solid black outline) and equivalent footprints (red dashed outline) modeled for 643-7E and 643-26E, respectively. NRCDA footprints are reconfigured as a square form with an equivalent footprint area for simplification of modeling. Note that both actual and equivalent footprints have the same center (footprint centroid).

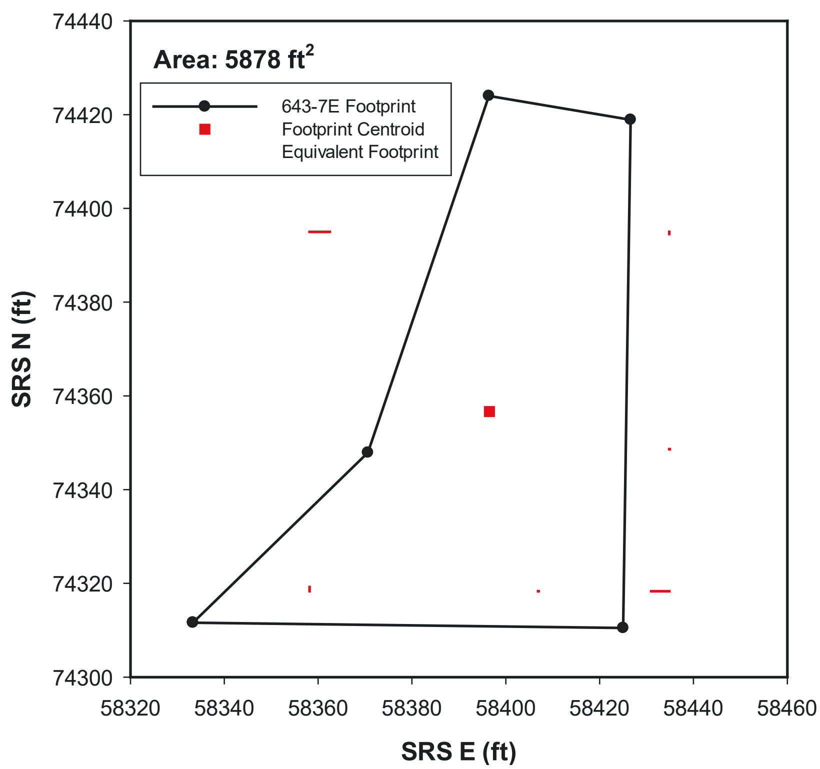


Figure 5. Footprint of NRCDA 643-7E

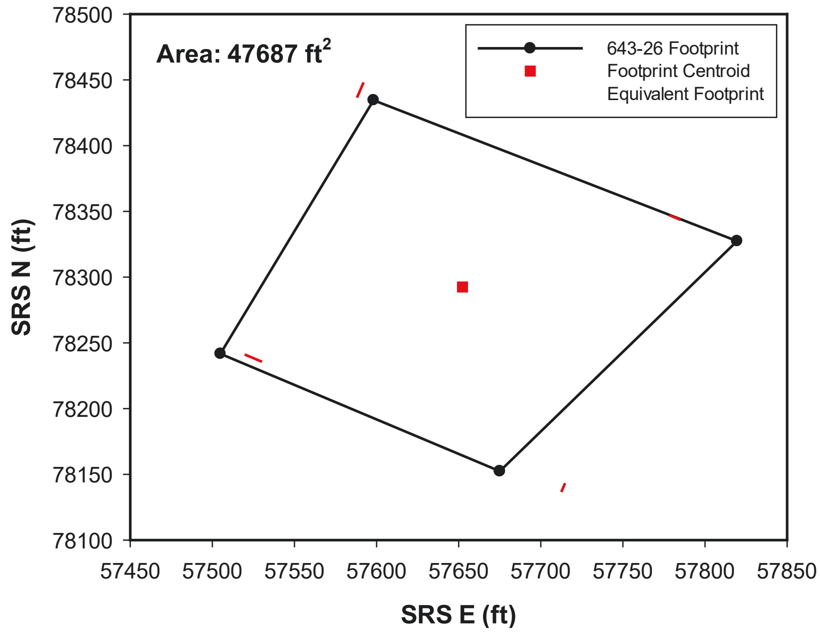


Figure 6. Footprint of NRCDA 643-26E

3.2.2 Model Domain Dimensions

Because of the different subsurface features and geometry, and disposal pad size described in Sections 2.3 and 3.2.1, respectively, NRCDA 643-7E and 643-26E require unique PORFLOW vadose zone flow and transport models. Due to their locations in E-Area relative to other DU's, different final closure cap configurations are applicable to the two NRCDAs. The 643-7E NRCDA is somewhat isolated from the other E-Area LLWF DU's (see Figure 1). At the end of the IC period, a final closure cap will be placed over 643-7E extending 40ft beyond the edge of the disposal pad on all sides. Beyond that is undisturbed soil out to the edge of the model domain. On the other hand, 643-26E is surrounded by other DU's (i.e., ET03, ET04, ST08) and can be represented in the model by an essentially infinite cap that runs to the edge of the model domain. Schematics for the 643-7E and 643-26E conceptual models are shown in Figure 7 and Figure 8, respectively. Note that the NRCDA vadose-zone models are 3D. Hence, the dimensions are the same in x- and y-directions.

Table 7 summarizes the relevant dimensions of the vadose zone conceptual models for both NRCDAs. In Figure 7 and Figure 8, the height of the KAPL CB/TS welded cask (18 ft high) and the double-stacked large SBDC bolted containers (8.2 ft high) are used to represent the waste zone thickness of the activated metal component waste fraction and ACP equipment waste fraction, respectively. Each waste form is modeled separately, and results are subsequently combined in the flux to the water table for aquifer PORFLOW analyses (scope beyond this effort). Additional modeling geometries may be evaluated as potential sensitivity cases based on other stacking scenarios for SBDC's and partial filling of the disposal pad footprint.

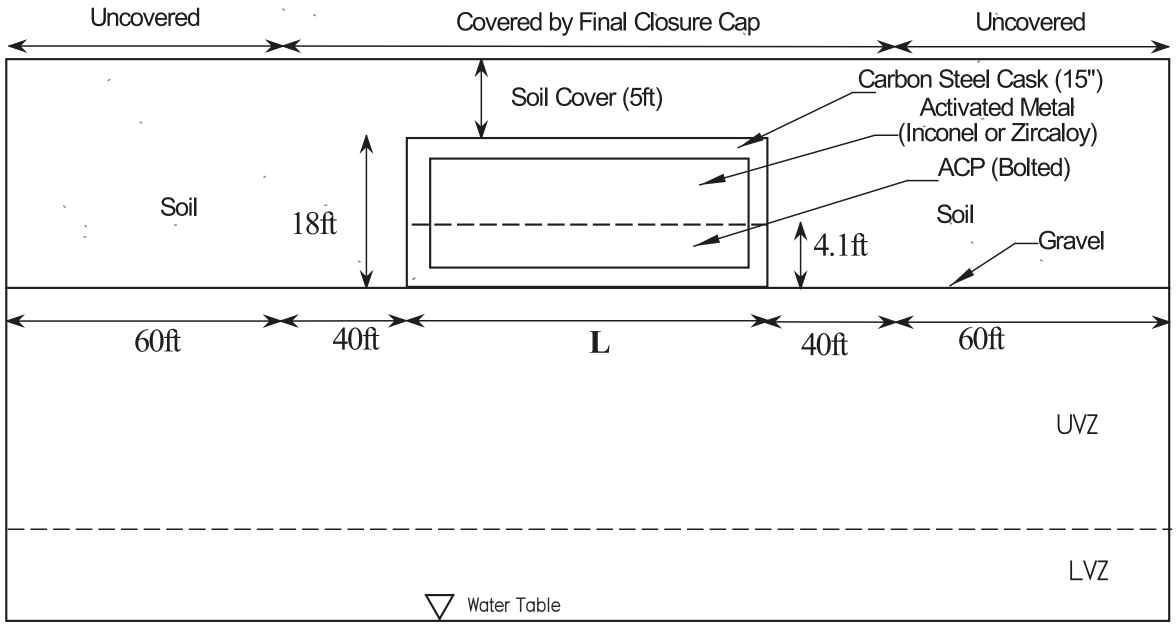


Figure 7. Schematic of NRCDA Vadose Zone Conceptual Model for 643-7E (Not Scaled)

