## Potential Gas Generation in a Salt Repository

Gas Generation Model – Results



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QDS- 10075A-T3-RESULTS Version 1

February 2023



## **Document Details**

Quintessa Document Owner: S Benbow Client: COVRA Security Status: Public

## **Document History**

Version	Date	Changes	Editor(s)	Reviewer(s)	Approver
1	15/02/2023		S Benbow	S Watson, J Bartol	A Bond

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## Summary

A high-level conceptualisation of potential gas generation processes for the waste types considered in COVRA's OPERA research programme (Verhoef et al., 2017) is given by Watson (2023). Benbow et al. (2023) presents a functional specification for a relatively simple model for estimating amounts and timescales associated with gas generation from a single representative waste package from each identified waste stream based on the conceptualisation provided by Watson (2023). Only gas generation from waste packages, and not from the overpack for HLW is considered in the model. The overpack is being considered separately by COVRA in other studies. Parameter values to represent a central case for analysis based on best estimates of waste inventories, package geometries and package and tunnel void spaces determined from the OPERA safety case and additional information on provisional salt repository tunnel geometries provided by COVRA are also given by Benbow et al. (2023), together with general parameters for determining rates of gas generation due to corrosion, organic degradation and radiolysis.

This report presents preliminary results from the model described in Benbow et al. (2023), implemented using Quintessa's QPAC software (Quintessa, 2013). Results for the central analysis case and some sensitivity cases are presented. The results that are presented are not precise predictions of the amount of gas that might be generated. They aim to be indicative estimates of gas production that might be occur if the specified brine inflows and water availability occur under repository conditions. In future, the model could be refined to add further realism in order to better estimate timings and amounts of gas.

The results of the model confirm the expected result that amounts of gas generation are strongly sensitive to water availability and help to distinguish contributions from water initially emplaced in the waste, water (brine) assumed to be initially adjacent to the exterior of the package in the repository (e.g. in a wetted crushed salt backfill) and the flux of water (brine) from the salt host formation.

The sensitivity analysis results suggest that gas generation can be significantly reduced if less water is made available to the packages. Limiting the geosphere flux alone is insufficient however, and in most cases it is necessary to also reduce the amount of water that is initially assumed to be available in the package and in the void space surrounding it to limit the amount of gas generated because in many cases the water that is initially present is sufficient to support all of the potential gas generation from the package.

Although the overpack is not considered in the models, the effect that it may have on isolating the waste packages from water initially in the repository void spaces, and from

the geosphere brine flux, is investigated in a delayed inflow sensitivity case. This was seen to have little effect unless the delay can be made to be very long by suitably engineering the overpack. A delay of 1,000 y was seen to lead to negligible differences in overall amounts of gas generated from the waste package, and only affected the timing of the build-up of gas in cases where this occurs early in the system evolution.

Of the waste groups considered, vitrified waste and depleted uranium give rise to the greatest amount of gas generated per package. For both of these cases the model does not currently account for the reduction in alpha radiolysis that might result from the waste form restricting direct access of water to the radionuclide inventory. Molybdenum and non-compactible LILW give rise to much smaller amounts of gas generated gas. The compactible LILW waste packages produce about twice as much gas as Molybdenum and non-compactible LILW and are present in very large numbers in the repository. It may be sensible to further analyse these cases in particular in future work where further realism could be added to the model. Various approaches are possible to minimise the gas pressure that might develop in the repository, including the use of gas permeable seals and specifically engineered void spaces in which gas can accumulate. These could provide a pathway and destination for gases that migrate from the emplaced waste packages.

## Contents

1	Introduction	1	
2	Central Analysis Case Results		
	2.1 Vitrified Waste		
	2.2 Research Reactor Spent Fuel	8	
	2.3 Uranium Collection Filters	12	
	2.4 Reprocessing Waste	16	
	2.5 Decommissioning Waste (Revised OPERA HLW Technical Waste)	20	
	2.6 Legacy Waste (Revised OPERA HLW Technical Waste)	25	
	2.7 Depleted Uranium	30	
	2.8 Molybdenum Waste	34	
	2.9 Non-Compactible LILW	38	
	2.10 Compactible LILW	42	
	2.11 Discussion	47	
3	Sensitivity Cases		
	3.1 Zero Geosphere Inflow Results	52	
	3.2 Slower Non-Zero Geosphere Inflows	60	
	3.3 Delayed Inflow Due to Overpack	61	
	3.4 Limiting Inflow with Pressure	63	
	3.5 Discussion	69	
4	Summary	70	
Re	ferences	72	

## 1 Introduction

A high-level conceptualisation of potential gas generation processes for the waste types considered in COVRA's OPERA research programme (Verhoef et al., 2017) is given by Watson (2023). Benbow et al. (2023) presents a functional specification for a relatively simple model for estimating amounts and timescales associated with gas generation from a single representative waste package from each identified waste group based on the conceptualisation provided by Watson. Only gas generation from the wasteform and waste packaging that forms part of the waste package during storage are considered in the model. Overpacks and waste containers for wastes that are repackaged for disposal are not considered. Parameter values to represent a central case for analysis based on best estimates of waste inventories, package geometries and package and tunnel void spaces determined from the OPERA research programme and additional information on provisional salt repository tunnel geometries provided by COVRA are also given by Benbow et al. (2023), together with general parameters for determining rates of gas generation due to corrosion, organic degradation and radiolysis.

This report presents preliminary results from the model described in Benbow et al. (2023), implemented using Quintessa's QPAC software (Quintessa, 2013). Results for the central analysis case are presented and some sensitivity cases are considered. The central analysis case conservatively assumes that a constant inflow of water from the geosphere will be available to sustain gas generating reactions throughout the one-million-year evolution of the package that is simulated. The sensitivity cases that are simulated include a dry case in which there is no inflow from the geosphere, a case in which inflows towards packages in the lower level of the repository are delayed due to the isolation from the geosphere provided by the steel overpack, and a case in which build-up of pressure around the packages is assumed to lead to limiting and eventual halting of inflows.

It should be noted that the results presented are not precise predictions of the amount of gas that might be generated. They aim to be indicative estimates of gas production that might be occur if the specified brine inflows and water availability occur under repository conditions. To make predictions of gas pressure would require a more detailed coupling of gas generation with water availability, including the consumption of water in reactions with the packaging that is not included in the current models, and a coupled water flow and gas transport model to allow the effect of pressurisation on inflow from the geosphere to be simulated and together with a representation of the way in which the excavations converge to reduce void space around the packages. More detailed coupling of gas generation and transport is possible in QPAC (e.g. Watson et al., 2012) but is beyond the scope of the current work.

1

Central analysis case results are presented in Section 2 and sensitivity case results are given in Section 3. General observations on the outcomes of the modelling are summarised in Section 4.