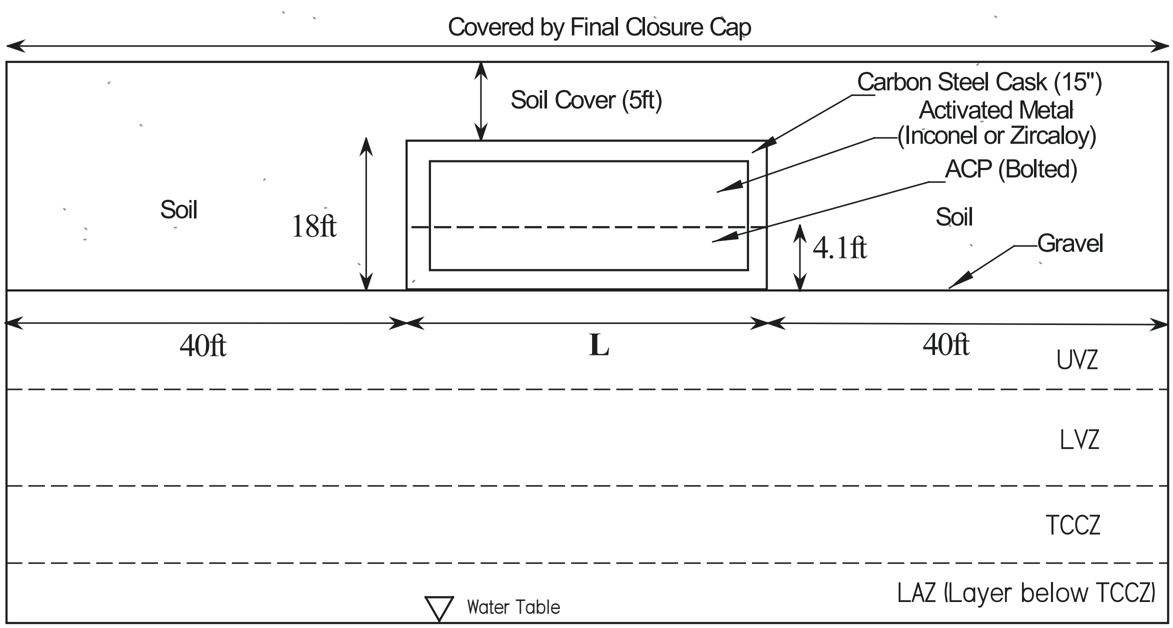


Figure 8. Schematic of NRCDA Vadose Zone Conceptual Model for 643-26E (Not Scaled)

Table 7. NRCDA Model Dimensions

	643-26E	643-7E
Footprint Area [1]	4430 m^2 (47687 ft^2)	546 m^2 (5878 ft^2)
Length L	66.6 m (218.375 ft)	23.37 m (76.67 ft)
Average Depth to WT [2]	75 ft	63 ft
Top of Subsurface Zones (Material) – Height above WT		
UVZ (UVZ)	75 ft	63 ft
LVZ (LVZ)	57 ft	27 ft
TCCZ (UVZ)	18 ft	0
LAZ (LVZ)	10 ft	0

(1) Hamm (2019); (2) Bagwell and Bennett (2017)

3.2.3 Hydraulic Properties

Hydraulic properties for each material type and corresponding material zones used in the PORFLOW models are given in Table 8 (Nichols and Butcher 2020).

Table 8. Hydraulic Properties.

Type	Zones	Density (g/ml)	Porosity	Diffusivity (cm^2/yr)	K_h (cm/yr)	K_v (cm/yr)
UVZ	UVZ, TCCZ	2.69	0.385	167.26	1956.57	274.55
LVZ	LVZ, LAZ	2.67	0.380	167.26	10414.01	2871.74
OSC1 [1]	BACKFILL	2.65	0.456	167.26	4102.49	4102.49
ETboxesBefore [2]	WASTE	2.65	0.893	167.26	788.94	788.94

(1) OSC1 – Operational soil cover before dynamic compaction
(2) ETboxesBefore – Engineered Trench containerized waste zone before dynamic compaction

3.2.4 Boundary Conditions and Infiltration Rates

The bottom of the final closure cap forms the top boundary of the PORFLOW VZ model. Infiltration through the closure cap is calculated separately and provided as input to the PORFLOW model (Dyer 2019). The initial infiltration rate for the intact closure cap case changes as the closure cap slowly degrades over time. The intact closure cap case is distinguished from subsided closure cap cases where localized catastrophic failures are assumed to occur with the structural collapse of containers. Due to the robust nature of NR container and cask designs, and density of the internal component/equipment they contain, significant subsidence is not considered feasible for the NRCDA's. Intact case infiltration rates for the 643-26E NRCDA over the 10,000-year post-closure modeling timeframe (plus 100-year IC period) are shown in Table 9 (Dyer 2019). These infiltration estimates for the final closure cap at a slope of 2% are applied to the top boundary of the PORFLOW model domain. Infiltration rates beyond this 10,100 yr period are set to the last value shown in Table 9.

Table 9. Intact Case Infiltration Rates

Relative Years	Intact Infiltration Rate (in/yr) [(1)]
0	0.1
100	0.0008
180	0.007
290	0.16
300	0.18
340	0.3
380	0.38
480	1.39
660	3.23
1100	6.82
1900	10.24
2723	11.10
3300	11.18
5700	11.30
10100	11.35

[(1)] Dyer (2019)
Year 0: Beginning of IC period. Interim runoff cover is installed and maintained for next 100 years.
Year 100: End of IC period; installation of final closure cap.

For 643-7E, the covered part of the top boundary (i.e., the closure cap and its extension to 40ft beyond the edge of the pad) assumes the intact case infiltration rates, while the nominal infiltration rate of 15.78 in/yr (40cm/yr) applies to the uncovered part (beyond 40ft cap extension).

3.2.5 NRCDA Modeling Approach

As first described in Section 1.0, the proposed conceptual model (Wohlwend and Butcher 2018) recommends the following to be implemented in the upcoming PA:

1. Model each NRCDA in the same manner as other E-Area LLWF disposal units [i.e., one gram-mole (gmole) inventories are scaled up to disposal limits based on Performance Objectives (PO)].
2. Entire waste is placed within disposal units at the time of first burial.
3. Bolted containers: Generic waste form is used. Perform calculations for two cases from which minimum disposal limits will be selected:
   - Case 1: Immediate release of radionuclides from the containers at SIC
   - Case 2: Release of radionuclides at 750 year corresponding with hydraulic failure of welded casks
4. Welded steel casks: Special waste form is considered. Perform calculations for two cases from which the minimum disposal limits will be selected:
   - Case 3: All radionuclides reside within Inconel with hydraulic failure at 750 yrs
   - Case 4: All radionuclides reside within Zircaloy with hydraulic failure at 750 yrs
5. Combined flux at the water table: The total flux for each radionuclide at the water table is a combination of the fluxes resulting from NR components in welded casks and ACP contaminated equipment in bolted containers based on corresponding inventory ratios.

3.2.5.1 Rate of Release of Generic Waste

For generic waste it is assumed that radioactive material contained within the Waste Zone is instantaneously available to be transported (i.e., no rate-limiting mechanism is accounted for). This point in time can be at any chosen point. In the cases listed in Table 1 the time of release for generic waste is:

- Start of institutional control or application of a soil cover; and
- 750 years after burial of the waste.

Once these points in time are reached the waste is assumed to be completely available for local interaction with the porous media and subsequent transport.

In PORFLOW transport simulations a generic waste is handled by setting a specified inventory uniformly distributed throughout the Waste Zone. Generally, one gmole of the parent nuclide of interest is placed within the Waste Zone. This inventory placement is made at the time of first burial and the material is assumed to be available for transport once hydraulically failure occurs.

3.2.5.2 Rate of Release of Special Waste

For special waste forms, a rate limiting mechanism and/or a delayed release (hold up) is taken into account. For the Inconel and Zircaloy reactor components the radioactive constituents are embedded throughout the metal material. For actual physical release and transport to occur, the surface material must first corrode away. Thus, for this special waste form we are assuming a corrosion-based rate limited process that proceeds from the surface to the interior of the component. The distribution throughout the metal component is assumed to be uniform where a constant peaking factor was applied to conservatively account for the spatially varying neutron flux field during reactor operations. The release rate from one of these metals (here either Inconel or Zircaloy) is the product of a corrosion rate time and inventory.

The overall release rate for any radionuclide from activated metal stored in a welded steel cask is given in Section 2.1.2. This special waste form (i.e., a corrosion-limited release mechanism) is handled within PORFLOW by use of source term tables entered through “INCLude” files for each species within the short chain. By combining the rate equation and the parameters listed in Table 3, the individual release rates for activated waste Inconel and Zircaloy components are derived as follows.

For Inconel activated metal:

$$R_i(t) = 6.2194x10^{-5} I_{Inconel,i}(t)$$

$I_{Inconel,i}(t)$: Total inventory of the radionuclide in activated metal Inconel

For Zircaloy activated metal:

$$R_i(t) = 9.5832x10^{-6} I_{Zircaloy,i}(t)$$

$I_{Zircaloy,i}(t)$: Total inventory of the radionuclide in activated metal Zircaloy

Note that these rate equations do include the radioactive decay of each member in the short chain (i.e., $I_i(t)$) that are computed external to the PORFLOW analysis and then brought into the analysis by way of timetables through INCLude files. As an example of these source term files, the following was extracted from the Pu-239 input deck:

```
/Inventory
! Source terms in units of gmole/yr
INCLude "Flx-Corrosion-gmole-Pu-239.dat"
INCLude "Flx-Corrosion-gmole-U-235.dat"
INCLude "Flx-Corrosion-gmole-Pa-231.dat"
```

The computed metal corrosion rates are in units of gmole/yr per gmole of parent buried. Radioactive decay (and ingrowth of progeny) begins at the time of burial, while actual corrosion does not start until hydraulic failure (i.e., leaking) of the casks is assumed (i.e., 750 yrs after burial). The release of material continues until the entire buried material has corroded away. Corrosion is assumed to be very limited while the casks are hydraulically isolated from the local environment since limited amounts of reactants exist within the casks upon their closure. Based on their corrosion rates and average component thicknesses the following corrosion time periods are considered for complete corrosion:

- for Inconel – 16,079 yrs; and
- for Zircaloy – 104,349 yrs.

An example of the source term from corrosion of Inconel is provided in Figure 9 and Figure 10 which shows the release rate over time for Pu-239 and its daughters U-235, Pa-231 and Ac-227. Note that a one gmole of Pu-239 inventory was assumed at time of burial (i.e., none of its decay daughter present initially). Also, the corrosion rate is assumed to be zero for 750 yr after burial, corrodes at a constant material rate for 16,079 yrs, and then returns to zero beyond that time (i.e., no remaining Inconel material left). As Figure 9 illustrates, the source term for Pu-239 continually declines during this period due to its decay, while U-235 builds in as it's a direct daughter of Pu-239 and has a very long half-life. Similar curves for Pa-231 and Ac-227 are provided separately in Figure 10 which show their flux values are significantly lower (i.e., shown in a semi-log plot).

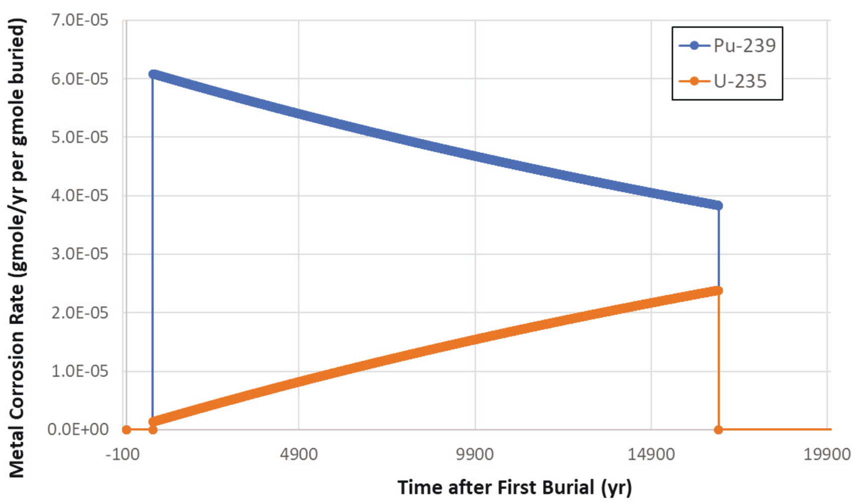


Figure 9. Metal corrosion rate release from Inconel for Pu-239 and its daughter U-235.

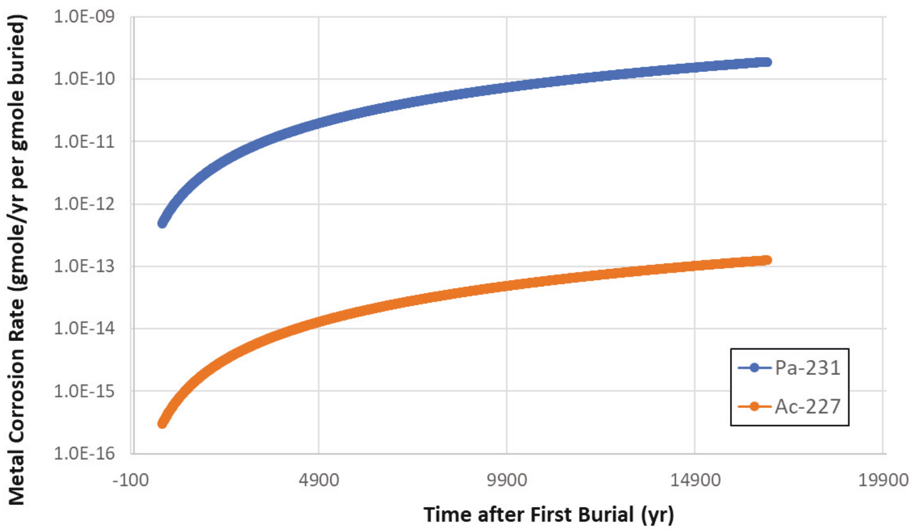


Figure 10. Metal corrosion rate release from Inconel for Pu-239's daughters Pa-231 and Ac-227.

Source term files, similar to these, for every parent (and its progeny) for both Inconel and Zircaloy have been created. Since the corrosion rates and release rates are independent of waste zone properties, these source term files can be computed externally and then employed within subsequent PORFLOW transport runs.

Source term files, similar to these, for every parent (and its progeny) for both Inconel and Zircaloy have been created. Since the corrosion rates and release rates are independent of waste zone properties, these source term files can be computed externally and then employed within subsequent PORFLOW transport runs.

3.2.5.3 Modeling the Generic and Special Waste Form

For simplification, the NRCDA waste zone composed of bolted containers (generic waste form) and welded casks (special waste form) is assigned the same material properties as the Engineered Trench waste zone before dynamic compaction (i.e., "ETboxesBefore") (see Table 8). Because the release of inventory for both the generic and the special waste forms is zero prior to them being available for transport, the transport properties for both waste forms (i.e., Waste Zones) can be set at the start of the PORFLOW transport run and remain unchanged throughout the simulation. ETboxesBefore is a blended set of properties made up of 20% by volume OSC1 (i.e., operational soil cover before dynamic compaction) and 80% by volume containers (i.e., impermeable objects without any chemical absorption properties). A complete input deck listing of the PORFLOW vadose zone transport model of Pu-238 for the Inconel activated metal/welded casks in NRCDA 643-7E is shown in Appendix A.

4.0 Model Results

The following cases were evaluated for both 643-7E and 643-26E (see Table 1):

- ACP (generic waste form) stored in bolted containers that hydraulically fail upon installation of the interim soil cover (Case 1).
- Activated Inconel metal (special waste form) contained in welded carbon-steel casks that hydraulically fail 750 years following placement on the disposal pad (Case 3).

For demonstration purposes, the following radionuclides are selected: C-14, I-129, Nb-94, Ni-59, Pu-239 and Tc-99 (see Table 2). Radionuclide decay properties for these radionuclides along with their corresponding elemental chemical sorption properties assigned to each layer in the model are shown in Table 10.