## 2 Central Analysis Case Results

Results are presented in the following sections for the simulations of the central analysis case described in Benbow et al. (2023) for each waste group. In the central analysis case the rate of inflow of water to the disposal tunnels is assumed to be 1 g/m/day. The inflow is scaled by the number of waste packages per unit length of tunnel in order to derive a geosphere inflow rate per package,  $Q_{geo}$  (mol/y), as described in Benbow et al. (2023).

The 1 g/m/day rate of inflow that is used is based on models of inflows to open tunnels at Waste Isolation Pilot Plant (WIPP) developed for the DECOVALEX 2023 project, as explained in Benbow et al. (2023). The continuing inflow in the central analysis case is based on an assumption that water will continue to be consumed in reactions with the waste which therefore continues to draw water toward the waste package. The central analysis case conservatively assumes that the inflows do not slow as the package and surrounding pore/void space pressurises as gas is produced, since modelling the disposition of the produced gas in the repository system is beyond the scope of the current model.

As noted in Section 1, the steel overpack for HLW packages in the lower level of the repository is not included in the scope of the current model and is being considered separately by COVRA in other studies. To some extent the results presented here can be "shifted" by the containment time provided by the overpack, with the exception that any contributions to gas generation from initially emplaced water or due to radiolysis of organics should not be shifted.

For each waste group a description of the phenomenology of the evolution of gas generation with time is given, which attempts to describe the process and couplings that control the evolution. The results for each waste group are structured in a similar manner to aid the reader in comparing results between waste groups. They can be read in isolation from each other and provide a basis to facilitate understanding of deviations to the central analysis case evolutions that are introduced by the modified assumptions in the sensitivity cases in Section 3. The Compactible LILW case is, perhaps, one of the most interesting cases in the sense that it includes most of the waste degradation processes that are included in the model and so clearly demonstrates the interplay of the water supply rate and the various gas-generating processes in the package.

The HLW Technical Waste group (Watson, 2023) is not included in the modelling since COVRA are now planning to separate this into two separate waste groups corresponding to decommissioning (in KONRAD packages) and legacy waste (in DDS packages).

## 2.1 Vitrified Waste

The time evolution of the inventories of metals, organics and water in the vitrified waste group are shown in Figure 2-1 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period, and the grey shaded region indicates the period after disposal.

The vitrified waste group metal inventory only comprises stainless steel for the outer packaging. Since there is initially no water inside the package, it only starts to corrode once placed in the repository. Since the package is sealed, the corrosion of the packaging is from the outside only. Conditions outside the package are neutral. With the imposed initial water saturation of 0.1 outside the package and geosphere inflow of 1 g/m/day, it takes ~5 × 10<sup>4</sup> y to fully corrode the outer packaging. At this point, water enters the package.

There is no organic inventory in the vitrified waste.

Figure 2-2 shows the gases produced inside and outside of the package (top-left and topright plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottomright plots respectively).

The waste package is sealed, so corrosion is only initially possible on the outside of the packaging. This leads to generation of H<sub>2</sub> outside the package, which halts at  $\sim 5 \times 10^4$  y when the package is fully corroded and  $\sim 2,000$  moles of H<sub>2</sub> has been produced by corrosion. Water can then enter the package. This allows radiolysis of H<sub>2</sub>O to begin inside the original package volume. In the period from  $\sim 5 \times 10^4$  y to  $10^6$  y, when the simulation ends, approximately  $2.5 \times 10^5$  moles of H<sub>2</sub> are produced by radiolysis inside the original package volume. A smaller amount of H<sub>2</sub> is produced by radiolysis outside the package due to the assumption that only one-thousandth of the gamma energy can escape the package (Benbow et al., 2023). This assumption continues to be made after the packaging is corroded, i.e. the corrosion products are assumed to adsorb a similar amount of energy as the pristine metal.

Rates of gas generation inside the package are shown in Figure 2-3. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of  $H_2O$  (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas

generation outside the package are shown in Figure 2-4. This only comprises contributions from corrosion (top) and radiolysis of H<sub>2</sub>O (bottom).

Corrosion of the outer packaging leads to H<sub>2</sub> generation rates of around  $4 \times 10^{-2}$  mol/y, whereas rates of H<sub>2</sub> generation from radiolysis of H<sub>2</sub>O inside the package, after it has fully corroded, are almost 10 times larger (around  $3 \times 10^{-1}$  mol/y). The small amount of corrosion inside the package after the package fails corrosively is due to the way in which amounts that approach zero are handled in the model. The corrosive failure of the outer packaging is assumed to occur when the packaging is 99.9% corroded. The small amount of remaining metal can then continue to corrode from the inside and outside after water enters the package. The ramping down of the corrosion rate when the metal amount is close to zero causes the prolonged period of corrosion at the negligible rate ( $< 10^{-10}$  mol/y). The apparent initial 'spike' in the rate of generation of H<sub>2</sub> due to radiolysis of H<sub>2</sub>O inside the package after it corrodes (Figure 2-3, bottom-left plot) is a consequence of the log time axis that is used in the plot. Figure 2-6 shows the same H<sub>2</sub> radiolysis data plotted alongside the alpha decay power data (which dominates the decay power) from Figure 2-5, using a linear time axis. The rate of gas generation can be seen to follow the decay power, as would be expected. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are initially around  $1 \times 10^{-3}$  mol/y, but this quickly falls as the gamma power of the waste falls.

The radiolysis calculations assume that the water has full access to the vitrified waste and so do not account for the cracking of the waste form that would be necessary for the water to access the waste. Therefore, they will tend to overestimate the amount of gas production since alpha energy that would be absorbed by the glass between the fractures is assumed to be available for radiolysis. Significant amounts of radiolysis due to alpha radiation would only be expected if the glass was highly cracked, and so the simulated rates of gas generation due to radiolysis are therefore almost certainly an upper bound.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-5. Alpha decays dominate the decay power. The decaying inventory is shown in the left-hand plot.



Figure 2-1 Vitrified waste: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-2 Vitrified waste: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.

5



Figure 2-3 Vitrified waste: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-4 Vitrified waste: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.

6



Figure 2-5 Vitrified waste: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-6 Curves showing the rate of generation of  $H_2$  due to radiolysis of  $H_2O$  inside the package (blue) and the alpha radiation decay power (orange), to explain the shape of the 'spike' in the rate of generation of  $H_2$  due to radiolysis shown in the bottomleft plot in Figure 2-3.

## 2.2 Research Reactor Spent Fuel

The time evolution of the inventories of metals, organics and water in the research reactor spent fuel waste group are shown in Figure 2-7 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The research reactor spent fuel waste group metal inventory comprises stainless steel for the outer packaging, with stainless steel and aluminium in the waste. In the model it is assumed that there is initially no water inside the package, so the waste package only starts to corrode once placed in the repository. Since the package is sealed, the corrosion of the packaging is from the outside only. Conditions outside the package are neutral. With the imposed initial water saturation of 0.1 outside the package and geosphere inflow of 1 g/m/day, it takes  $\sim 3.3 \times 10^4$  y to fully corrode the outer packaging. At this point, water enters the package.

The outside of the package is fully saturated at  $\sim 3.3 \times 10^4$  y when the package is fully corroded. This, combined with the assumed water inflow rate of 1 g/m/day, is sufficient to maintain full saturation inside the package. Aluminium corrodes faster than stainless steel and is corroded by  $4.5 \times 10^4$  y. Stainless steel waste corrosion is slower, taking until around  $6.3 \times 10^4$  y to fully corrode.

There is no organic inventory in the research reactor spent fuel waste group.

Figure 2-8 shows the gases produced inside and outside of the package (top-left and topright plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottomright plots respectively).

Corrosion of the packaging (from the outside) leads to generation of H<sub>2</sub> outside the package, which halts at  $\sim 3.3 \times 10^4$  y when it is fully corroded. By this time  $\sim 2,500$  moles of H<sub>2</sub> is produced by corrosion. At this point water can enter the package and so corrosion and radiolysis can begin inside the package, which leads to a large amount of H<sub>2</sub> generation inside the package. In the period from  $\sim 3.3 \times 10^4$  y to  $10^6$  y, approximately  $2.6 \times 10^4$  moles of H<sub>2</sub> are produced inside the package, the majority of this ( $\sim 2.1 \times 10^4$  moles) being due to corrosion of the waste metal.

Only a small amount of  $H_2$  is produced by radiolysis outside the package due to the assumption that only one-thousandth of the gamma energy can escape the package. This assumption continues to be made after the packaging is corroded, i.e. the corrosion products are assumed to adsorb a similar amount of energy as the pristine metal.

Rates of gas generation inside the package are shown in Figure 2-9. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of

 $\rm H_2O$  (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas generation outside the package are shown in Figure 2-10. This only comprises contributions from corrosion (top-left) and radiolysis of  $\rm H_2O$  (bottom-left).

Corrosion of the outer packaging leads to H<sub>2</sub> generation rates of around  $7 \times 10^{-2}$  mol/y. Inside the package, after the outer packaging has been fully corroded, metal corrosion leads to H<sub>2</sub> generation rates of around 1 mol/y until the metals are corroded. Rates of H<sub>2</sub> generation from radiolysis of H<sub>2</sub>O inside the package fall from a peak of around  $1.7 \times 10^{-2}$  mol/y at the point at which the metal waste is corroded to  $2.2 \times 10^{-3}$  mol/y over the period  $3.3 \times 10^4$  to  $10^6$  y. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are smaller than that due to corrosion because of the limited gamma energy that escapes from the package. The shape of the radiolysis rate curve is caused by a combination of the rising saturation outside the package at early times (up to ~10<sup>4</sup> y) and the falling gamma energy with time.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-11. Alpha decays dominate the decay power. The decaying inventory is shown in the left-hand plot.



Figure 2-7 Research Reactor Spent Fuel: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-8 Research Reactor Spent Fuel: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-9 Research Reactor Spent Fuel: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.

10



Figure 2-10 Research Reactor Spent Fuel: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-11 Research Reactor Spent Fuel: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

## 2.3 Uranium Collection Filters

The time evolution of the inventories of metals, organics and water in the uranium collection filters waste group are shown in Figure 2-12 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The uranium collection filters waste group metal inventory comprises stainless steel for the outer packaging, with stainless steel filters and filter housing and aluminium in the waste. In the model it is assumed that there is initially no water inside the package, it only starts to corrode once placed in the repository. Since the package is sealed, the initial corrosion of the packaging is from the outside only. Conditions outside the package are neutral. With the imposed initial water saturation of 0.1 outside the package and geosphere inflow of 1 g/m/day, it takes  $\sim 3.4 \times 10^4$  y to fully corrode the outer packaging. At this point, water enters the package.

The outside of the package is fully saturated at the time when the package is fully corroded. This, combined with the assumed water inflow rate of 1 g/m/day, is sufficient to cause the inside of the package to rapidly become fully saturated and stay fully saturated throughout the remainder of the simulated period. Aluminium corrodes faster than stainless steel and is fully corroded by  $\sim 5.7 \times 10^4$  y. Stainless steel in the waste is fully corroded by  $\sim 5 \times 10^5$  y.

There is no organic inventory in the uranium collection filters waste group.

Figure 2-13 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

Corrosion of the packaging (from the outside) leads to generation of H<sub>2</sub> outside the package, which halts at  $\sim 3.4 \times 10^4$  y when it is fully corroded. By this time  $\sim 2,500$  moles of H<sub>2</sub> is produced by corrosion. At this point water can enter the package and so corrosion and radiolysis can begin inside the package, which leads to a large amount of H<sub>2</sub> generation inside the package. Steel corrosion is rapid since the surface area of the combined stainless steel material is dominated by the surface area of the filters. This causes steel to corrode more rapidly than the aluminium. In the period from  $\sim 3.4 \times 10^4$  y to  $5.6 \times 10^4$  y, approximately  $3.7 \times 10^4$  moles of H<sub>2</sub> are produced inside the package.

Only a small amount of  $H_2$  is produced by radiolysis outside the package due to the assumption that only one-thousandth of the gamma energy can escape the package. This assumption continues to be made after the packaging is corroded, i.e. the corrosion products are assumed to adsorb a similar amount of energy as the pristine metal.

Rates of gas generation inside the package are shown in Figure 2-14. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of H<sub>2</sub>O (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas generation outside the package are shown in Figure 2-15. This only comprises contributions from corrosion (top) and radiolysis of H<sub>2</sub>O (bottom).

Corrosion of the outer packaging leads to H<sub>2</sub> generation rates of around  $7 \times 10^{-2}$  mol/y. Inside the package, after the outer packaging has been fully corroded, metal corrosion briefly leads to H<sub>2</sub> generation rates of around 10 mol/y due to the large reactive surface area of the combined stainless steel inventory, falling to  $2 \times 10^{-1}$  mol/y when only aluminium is remaining. Rates of H<sub>2</sub> generation from radiolysis of H<sub>2</sub>O inside the package are around  $2.4 \times 10^{-3}$  mol/y over most of the period from  $3.4 \times 10^4$  to  $10^6$  y. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are several orders of magnitude smaller due to the limited gamma energy that escapes from the package.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-16. Alpha decays dominate the decay power. The decaying inventory is shown in the left-hand plot.



Figure 2-12 Uranium Collection Filters: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-13 Uranium Collection Filters: gases produced inside (top-left) and outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-14 Uranium Collection Filters: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right – none for this waste group). Pink shading – storage period; grey shading – period after disposal.