Table 10. Radionuclide and Chemical Properties.

Parent Nuclide	Progeny Nuclide	Half-Life (yr)	K_d (ml/g)		
			LAZ/LVZ	TCCZ/UVZ	BACKFILL/WASTE
C-14		5.7000E+03	1	30	30
I-129		1.5700E+07	1	3	3
Nb-94		2.0300E+04	1000	1000	1000
Ni-59		7.6000E+04	7	30	30
Pu-239		2.4110E+04	650	6000	6000
	U-235	7.0400E+08	300	400	400
	Pa-231	3.2760E+04	3	9	9
	Ac-227	2.1772E+01	1100	8500	8500
Tc-99		2.1110E+05	0.6	1.8	1.8

I-129 and Tc-99 have low K_d values (i.e., 3 and 1.8, respectively) in the waste zone, resulting in an early appearance of its peak flux at the water table. C-14 and Ni-59 have moderate K_d values (i.e., 30). Pu-239 generates U-239, Pa-231, and Ac-227 as daughter products. Both Nb-94 and Pu-239 have large K_d values (i.e., 1000 and 6000, respectively), causing delay of their peak flux at the water table. The model results are shown below in Figure 11 to Figure 14. Figure 11 and Figure 12 display the results for 643-7E containers and casks, respectively. Figure 13 and Figure 14 show the results for 643-26E containers and casks, respectively. In Figure 12 and Figure 14, the results show a steep decline in the flux values for nuclides with low and moderate K_d due to completion of radionuclide inventory release from the metal alloy (i.e., end of metal corrosion). Note that PORFLOW runs are generally made based on one gmole of parent being buried. However, fluxes to the water table, as shown in Figure 11 through Figure 14 are presented in units of Ci/yr per Ci of parent being buried.

As can be seen in Figure 11 through Figure 14, fluxes to the water table peak at times beyond ~1,000 years. Tc-99 is the most mobile of the list of parent nuclides considered and shows peaks around 1,000 years. This is a direct result of the effect of the final cover on retarded phasic velocities during the first ~1,000 years. The fluxes to the water table results provided in Figure 12 (Case 3) and in Figure 13 (Case 1) were then calibrated to 1D GoldSim models using the final set of PORFLOW transport model runs and are described separately in Smith (2020).

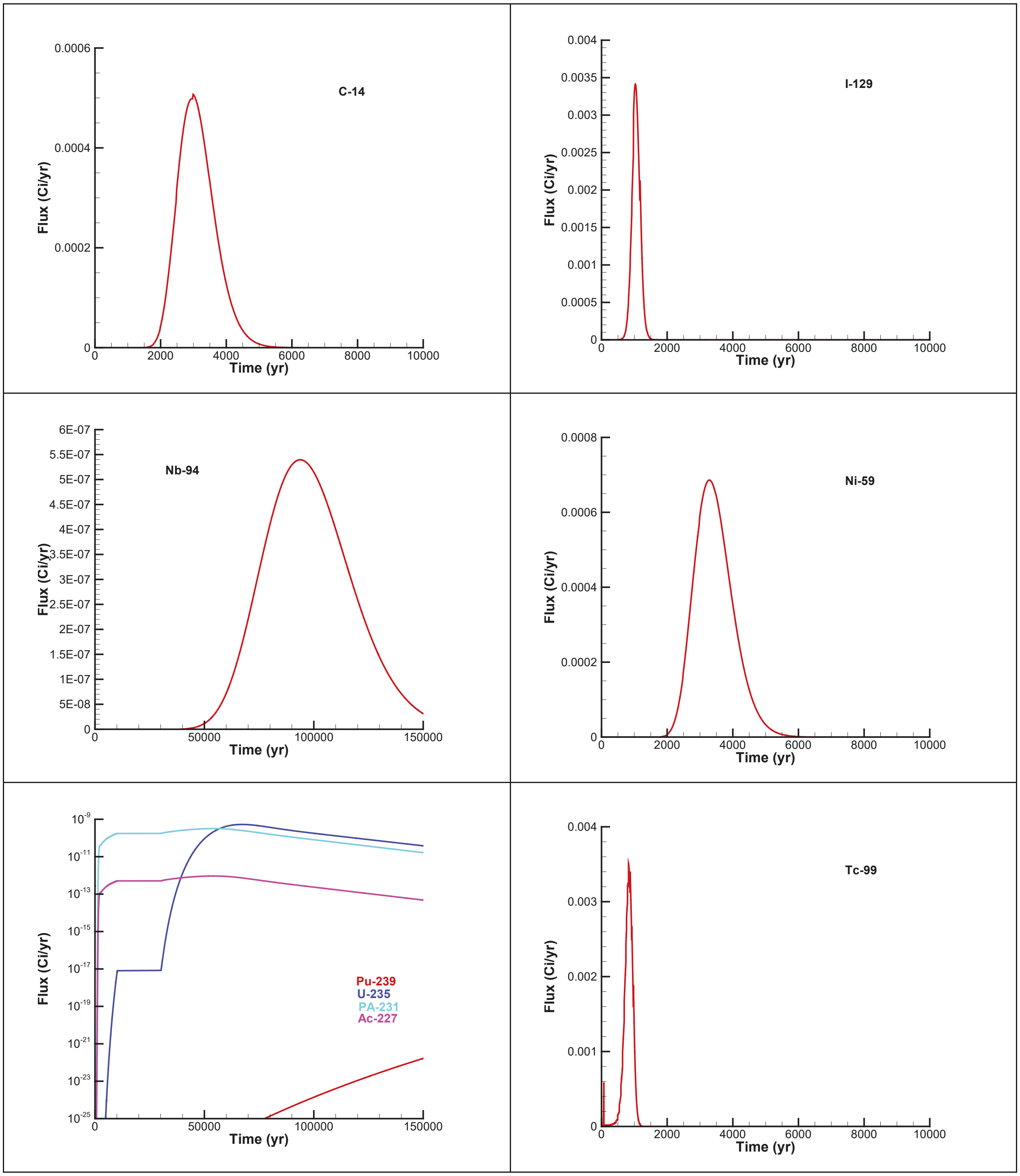


Figure 11. Flux at WT (643-7E, Generic Waste Form, Bolted Containers, Case 1).