Figure 2-15 Uranium Collection Filters: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-16 Uranium Collection Filters: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

## 2.4 Reprocessing Waste

The time evolution of the inventories of metals, organics and water in the reprocessing waste group are shown in Figure 2-17 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The reprocessing waste group metal inventory comprises stainless steel for the outer packaging, with stainless steel and zircaloy in the waste. In the model it is assumed that there is initially no water inside the package, it only starts to corrode once placed in the repository. Since the package is sealed, the corrosion of the packaging is from the outside only. Conditions outside the package are neutral. With the imposed initial water saturation of 0.1 outside the package and geosphere inflow of 1 g/m/day, it takes  $\sim 5 \times 10^4$  y to fully corrode the outer packaging. At this point, water enters the package.

The outside of the package is fully saturated at  $\sim 5 \times 10^4$  y when the package is fully corroded. This, combined with the assumed water inflow rate of 1 g/m/day, is sufficient to rapidly saturate the inside of the package and to maintain full saturation thereafter. The waste steel corrodes more quickly than zircaloy and is fully corroded by  $\sim 7.7 \times 10^4$  y. Zircaloy is fully corroded by  $\sim 2.2 \times 10^5$  y.

There is no organic inventory in the reprocessing waste group.

Figure 2-18 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

Corrosion of the packaging (from the outside) leads to generation of H<sub>2</sub> outside the package, which halts at  $\sim 5 \times 10^4$  y when it is fully corroded. By this time  $\sim 2,000$  moles of H<sub>2</sub> is produced by corrosion. At this point water can enter the package and so corrosion and radiolysis can begin inside the package, which leads to a large amount of H<sub>2</sub> generation inside the package. In the period from  $\sim 5 \times 10^4$  y to  $10^6$  y, approximately  $1.3 \times 10^4$  moles of H<sub>2</sub> are produced inside the package. Only a small amount of H<sub>2</sub> is produced by radiolysis outside the package due to the assumption that only one-thousandth of the gamma energy can escape the package. This assumption continues to be made after the packaging is corroded, i.e. the corrosion products are assumed to adsorb a similar amount of energy as the pristine metal.

Rates of gas generation inside the package are shown in Figure 2-19. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of H<sub>2</sub>O (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas generation outside the package are shown in Figure 2-20. This only comprises contributions from corrosion (top) and radiolysis of H<sub>2</sub>O (bottom).

Corrosion of the outer packaging leads to H<sub>2</sub> generation rates of around  $3 \times 10^{-2}$  mol/y. Inside the package, after the outer packaging has been fully corroded, metal corrosion leads to H<sub>2</sub> generation rates of around  $1.4 \times 10^{-1}$  mol/y while steel is present and then  $4.3 \times 10^{-2}$  mol/y when only zircaloy is remaining (despite the lower specific corrosion rate of zircalloy, the net rate is closer to steel due to the larger surface area of zircaloy in the waste). Rates of H<sub>2</sub> generation from radiolysis of H<sub>2</sub>O inside the package fall from  $\sim 1.6 \times 10^{-2}$  mol/y when the package is corroded to  $\sim 3 \times 10^{-4}$  at  $10^{6}$  y. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are small because of the limited gamma energy that escapes from the package.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-21. Alpha decays dominate the decay power. The decaying inventory is shown in the left-hand plot.



Figure 2-17 Reprocessing Waste: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-18 Reprocessing Waste: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-19 Reprocessing Waste: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-20 Reprocessing Waste: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-21 Reprocessing Waste: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

# 2.5 Decommissioning Waste (Revised OPERA HLW Technical Waste)

The decommissioning waste is packaged in a KONRAD container, which is not included in the analysis as it is unclear whether this container will be used for disposal or whether the waste will be repackaged. "The package" in the commentary below refers to only the interior portion of the waste package.

The time evolution of the inventories of metals, organics and water in the decommissioning waste group are shown in Figure 2-22 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The decommissioning waste group metal inventory comprises aluminium and stainless steel. There is initially only a trace amount of water inside the package ( $8.4 \times 10^{-3}$  mol). This equates to approximately 0.2 g of water, which is less than the cut-off value of 1 g that is applied in the model as the required amount of water for reactions to occur inside the package, in the absence of an inflow of water. Therefore, no corrosion occurs during the storage period.

The KONRAD container is assumed to not offer any barrier to the 1 g/m/day flux of water from the geosphere reaching the package being considered, so when the package is placed in the repository, corrosion of the waste can begin immediately. As described in Benbow et al. (2023), since there is no outer packaging for this waste group included in the model, all water arriving from the geosphere is directed to the "inside" of the package to maximise gas generation. Once the "inside" is saturated the "outside" can then start to saturate with an excess water that arrives. As noted in Benbow et al. (2023), given that there is no outer packaging, the initial water saturation outside the package volume is assumed to be zero for this case to avoid an unrealistically large flux of water towards the interior as soon as the waste is emplaced. Water availability is therefore entirely controlled by the flux from the geosphere.

Aluminium and steel begin to corrode when the waste is exposed to the supply of water from the geosphere. The combined corrosion rate is not sufficient to consume all of the arriving water so the saturation inside the package begins to slowly rise while the metals are corroding. The combination of initial amounts of metal, their surface areas and their corrosion rates in neutral conditions leads to aluminium and steel completely corroding at almost exactly the same time at  $\sim 5 \times 10^3$  y.

There is no organic inventory in the decommissioning waste group.

Figure 2-23 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded, which

is irrelevant for the KONRAD case, and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

Corrosion of the metal waste and radiolysis of H<sub>2</sub>O leads to generation of H<sub>2</sub> inside the package. Approximately 220 moles of H<sub>2</sub> is produced before the waste metal is fully corroded. Radiolysis continues to produce a total of around 3,600 moles of H<sub>2</sub> at 10<sup>6</sup> y. Little H<sub>2</sub> is produced outside of the package due to radiolysis, since until the interior of the package is saturated (at ~7.5 × 10<sup>4</sup> y) all incoming water from the geosphere is directed to the interior of the package, meaning that outside the saturation is zero and radiolysis cannot occur. After the interior saturates, the exterior quickly saturates (Figure 2-22) and radiolysis begins outside the package, but only at a slow rate due to the assumption that only one-thousandth of the gamma energy can escape the package.

Rates of gas generation inside the package are shown in Figure 2-24. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of H<sub>2</sub>O (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas generation outside the package are shown in Figure 2-25. This only comprises contributions from corrosion (top-left) and radiolysis of H<sub>2</sub>O (bottom-left). Since the KONRAD container is not modelled, corrosion rates outside the modelled package are zero in this case. Radiolysis rates are only non-zero after the interior of the package volume becomes saturated, when excess water arriving from the geosphere is then redirected to the volume outside the package.

The combined corrosion rate of aluminium and steel leads to H<sub>2</sub> generation rates of around  $3.2 \times 10^{-2}$  mol/y inside the package. Long-term rates of H<sub>2</sub> production from radiolysis are around  $6 \times 10^{-3}$  mol/y, falling to around  $1 \times 10^{-3}$  mol/y at  $10^{6}$  y. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are small as noted above.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-26. Alpha and beta decays dominate the decay power. The decaying inventory is shown in the left-hand plot.

As is noted in Benbow et al. (2023), it is suspected that initial waste metal inventory is underestimated for this waste group.



Figure 2-22 Decommissioning Waste (Revised OPERA HLW Technical Waste): metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-23 Decommissioning Waste (Revised OPERA HLW Technical Waste): gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-24 Decommissioning Waste (Revised OPERA HLW Technical Waste): gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-25 Decommissioning Waste (Revised OPERA HLW Technical Waste): gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-26 Decommissioning Waste (Revised OPERA HLW Technical Waste): radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

## 2.6 Legacy Waste (Revised OPERA HLW Technical Waste)

The time evolution of the inventories of metals, organics and water in the legacy waste group are shown in Figure 2-27 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The legacy waste group metal inventory comprises stainless steel for the outer packaging, with stainless steel and a small amount of aluminium in the waste. There is initially only a trace amount of water inside the package ( $4 \times 10^{-4}$  mol). This equates to approximately 0.01 g of water, which is less than the cut-off value of 1 g that is applied in the model as the required amount of water for reactions to occur inside the package, in the absence of an inflow of water. Therefore, no corrosion occurs during the storage period.

The waste is packaged in a DDS drum. The DDS will most likely be placed in a concrete overpack. This is assumed in the analysis. The DDS is vented, so once it is placed in the repository water becomes available to both the exterior and interior of the package. The aluminium waste is completely corroded by ~170 y. Corrosion of the waste and packaging stainless steel is slower as a result of the high pH conditions due to the concrete overpacks, allowing the saturation of water inside and outside the package to rise at a rate controlled by the geosphere inflow and the corrosion, organic degradation and radiolysis reactions. The steel packaging is fully corroded by ~3 × 10<sup>5</sup> y and the waste steel is fully corroded by ~4 × 10<sup>5</sup> y.

Water is present in the interior of the package after it is placed in the repository, which allows organic hydrolysis reactions to occur throughout most of the simulated time period. The hydrolysis reactions are sufficiently fast that reactive amounts of cellulose are held close to zero, meaning that the overall rate of hydrolysis is controlled by the rate of the scission reactions from the stopped phases. The amorphous and crystalline phases are exhausted by  $\sim 3 \times 10^4$  y and  $3 \times 10^5$  y respectively.

Figure 2-28 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

Corrosion of the packaging (from the outside) leads to generation of H<sub>2</sub> outside the package, which halts at  $\sim 3 \times 10^5$  y when it is fully corroded. By this time  $\sim 1,100$  moles of H<sub>2</sub> is produced by corrosion outside the package. Only a small amount of H<sub>2</sub> is produced by radiolysis outside the package due to the assumption that only one-thousandth of the gamma energy can escape the package. This assumption continues to

be made after the packaging is corroded, i.e. the corrosion products are assumed to adsorb a similar amount of energy as the pristine metal.

Inside the package,  $H_2$  is produced from steel corrosion (both waste steel and the interior side of the packaging) and radiolysis of  $H_2O$  and  $CO_2$  and  $CH_4$  are produced by cellulose degradation. Hydrolysis reactions dominate the cellulose degradation, radiolysis is less significant, and so  $CO_2$  and  $CH_4$  are produced in almost identical amounts (which are indistinguishable in the plot).

Rates of gas generation inside the package are shown in Figure 2-29. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of H<sub>2</sub>O (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas generation outside the package are shown in Figure 2-30. This only comprises contributions from corrosion (top) and radiolysis of H<sub>2</sub>O (bottom).

Corrosion of the outer packaging leads to H<sub>2</sub> generation rates of around  $3 \times 10^{-3}$  mol/y. Inside the package, metal corrosion leads to H<sub>2</sub> generation rates of around  $10^{-1}$  mol/y while aluminium is present and then  $5 \times 10^{-3}$  mol/y when only steel is remaining. Rates of H<sub>2</sub> generation from radiolysis of H<sub>2</sub>O inside the package are smaller, rising to a peak of  $\sim 10^{-4}$  mol/y at  $\sim 2 \times 10^{5}$  y. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are small because of the limited gamma energy that escapes from the package. The shape of the radiolysis curves is caused by a combination of the rising saturation outside the package and the falling gamma energy.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-31. Alpha and beta decays dominate the decay power. The decaying inventory is shown in the left-hand plot.

As is noted in Benbow et al. (2023), it is suspected that initial waste metal inventory is underestimated for this waste group.



Figure 2-27 Legacy Waste (Revised OPERA HLW Technical Waste): metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-28 Legacy Waste (Revised OPERA HLW Technical Waste): gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-29 Legacy Waste (Revised OPERA HLW Technical Waste): gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-30 Legacy Waste (Revised OPERA HLW Technical Waste): gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-31 Legacy Waste (Revised OPERA HLW Technical Waste): radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

## 2.7 Depleted Uranium

The depleted uranium waste is expected to be packaged for disposal in a KONRAD container, which is not included in the analysis. "The package" in the commentary below refers to only the interior portion of the waste package. The package is grouted with an assumed large water : cement ratio (so that the grout is sufficiently fluid to access all voids) and so it has a high initial water saturation.

The time evolution of the inventories of metals, organics and water in the depleted uranium waste group are shown in Figure 2-32 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

There are no disposed metals or organics in the depleted uranium waste group so the only gas generating process that occurs in the package is radiolysis of H<sub>2</sub>O. Since the radionuclide inventory is only known at 2130, when the package is assumed to be placed in the repository, radiolysis is not simulated while in storage. Gas generation is therefore only possible in the model after the package is placed in the repository.

The KONRAD container is assumed to not offer any barrier to the 1 g/m/day flux of water from the geosphere reaching the package being considered, so when the package is placed in the repository, radiolysis can begin immediately.

Figure 2-33 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded, which is irrelevant for the KONRAD case, and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

After  $10^6$  y,  $\sim 7.3 \times 10^5$  moles of H<sub>2</sub> is produced by radiolysis of H<sub>2</sub>O inside the package (i.e. inside the volume associated with the waste – see above). H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are small due to the small fraction of gamma energy that escape the package.

Rates of gas generation inside the package are shown in Figure 2-34. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of  $H_2O$  (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas generation outside the package are shown in Figure 2-35. This only comprises contributions from corrosion (top) and radiolysis of  $H_2O$  (bottom).