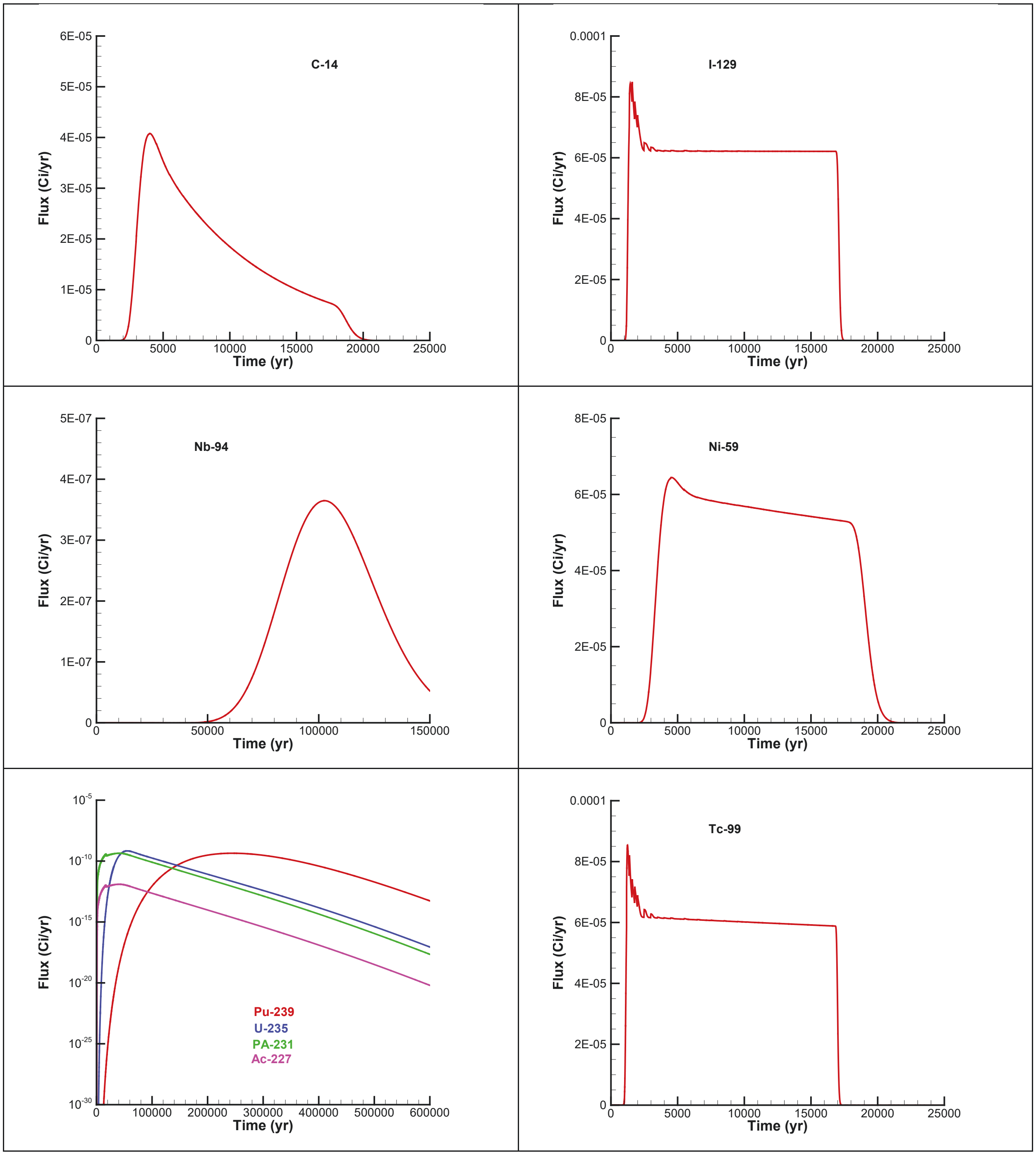


Figure 12. Flux at WT (643-7E, Special Waste Form, Activated Inconel, Welded Casks, Case 3).

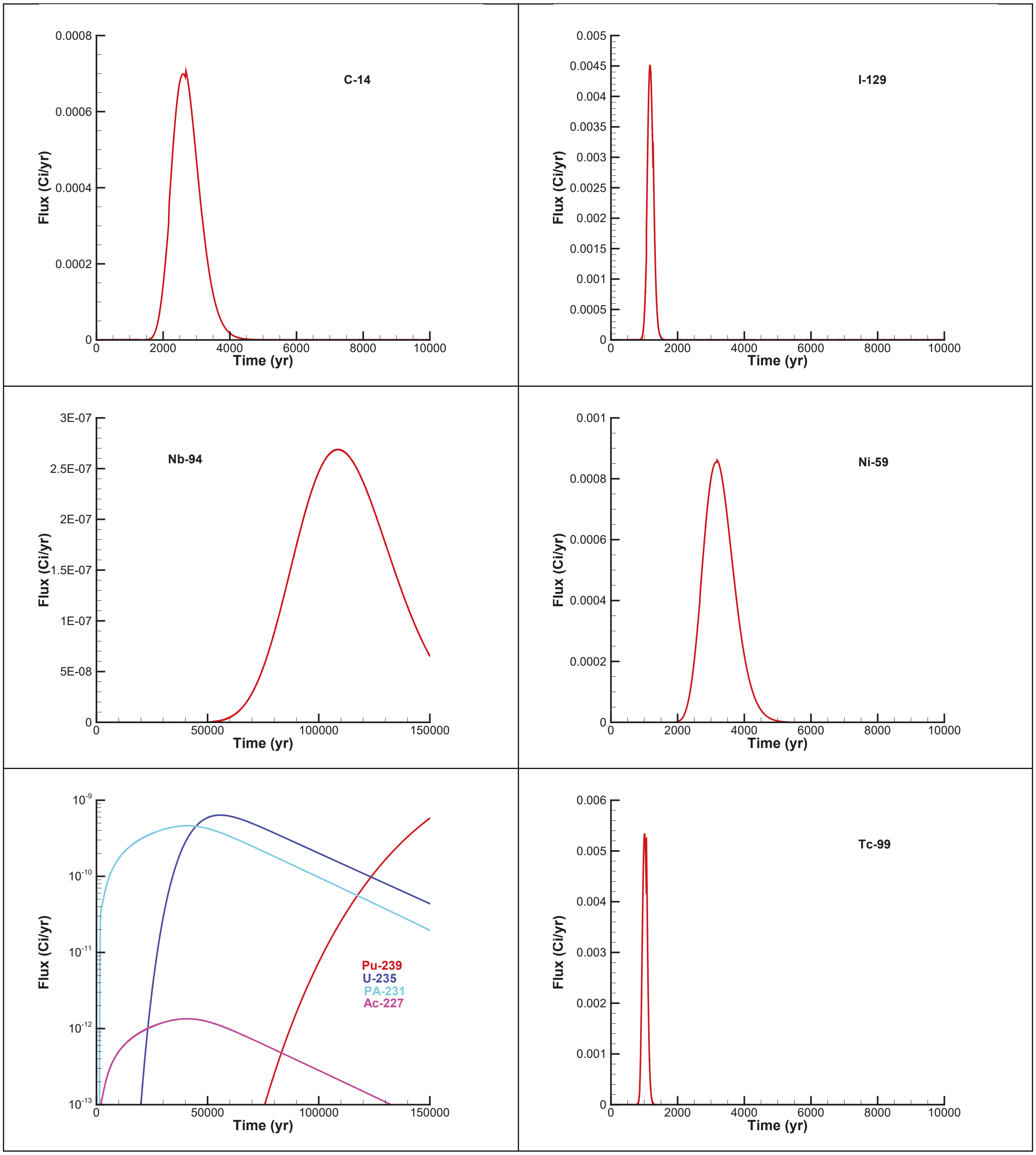


Figure 13. Flux at WT (643-26E, Generic Waste Form, Bolted Containers, Case 1).