As noted above, gas generation rates are zero except for radiolysis of H<sub>2</sub>O. H<sub>2</sub> is produced at a rate of ~0.7 mol/y inside the package and ~ $10^{-5}$  mol/y outside the package for the majority of the evolution. The rate is increasing for most of the simulated evolution as the decay energy increases with ingrowth.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-36. Alpha decays dominate the decay power. The decaying inventory is shown in the left-hand plot.



Figure 2-32 Depleted Uranium: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.


Figure 2-33 Depleted Uranium: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-34 Depleted Uranium: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-35 Depleted Uranium: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-36 Depleted Uranium: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

# 2.8 Molybdenum Waste

The time evolution of the inventories of metals, organics and water in the molybdenum waste group are shown in Figure 2-37 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The molybdenum waste group has no metal packaging. The waste metal inventory comprises stainless steel (drum and stirrer) and galvanised steel (rebar). As a bounding assumption, the pore/void space in the package is assumed to be initially saturated with water so that corrosion can begin immediately. Steel corrosion rates are slow however, and so only a small amount of corrosion occurs during the storage period, where the oxic conditions do not lead to consumption of water in the corrosion reaction.

Once placed in the repository, since the 200 l drums are not assumed to be watertight, inflows of water from the geosphere, which are conditioned by the concrete container and grouted waste, can approach both the interior and exterior of the package. Corrosion of the galvanised steel is faster than that of stainless steel and so the galvanised steel is fully corroded by  $\sim 4 \times 10^4$  y. The stainless steel is fully corroded by  $\sim 5 \times 10^5$  y.

Corrosion rates are sufficiently slow that complete saturation of the waste is maintained at all times and the pore/void space surrounding the package continues to increase in saturation until it is fully saturated. Therefore, gas generation is not limited by the supply of water for the entire evolution of the package.

There is no organic inventory in the molybdenum waste group.

Figure 2-38 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively). There is no outer packing for the 1000L concrete container, so the fraction corroded is set to 1 from the start of the simulation.

Radiolysis is the only process that generates  $H_2$  outside the package, but the amount produced is trivial due to the low activity of the waste and the small fraction of the gamma energy that is assumed to escape the inner part of the package. Inside the package, corrosion of the galvanised steel leads to the most rapid increase in  $H_2$ generation, after which it slows when only stainless steel remains. Around  $6.7 \times 10^3$ moles of  $H_2$  is produced in total.

Rates of gas generation inside the package are shown in Figure 2-39. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of  $H_2O$  (bottom left) and radiolysis of organics (bottom-right) are shown. Rates of gas

generation outside the package are shown in Figure 2-40. This only comprises contributions from corrosion (top) and radiolysis of H<sub>2</sub>O (bottom).

 $H_2$  generation rates outside the package are small as noted above. Inside the package, rates of  $H_2$  generation are around  $10^{-1}$  mol/y while galvanised steel is present, falling to  $\sim 3 \times 10^{-3}$  mol/y when only stainless steel is remaining. Rates of  $H_2$  generation from radiolysis of  $H_2O$  inside the package are smaller, being less than  $10^{-5}$  mol/y after  $\sim 300$  y.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-41. Alpha decays dominate the decay power, but the overall activity is small. The decaying inventory is shown in the left-hand plot.



Figure 2-37 Molybdenum Waste: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-38 Molybdenum Waste: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-39 Molybdenum Waste: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right – none for this waste group); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-40 Molybdenum Waste: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-41 Molybdenum Waste: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

# 2.9 Non-Compactible LILW

The time evolution of the inventories of metals, organics and water in the noncompactible LILW waste group (from OPERA) are shown in Figure 2-42 (top-left, topright and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The non-compactible LILW waste group has no metal packaging. The waste metal inventory comprises stainless steel and galvanised steel (rebar) in the waste. Like the molybdenum waste group (Section 2.8) a large water to cement ratio is assumed for the grout. The residual water begins to corrode the package interior (waste and interior side of the packaging) while the package is in storage. However, since the steel corrosion reactions under oxic conditions are assumed to not consume water, the initial water inventory is not changed during the storage period.

Once placed in the repository, since the 200 l drums are not assumed to be watertight, inflows of water from the geosphere can approach both the interior and exterior of the package. Corrosion of the galvanised steel is faster than that of stainless steel and so the galvanised steel is fully corroded by  $\sim 4 \times 10^4$  y. The stainless steel is fully corroded by  $\sim 5 \times 10^5$  y.

Corrosion rates are sufficiently slow that complete saturation of the waste is maintained at all times and the pore/void space surrounding the package continues to increase in saturation until it is fully saturated. Therefore, gas generation is not limited by the supply of water for the entire evolution of the package.

The only organics in the waste are ion exchange resins, which are assumed to not hydrolyse and are therefore only subject to radiolysis.

Figure 2-43 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

 $H_2$  is generated steadily throughout the evolution of the package.  $CH_4$  is also produced by radiolysis of resins, but in much lower quantities that are not visible on the linear scale of the plot, and over a short timescale due to the short-lived inventory.

The small fraction of gas produced from radiolysis can be inferred from the rates of gas generation inside the package, shown in Figure 2-44. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of H<sub>2</sub>O (bottom left) and radiolysis of organics (bottom-right) are shown. H<sub>2</sub> generation by metal corrosion dominates the gas production rate by several orders of magnitude, until late times when the metal inventory is exhausted, by which time rates of production due to radiolysis are

negligible. Rates of gas generation outside the package are shown in Figure 2-45. This only comprises radiolysis of  $H_2O$  (bottom) which is negligible.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-46. Beta and gamma decays dominate the decay power, but the overall activity is small. The decaying inventory is shown in the left-hand plot.



Figure 2-42 Non-Compactible LILW: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-43 Non-Compactible LILW: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-44 Non-Compactible LILW: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-45 Non-Compactible LILW: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-46 Non-Compactible LILW: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

# 2.10 Compactible LILW

The time evolution of the inventories of metals, organics and water in the compactible LILW waste group (from OPERA) are shown in Figure 2-47 (top-left, top-right and bottom-left plots respectively). The water saturations inside and outside of the waste package are also shown (bottom-right plot). The pink shaded region indicates the storage period and the grey shaded region indicates the period after disposal.

The compactible LILW waste group metal inventory comprises galvanised steel for the outer packaging, with stainless steel, galvanised steel and aluminium in the waste. An average package is simulated, since the precise waste content will vary by package. Since there is some water initially disposed inside the package, the package interior (waste and interior side of the packaging) begins to corrode in alkaline conditions while the package is in storage. The aluminium corrosion rate is greater than that of steel and leads to complete consumption of the initial water after  $\sim 6$  y, while the package is still in storage. Gas generation in storage then stops.

After the package is placed in the repository, the outside of the packaging begins to corrode from the outside due to the imposed initial water saturation of 0.1 outside the package and geosphere inflow of 1 g/m/day. Since the package is open/vented, water also becomes available to the interior of the package.

In the pH neutral brine conditions outside the package, the corrosion rate of galvanised steel is greater than the corrosion rate of aluminium in the alkaline conditions inside the package. This, combined with the fact that 90% of the inflow from the geosphere is initially directed towards the outside of the package leads to rapid corrosion of the packaging while maintaining dry conditions inside the package. The outer packaging is fully corroded by  $\sim$ 130 y.

When the package fails, the water inventory outside the package becomes available to the interior of the package and the full geosphere flux is directed to the interior package region. This causes rapid corrosion of a small portion of the aluminium inventory until the water supply is exhausted. At this point, saturations fall to zero and the rates of corrosion become limited by the supply of water from the geosphere. Corrosion of the remaining inventory of aluminium takes until  $\sim 9 \times 10^3$  y. After the aluminium is exhausted, the stainless and galvanised steel waste metals continue to corrode. The combined corrosion rates of the galvanised and stainless steel are sufficient to continue to maintain dry conditions inside the package. The galvanised steel is fully corroded by  $\sim 1.8 \times 10^4$  y. Then only stainless steel remains and since its corrosion rate is slower, the supply of water from the geosphere begins to raise the saturation inside the package. It takes until  $\sim 6.7 \times 10^4$  y for the stainless steel to completely corrode.

While water is present inside the package organic hydrolysis reactions occur. During the period of aluminium and galvanised steel corrosion, while the interior of the package

is dry, only a small amount of cellulose degradation occurs, which is limited by the supply of water from the geosphere. The rate is slower than rate of the scission reactions from the stopped to the reactive phases and so the cellulose inventory is driven towards equilibrium between the stopped and reactive phases. After aluminium and galvanised steel are exhausted, water availability for cellulose degradation increases and the reactive phase amounts quickly fall to zero, when the rate of degradation becomes limited by the rate of the scission reactions. Amorphous and crystalline cellulose inventories are exhausted by  $\sim 3.5 \times 10^4$  y and  $\sim 3 \times 10^5$  y respectively.

Figure 2-48 shows the gases produced inside and outside of the package (top-left and top-right plots respectively). The fraction of the outer packaging that is corroded and the imposed temperature (see Benbow et al., 2023) are also shown (bottom-left and bottom-right plots respectively).

Aluminium corrosion in the water initially in the package causes generation of some  $H_2$  in storage until the water is consumed. In the repository, while galvanised steel and aluminium are present the gas produced is mostly  $H_2$  with a smaller amount of CO<sub>2</sub> and CH<sub>4</sub> (the amounts are identical, although this is not distinguishable in the plot) from the smaller portion of the water consumed in hydrolysis reactions with the cellulose. After the aluminium and galvanised steel is fully corroded, the portion of CO<sub>2</sub> and CH<sub>4</sub> produced is larger due to the weaker competition from the stainless steel corrosion reaction, but H<sub>2</sub> production from the corrosion reaction still dominates the produced gases. After 10<sup>6</sup> y, ~8.2 × 10<sup>3</sup> moles of H<sub>2</sub> and ~1.8 × 10<sup>3</sup> moles of CO<sub>2</sub> and CH<sub>4</sub> are produced.

Only a small fraction of gas is produced from radiolysis as can be seen by the rates of gas generation inside the package, shown in Figure 2-49. Separate contributions from corrosion (top-left), organic degradation (top-right), radiolysis of H<sub>2</sub>O (bottom left) and radiolysis of organics (bottom-right) are shown in the plot. Rates of gas generation outside the package are shown in Figure 2-50. This only comprises contributions from corrosion (top) and radiolysis of H<sub>2</sub>O (bottom).

During storage, H<sub>2</sub> generation rates are around 60 mol/y while aluminium is present, falling to zero when the initial water is depleted. In the repository, H<sub>2</sub> generation rates inside the package are limited by the supply of water to around  $10^{-1}$  mol/y inside the package until the metal inventory is fully corroded, after which time H<sub>2</sub> is only generated by radiolysis of H<sub>2</sub>O at a rate of ~ $10^{-5}$  mol/y. Rates of production of CO<sub>2</sub> and CH<sub>4</sub> from cellulose are around  $10^{-2}$  mol/y while cellulose is present, with gas production rates from cellulose radiolysis being about 100 to 1,000 times smaller. Rates of gas generation outside the package are only significant at early times when the packaging is corroding from the outside. H<sub>2</sub> generation rates from radiolysis of H<sub>2</sub>O outside the package are small because of the limited gamma energy that escapes from the package and the low water saturation until aluminium and galvanised steel are fully corroded in the waste.

The evolving alpha, beta and gamma decay power of the waste is shown in the righthand plot of Figure 2-51. Alpha decays dominate the decay power, but the overall activity is small. The decaying inventory is shown in the left-hand plot.



Figure 2-47 Compactible LILW: metals inventory (top-left); organics inventory (top-right); water inventory (bottom-left); and water saturation (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-48 Compactible LILW: gases produced inside (top-left); gases produced outside (top-right); package fraction corroded (bottom-left); and temperature (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-49 Compactible LILW: gas rate inside from corrosion (top-left); gas rate inside from organic degradation (top-right); gas rate inside from radiolysis of water (bottom-left); and gas rate inside from radiolysis of organics (bottom-right). Pink shading – storage period; grey shading – period after disposal.



Figure 2-50 Compactible LILW: gas rate outside from corrosion (top); and gas rate outside from radiolysis of water (bottom). Pink shading – storage period; grey shading – period after disposal.



Figure 2-51 Compactible LILW: radionuclide inventory (left); and decay power (right). Pink shading – storage period; grey shading – period after disposal.

# 2.11 Discussion

For each waste group, the amount of gas generated for the central analysis case parameterisation of the model in the  $10^6$  y period of evolution that was simulated is summarised in Table 2-1.

It is difficult to determine whether the estimated amounts of gas generation are entirely optimistic or pessimistic since, unavoidably, a mixture of assumptions are made in the specification of the model due to the defined scope of the modelling and the simplifying assumptions that it was necessary to make. The main optimistic assumption that has been made, which would tend to underestimate the amount of gas that is generated, is:

▲ Gas generated by corrosion of the overpack (and any other operational engineering structures), which is outside the scope of the modelling, is ignored.

The pessimistic assumptions, which would tend to overestimate the amount of gas production include:

- ▲ Inflows do not slow as the package and surrounding pore/void space pressurises as gas is produced and as salt creep closes the excavated voidage;
- ▲ The imposed constant rate of water available to the package is (perhaps) greater than might be expected especially if interactions with the overpack were to be considered;
- ▲ Radiolysis calculations assume 'complete mixing' of the water with the waste form (this is especially unlikely for vitrified waste forms);
- ▲ Microbes are assumed to be active in the highly saline porewaters; and
- ▲ The generated gas is assumed to not react (e.g. in reality CO<sub>2</sub> may dissolve or react with cementitious materials), which would reduce the amount of gas.