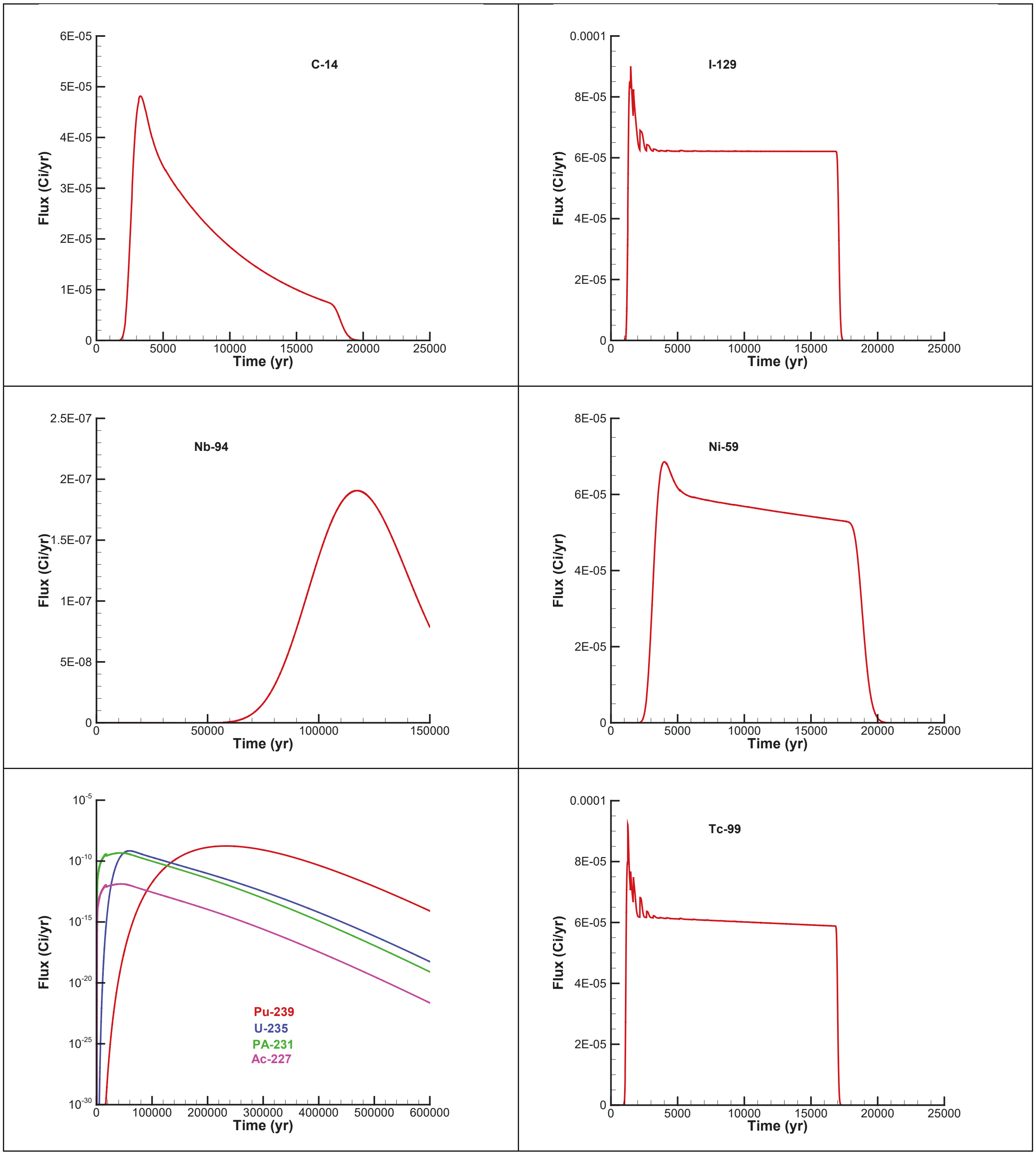


Figure 14. Flux at WT (643-26E, Special Waste Form, Activated Inconel, Welded Casks, Case 3).

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Appendix A. PORFLOW Input File for Vadose Zone Pu-239 Transport Modeling

Below is an example of a PORFLOW input deck. The example chosen is for the Inconel Welded Cask (i.e., Case 3) within 643-7E for the Pu-239 chain:

Pu-239 → U-235 → Pa-231 → Ac-227

The corrosion-based source terms are computed externally to PORFLOW and are brought into the PORFLOW run by way of included files (i.e., in a tabular form within individual ASCI files for each member of the short chain).

Note that the following external input files are inserted into this input deck upon execution of PORFLOW:

- MESH.dat – 3D mesh definition
- LOCA.dat – material zone definitions
- Flx-Corrosion-gmole-Pu-239.dat – Pu-238 Inconel source term (gmole/yr)
- Flx-Corrosion-gmole-U-235.dat – U-235 Inconel source term (gmole/yr)
- Flx-Corrosion-gmole-Pa-231.dat – Pa-231 Inconel source term (gmole/yr)
- Flx-Corrosion-gmole-Ac-227.dat – Ac-227 Inconel source term (gmole/yr)

Pu-239 Case 3 PORFLOW input deck for 643-7E

```
/ Main input file
TITLe 3D VADOSE ZONE TRANSPORT MODEL, Case01, 7E_InconelCask, Pu-239 (manual sourceterms)
!
/ Allocate space for user-defined variables as needed
ALLOcate space for 1000000 words in user input TABLes
!              C   !Pu-239 (in fluid)
ALLOCATE       C2  !U-235  (in fluid)
ALLOCATE       C3  !Pa-231 (in fluid)
ALLOCATE       C4  !Ac-227 (in fluid)
!
/ Finite-element mesh
INCLude '../../../Common/MESH.dat'
!
/Material Types and Boundary Conditions
INCLude "../../../Common/LOCA.dat"
!
/ Material and nuclide properties
!see transient specification before each SOLVe
PROPerty for C C2 C3 C4 is HARMonic
PROPerty for C C2 C3 C4 is TOTAl
!
/ Nuclide properties
!(in fluid)
DECAy half LIFE for C   is 2.4110E+04 years ! Pu-239
DECAy half LIFE for C2  is 7.0400E+08 years ! U-235
DECAy half LIFE for C3  is 3.2760E+04 years ! Pa-231
DECAy half LIFE for C4  is 2.1772E+01 years ! Ac-227
REGEneration of C2  from C   is 1.00000E+00 ! U-235   from Pu-239
REGEneration of C3  from C2  is 1.00000E+00 ! Pa-231  from U-235
REGEneration of C4  from C3  is 1.00000E+00 ! Ac-227  from Pa-231
!
/ Boundary conditions
BOUN C  X- FLUX = 0
BOUN C2 X- FLUX = 0
BOUN C3 X- FLUX = 0
BOUN C4 X- FLUX = 0

BOUN C  X+ FLUX = 0
BOUN C2 X+ FLUX = 0
BOUN C3 X+ FLUX = 0
BOUN C4 X+ FLUX = 0
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BOUN C  Y- FLUX = 0
BOUN C2 Y- FLUX = 0
BOUN C3 Y- FLUX = 0
BOUN C4 Y- FLUX = 0

BOUN C  Y+ FLUX = 0
BOUN C2 Y+ FLUX = 0
BOUN C3 Y+ FLUX = 0
BOUN C4 Y+ FLUX = 0

BOUN C  Z- FLOW = 0
BOUN C2 Z- FLOW = 0
BOUN C3 Z- FLOW = 0
BOUN C4 Z- FLOW = 0

BOUN C  Z+ FLUX = 0
BOUN C2 Z+ FLUX = 0
BOUN C3 Z+ FLUX = 0
BOUN C4 Z+ FLUX = 0
!
/ Diagnostic information
DIAGnostic output: TIME  C C2 C3 C4 for node (36,36,36) every 100 steps
!
HISTory of STORage for C  in ID=WASTE to "C_STOR.out"
HISTory of STORAGE for C2 in ID=WASTE to "C2_STOR.out"
HISTory of STORAGE for C3 in ID=WASTE to "C3_STOR.out"
HISTory of STORAGE for C4 in ID=WASTE to "C4_STOR.out"
!
HISTory of SOURce  for C  in ID=WASTE to "C_SOUR.out"
HISTory of SOURce  for C2 in ID=WASTE to "C2_SOUR.out"
HISTory of SOURce  for C3 in ID=WASTE to "C3_SOUR.out"
HISTory of SOURce  for C4 in ID=WASTE to "C4_SOUR.out"
!
/ Flux output
FLUX C C2 C3 C4 for ID=DOMAIN by TIME every 1 years to "FLUX.out"
SAVE C C2 C3 C4 for ID=INSIDE to "C.sav"  at TIME interval of 50 years
!
/ Solution controls
/ Don't use MATRix LUDE for large problem > 20000 elements
MATRix in X and Y and Z for C  in 3 sweeps using ADI
MATRix in X and Y and Z for C2 in 3 sweeps using ADI
MATRix in X and Y and Z for C3 in 3 sweeps using ADI
MATRix in X and Y and Z for C4 in 3 sweeps using ADI
CONVergence for C  REFE GLOBal 1.e-9, max iterations = 10
CONVergence for C2 REFE GLOBal 1.e-9, max iterations = 10
CONVergence for C3 REFE GLOBal 1.e-9, max iterations = 10
CONVergence for C4 REFE GLOBal 1.e-9, max iterations = 10
LIMIt for C  0.0
LIMIt for C2 0.0
LIMIt for C3 0.0
LIMIt for C4 0.0
!
/ No flow calculation
DISAble FLOW
!
/ Solve transient transport; save fluxes and concentrations
CPU 4
!
/ Turn off output of material type index
OUTPut OFF
!
!                                                           TI01    -8.0 to 0.0 yrs
/Inventory
! Source terms in units of gmole/yr
INCLude "Flx-Corrosion-gmole-Pu-239.dat"
INCLude "Flx-Corrosion-gmole-U-235.dat"
INCLude "Flx-Corrosion-gmole-Pa-231.dat"
INCLude "Flx-Corrosion-gmole-Ac-227.dat"
!
!                                                                   LVZ
DENSity SOLId  ID=LVZ DENSity  2.67                 !LowerVadoseZone  rock grain density (g/cm^3)
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POROsity    ID=LVZ 0.38                                        !LowerVadoseZone   rock grain density
(g/cm^3)
TRANsport ID=LVZ for C  Kd=650.0  De=167.25528 aL=0 aT=0    !Pu-239 TI01 Sandy/LowerVadoseZone
TRANsport ID=LVZ for C2 Kd=300.0  De=167.25528 aL=0 aT=0    !U-235  TI01 Sandy/LowerVadoseZone
TRANsport ID=LVZ for C3 Kd=3.0    De=167.25528 aL=0 aT=0    !Pa-231 TI01 Sandy/LowerVadoseZone
TRANsport ID=LVZ for C4 Kd=1100.0 De=167.25528 aL=0 aT=0    !Ac-227 TI01 Sandy/LowerVadoseZone
!
!                                                                   UVZ
DENSity SOLId  ID=UVZ DENSity  2.69                  !UpperVadoseZone  rock grain density (g/cm^3)
POROsity    ID=UVZ 0.385                             !UpperVadoseZone  rock grain density (g/cm^3)
TRANsport ID=UVZ for C   Kd=6000.0 De=167.25528 aL=0 aT=0   !Pu-239 TI01 Clayey/UpperVadoseZone
TRANsport ID=UVZ for C2  Kd=400.0  De=167.25528 aL=0 aT=0   !U-235  TI01 Clayey/UpperVadoseZone
TRANsport ID=UVZ for C3  Kd=9.0    De=167.25528 aL=0 aT=0   !Pa-231 TI01 Clayey/UpperVadoseZone
TRANsport ID=UVZ for C4  Kd=8500.0 De=167.25528 aL=0 aT=0   !Ac-227 TI01 Clayey/UpperVadoseZone
!
!                                                                   BACKFILL
DENSity SOLId  ID=BACKFILL DENSity  2.65             !OscBefore  rock grain density (g/cm^3)
POROsity    ID=BACKFILL 0.456                        !OscBefore  rock grain density (g/cm^3)
TRANsport ID=BACKFILL for C   Kd=6000.0 De=167.25528 aL=0 aT=0      !Pu-239 TI01 Clayey/OscBefore
TRANsport ID=BACKFILL for C2  Kd=400.0  De=167.25528 aL=0 aT=0      !U-235  TI01 Clayey/OscBefore
TRANsport ID=BACKFILL for C3  Kd=9.0    De=167.25528 aL=0 aT=0      !Pa-231 TI01 Clayey/OscBefore
TRANsport ID=BACKFILL for C4  Kd=8500.0 De=167.25528 aL=0 aT=0      !Ac-227 TI01 Clayey/OscBefore
!
!                                                                   WASTE
DENSity SOLId  ID=WASTE DENSity  2.65                !ETboxesBefore  rock grain density (g/cm^3)
POROsity    ID=WASTE 0.893                           !ETboxesBefore  rock grain density (g/cm^3)
TRANsport ID=WASTE for C   Kd=6000.0 De=167.25528 aL=0 aT=0 !Pu-239 TI01 Clayey/ETboxesBefore
TRANsport ID=WASTE for C2  Kd=400.0  De=167.25528 aL=0 aT=0 !U-235  TI01 Clayey/ETboxesBefore
TRANsport ID=WASTE for C3  Kd=9.0    De=167.25528 aL=0 aT=0 !Pa-231 TI01 Clayey/ETboxesBefore
TRANsport ID=WASTE for C4  Kd=8500.0 De=167.25528 aL=0 aT=0 !Ac-227 TI01 Clayey/ETboxesBefore
!
SAVE MTYP COMPACT to "MAIN.sav" NOW
READ 1 '../../../../Flow/Case01/TI01/FLOW.sav' and make fresh STARt
TIME -8.0
!
SOLVE C C2 C3 C4   8.0 yrs dt=1 inc=1 max=1
SAVE  C C2 C3 C4   for ID=INSIDE to 'C.sav'  NOW
!
!                                                           TI02   0.0 to 11.0 yrs
!
READ 1 '../../../../Flow/Case01/TI02/FLOW.sav'
TIME 0.0
!
SOLVE C C2 C3 C4   11.0 yrs dt=1 inc=1 max=1
!
!                                                           TI03   11.0 to 71.0 yrs
!
READ 1 '../../../../Flow/Case01/TI03/FLOW.sav'
TIME 11.0
!
SOLVE C C2 C3 C4  60.0 yrs dt=1 inc=1 max=1
!
!                                                           TI04   71.0 to 171.0 yrs
!
READ 1 '../../../../Flow/Case01/TI04/FLOW.sav'
TIME 71.0
!
SOLVE C C2 C3 C4   100.0 yrs dt=1 inc=1 max=1
!
!                                                           TI05   171.0 to 191.0 yrs
!
READ 1 '../../../../Flow/Case01/TI05/FLOW.sav'
TIME 171.0
!
SOLVE C C2 C3 C4   20.0 yrs dt=1 inc=1 max=1
!
!                                                           TI06   191.0 to 211.0 yrs
!
READ 1 '../../../../Flow/Case01/TI06/FLOW.sav'
TIME 191.0
!
```

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SOLVE C C2 C3 C4   20.0 yrs dt=1 inc=1 max=1
!
!                                                            TI07   211.0 to 231.0 yrs
!
READ 1 '../../../../Flow/Case01/TI07/FLOW.sav'
TIME 211.0
!
SOLVE C C2 C3 C4   20.0 yrs dt=1 inc=1 max=1
!
!                                                            TI08   231.0 to 251.0 yrs
!
READ 1 '../../../../Flow/Case01/TI08/FLOW.sav'
TIME 231.0
!
SOLVE C C2 C3 C4   20.0 yrs dt=1 inc=1 max=1
!
!                                                            TI09   251.0 to 291.0 yrs
!
READ 1 '../../../../Flow/Case01/TI09/FLOW.sav'
TIME 251.0
!
SOLVE C C2 C3 C4   40.0 yrs dt=1 inc=1 max=1
!
!                                                            TI10   291.0 to 341.0 yrs
!
READ 1 '../../../../Flow/Case01/TI10/FLOW.sav'
TIME 291.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                            TI11   341.0 to 391.0 yrs
!
READ 1 '../../../../Flow/Case01/TI11/FLOW.sav'
TIME 341.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                            TI12   391.0 to 441.0 yrs
!
READ 1 '../../../../Flow/Case01/TI12/FLOW.sav'
TIME 391.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                            TI13   441.0 to 491.0 yrs
!
READ 1 '../../../../Flow/Case01/TI13/FLOW.sav'
TIME 441.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                            TI14   491.0 to 541.0 yrs
!
READ 1 '../../../../Flow/Case01/TI14/FLOW.sav'
TIME 491.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                            TI15   541.0 to 591.0 yrs
!
READ 1 '../../../../Flow/Case01/TI15/FLOW.sav'
TIME 541.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                            TI16   591.0 to 641.0 yrs
!
READ 1 '../../../../Flow/Case01/TI16/FLOW.sav'
TIME 591.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
```

```
!
!                                                             TI17   641.0 to 691.0 yrs
!
READ 1 '../../../../Flow/Case01/TI17/FLOW.sav'
TIME 641.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                             TI18   691.0 to 742.0 yrs
!
READ 1 '../../../../Flow/Case01/TI18/FLOW.sav'
TIME 691.0
!
SOLVE C C2 C3 C4   51.0 yrs dt=1 inc=1 max=1
!
!                                                             TI19   742.0 to 762.0 yrs
!
READ 1 '../../../../Flow/Case01/TI19/FLOW.sav'
TIME 742.0
SOLVE C C2 C3 C4   20.0 yrs dt=1 inc=1 max=1
!
!                                                             TI20   762.0 to 792.0 yrs
!
READ 1 '../../../../Flow/Case01/TI20/FLOW.sav'
TIME 762.0
!
SOLVE C C2 C3 C4   30.0 yrs dt=1 inc=1 max=1
!
!                                                             TI21   792.0 to 822.0 yrs
!
READ 1 '../../../../Flow/Case01/TI21/FLOW.sav'
TIME 792.0
!
SOLVE C C2 C3 C4   30.0 yrs dt=1 inc=1 max=1
!
!                                                             TI22   822.0 to 872.0 yrs
!
READ 1 '../../../../Flow/Case01/TI22/FLOW.sav'
TIME 822.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                             TI23   872.0 to 922.0 yrs
!
READ 1 '../../../../Flow/Case01/TI23/FLOW.sav'
TIME 872.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                             TI24   922.0 to 972.0 yrs
!
READ 1 '../../../../Flow/Case01/TI24/FLOW.sav'
TIME 922.0
!
SOLVE C C2 C3 C4   50.0 yrs dt=1 inc=1 max=1
!
!                                                             TI25   972.0 to 1171.0 yrs
!
READ 1 '../../../../Flow/Case01/TI25/FLOW.sav'
TIME 972.0
!
SOLVE C C2 C3 C4   199.0 yrs dt=1 inc=1 max=1
!
!                                                             TI26   1171.0 to 1371.0 yrs
!
READ 1 '../../../../Flow/Case01/TI26/FLOW.sav'
TIME 1171.0
!
SOLVE C C2 C3 C4   200.0 yrs dt=1 inc=1.05 max=20
!
!                                                             TI27   1371.0 to 1571.0 yrs
```

```
!
READ 1 '../../../../Flow/Case01/TI27/FLOW.sav'
TIME 1371.0
!
SOLVE C C2 C3 C4   200.0 yrs dt=20 inc=1 max=20
!
!                                                           TI28   1571.0 to 1771.0 yrs
!
READ 1 '../../../../Flow/Case01/TI28/FLOW.sav'
TIME 1571.0
!
SOLVE C C2 C3 C4   200.0 yrs dt=20 inc=1 max=20
!
!                                                           TI29   1771.0 to 1971.0 yrs
!
READ 1 '../../../../Flow/Case01/TI29/FLOW.sav'
TIME 1771.0
!
SOLVE C C2 C3 C4   200.0 yrs dt=20 inc=1 max=20
!
!                                                           TI30   1971.0 to 2471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI30/FLOW.sav'
TIME 1971.0
!
SOLVE C C2 C3 C4   500.0 yrs dt=20 inc=1 max=20
!
!                                                           TI31   2471.0 to 2971.0 yrs
!
READ 1 '../../../../Flow/Case01/TI31/FLOW.sav'
TIME 2471.0
!
SOLVE C C2 C3 C4   500.0 yrs dt=20 inc=1 max=20
!
!                                                           TI32   2971.0 to 3471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI32/FLOW.sav'
TIME 2971.0
!
SOLVE C C2 C3 C4   500.0 yrs dt=20 inc=1 max=20
!
!                                                           TI33   3471.0 to 3971.0 yrs
!
READ 1 '../../../../Flow/Case01/TI33/FLOW.sav'
TIME 3471.0
!
SOLVE C C2 C3 C4   500.0 yrs dt=20 inc=1 max=20
!
!                                                           TI34   3971.0 to 4471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI34/FLOW.sav'
TIME 3971.0
!
SOLVE C C2 C3 C4   500.0 yrs dt=20 inc=1 max=20
!
!                                                           TI35   4471.0 to 5471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI35/FLOW.sav'
TIME 4471.0
!
SOLVE C C2 C3 C4   1000.0 yrs dt=20 inc=1 max=20
!
!                                                           TI36   5471.0 to 6471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI36/FLOW.sav'
TIME 5471.0
!
SOLVE C C2 C3 C4   1000.0 yrs dt=20 inc=1 max=20
!
!                                                           TI37   6471.0 to 7471.0 yrs
!
```

```
READ 1 '../../../../Flow/Case01/TI37/FLOW.sav'
TIME 6471.0
!
SOLVE C C2 C3 C4   1000.0 yrs dt=20 inc=1 max=20
!
!                                                           TI38   7471.0 to 8471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI38/FLOW.sav'
TIME 7471.0
!
SOLVE C C2 C3 C4   1000.0 yrs dt=20 inc=1 max=20
!
!                                                           TI39   8471.0 to 9471.0 yrs
!
READ 1 '../../../../Flow/Case01/TI39/FLOW.sav'
TIME 8471.0
!
SOLVE C C2 C3 C4   1000.0 yrs dt=20 inc=1 max=20
!
!                                                           TI40   9471.0 to 10171.0 yrs
!
READ 1 '../../../../Flow/Case01/TI40/FLOW.sav'
TIME 9471.0
!
SOLVE C C2 C3 C4   700.0 yrs dt=20 inc=1 max=20
!
!                                                           TI41   10171.0 to 11171.0 yrs
!
READ 1 '../../../../Flow/Case01/TI41/FLOW.sav'
TIME 10171.0
!
SOLVE C C2 C3 C4   6650.0 yrs dt=20 inc=1 max=20
!
TIME 16821                                          ! Complete corrosion
SOLVE C C2 C3 C4  14350.0 yrs dt=20 inc=1 max=20
!
TIME 31171.0
SOLVE C C2 C3 C4   5000.0 yrs dt=20 inc=1.05 max=100
!
TIME 36171.0
SOLVE C C2 C3 C4   5000.0 yrs dt=100 inc=1 max=100
!
TIME 41171.0
SOLVE C C2 C3 C4   5000.0 yrs dt=100 inc=1 max=100
!
TIME 46171.0
SOLVE C C2 C3 C4   5000.0 yrs dt=100 inc=1 max=100
!
TIME 51171.0
SOLVE C C2 C3 C4   5000.0 yrs dt=100 inc=1 max=100
!
TIME 56171.0
SOLVE C C2 C3 C4   5000.0 yrs dt=100 inc=1 max=100
!
TIME 61171.0
SOLVE C C2 C3 C4   10000.0 yrs dt=100 inc=1.05 max=200
!
TIME 71171.0
SOLVE C C2 C3 C4   10000.0 yrs dt=200 inc=1 max=200
!
TIME 81171.0
SOLVE C C2 C3 C4   10000.0 yrs dt=200 inc=1 max=200
!
TIME 91171.0
SOLVE C C2 C3 C4   10000.0 yrs dt=200 inc=1 max=200
!
TIME 101171.0
SOLVE C C2 C3 C4   10000.0 yrs dt=200 inc=1 max=200
!
TIME 111171.0
SOLVE C C2 C3 C4   20000.0 yrs dt=200 inc=1 max=200
```

```
!
TIME 131171.0
SOLVE C C2 C3 C4   20000.0 yrs dt=200 inc=1 max=200
!
TIME 151171.0
SOLVE C C2 C3 C4   850000.0 yrs dt=200 inc=1.05 max=1000
!
END
QUIT
```

Distribution:

sebastian.aleman@srnl.doe.gov
paul.andrews@srs.gov
cj.bannochie@srnl.doe.gov
alex.cozzi@srnl.doe.gov
kerri.crawford@srs.gov
Thomas.Danielson@srnl.doe.gov
kenneth.dixon@srnl.doe.gov
James.Dyer@srnl.doe.gov
peter.fairchild@srs.gov
luther.hamm@srnl.doe.gov
thong.hang@srnl.doe.gov
connie.herman@srnl.doe.gov
dennis.jackson@srnl.doe.gov
daniel.kaplan@srnl.doe.gov
walt.kubilius@srnl.doe.gov
brady.lee@srnl.doe.gov
patricia.lee@srnl.doe.gov
Dien.Li@srs.gov
Joseph.Manna@srnl.doe.gov
john.mayer@srnl.doe.gov
daniel.mccabe@srnl.doe.gov
steven.mentrup@srs.gov
Gregg.Morgan@srnl.doe.gov
verne.mooneyhan@srs.gov
ralph.nichols@srnl.doe.gov
frank.pennebaker@srnl.doe.gov
William.Ramsey@srnl.doe.gov
Virgina.Rigsby@srs.gov
larry.romanowski@srs.gov
Jansen.Simmons@srs.gov
eric.skidmore@srnl.doe.gov
Ira.Stewart@srs.gov
michael.stone@srnl.doe.gov
kevin.tempel@srs.gov
Boyd.Wiedenman@srnl.doe.gov
Tad.Whiteside@srnl.doe.gov
Jennifer.Wohlwend@srnl.doe.gov

heather.capogreco@srnl.doe.gov
Records Administration (EDWS)