The total amount of gas that can potentially be produced from each package is, except for waste groups where gas generation is dominated by radiolysis, a function of the amount of waste metal and organics in the inventory. The above uncertainties will mostly only control the rate at which gas is generated from the waste packages, and not the total amount that could ever be produced, which for most cases is bounded by the amount of metal and organics that are disposed. The total amount of gas that can be produced by radiolysis is a function of both radionuclide inventory and the waste/waste package materials because some of the decay energy is absorbed by waste and packaging metals and other inert material, which does not result in generation of gases. Table 2-1 Amounts of gas produced in 10<sup>6</sup> y for each waste group. Numbers of packages were initially calculated from information in the OPERA reports. Revised numbers (shown in parenthesis) were subsequently obtained from COVRA<sup>1</sup>

Waste Group	Number of Packages (From OPERA, with revised numbers <sup>1</sup> shown in parentheses)	Amount of gas produced per package (mol)	Total amount of gas produced per waste group (using revised package numbers) (mol)	Fraction of total gas produced in upper and lower levels (using revised package numbers)
Repository lower level				
Vitrified Waste	478 (616)	258,263	1.59E+08	0.9073
Research Reactor Spent Fuel	150 (27HEU+164LEU)	28,364	4.25E+06	0.0243
Uranium Collection Filters	53 (53)	42,236	2.24E+06	0.0128
Reprocessing Waste	600 (670)	14,566	9.76E+06	0.0557
Repository upper level				
Decommissioning Waste (Revised OPERA HLW Technical Waste)	N/A (826)	3,624	2.99E+06	0.0004
Legacy Waste (Revised OPERA HLW Technical Waste)	N/A (512)	4,427	2.27E+06	0.0003
Depleted Uranium	9,060 (specified as volume)	732,417	6.64E+09	0.8362
Molybdenum	8,000 (5,600)	6,715	3.76E+07	0.0047
Non-Compactible LILW	4,000 (3,100)	6,714	2.08E+07	0.0026
Compactible LILW	140,000 (100,100)	12,347	1.24E+09	0.1558

<sup>&</sup>lt;sup>1</sup> Updated\_Waste\_Inventory.xlsx (email from COVRA, 25/11/2022)

Of the high-level waste groups, the research reactor spent fuel, uranium collection filters and reprocessing waste groups all exhibit low levels of potential gas generation. The vitrified waste package produces an order of magnitude more gas, which is almost entirely due to radiolysis of water entering the package after the CSD container has fully corroded at  $\sim 5 \times 10^4$  y. It accounts for  $\sim 91\%$  of the gas generated in the lower level of the repository. Corrosion of the waste packaging is not limited by the availability of water, since saturations outside the package are greater than zero for the entire evolution. If water availability was less than that assumed in the central analysis case, then it is possible that the packaging could survive for longer, delaying the onset of radiolysis and reducing the amount of gas generated in the simulated period. However, the decay power of the waste is not significantly falling at 10<sup>6</sup> y and so the package lifetime would need to be significantly extended if similar amounts of gas were to be avoided in the far future. The assumption that water will become intimately mixed with the vitrified wasteform is highly pessimistic. Water will penetrate the wasteform along cracks, which will probably result in sufficient glass being present between the decaying radionuclides and the water to significantly reduce alpha radiolysis. Fracturing of the glass will increase with degradation, but would also be associated with transport of radionuclides out of the waste package, which would imply a system with significant water, and likely gas, movement.

The new decommissioning and legacy waste groups produce the smallest amounts of gas per package of the waste groups in the upper level of the repository. As noted in Benbow et al. (2023), there are some uncertainties in the initial waste metal inventories for these waste groups. It is suspected that they may be underestimated. It is also suspected that the implied void space in these new waste packages is unrealistically large and, for example, the decommissioning wastes may include significantly more concrete than is in the current inventory.

Amounts of gas produced for the depleted uranium waste group are particularly large, accounting for ~84% of the potential gas production in the upper level of the repository. This is entirely due to radiolysis of H<sub>2</sub>O inside the package, with a rate that increases with time over the simulated period due to ingrowth in the radionuclide inventory. The current assumption that the grouted uranium oxide powder is in direct contact with water is pessimistic and the grout is likely to reduce water access and hence alpha radiolysis, despite being an initial source of water inside the package.

Molybdenum and the non-compactible LILW waste groups evolve similarly and lead to a similar amount of gas per package as the new decommissioning and legacy waste packages, but around an order of magnitude more gas overall due to the greater number of packages in the repository. The molybdenum and non-compactible waste are also packed more tightly in the repository than the legacy waste and so will have a smaller available void space to accommodate the gas, so the consequences of gas from these waste groups are potentially more significant than that from the new waste groups. The compactible LILW waste package produces around twice as much gas per-package as the molybdenum and non-compactible LILW packages and has a smaller per-package voidage both inside and outside the package in which to accommodate the gas. The compactible LILW waste group has the greatest number of packages per waste group, resulting in ~16% of the potential gas production in the upper level of the repository. However, since the gas production from the depleted uranium waste is likely to be overestimated, compactible LILW is likely to lead to a larger fraction of the total gas production than estimated here. For this waste group, the rates of gas generation are water-limited for the geosphere flow rate assumed in the central analysis case, with saturations held close to zero while aluminium and galvanised steel are rapidly corroding in the waste (to ~2 × 10<sup>4</sup> y). A slower geosphere inflow rate would therefore directly reduce the rate of gas that is generated for this case, but would not reduce the total amount of gas overall unless the flow was so slow as to prevent complete corrosion during the simulation.

One approach to mitigating the high pressures that may develop for some of the waste groups would be to use gas-permeable seals in the repository and engineer permanent void space in the repository through the use of a non-compactible backfill in an engineered zone that is designed to accumulate gas. This could provide a pathway and destination for gases that migrate from the emplaced waste packages. Since it is assumed that all waste packages of a given type evolve identically, the necessary gas volumes can be calculated from the number of waste packages, the amount of gas generated per package and the target temperature and pressure.

Disposal concepts for salt rely on the salt restricting the flow of water through the geosphere to minimise both gas generation and aqueous transport of radionuclides. This is the basis for repositories in salt host rocks that have been licensed (e.g. WIPP). A fundamental consideration in the design of the overpack proposed by BGE for use in a salt rock by COVRA will be that the host rock is very dry and will remain so meaning that the volume of gas generated by corrosion of the thick steel overpack will not result in over-pressurisation of the host rock. While the geosphere flow rate used in the central analysis case is low (derived from observations in bedded salt), it is assumed that groundwater flow persists for the whole of the simulation. In reality, two processes are likely to restrict the supply of groundwater:

- ▲ creep convergence and healing of the EDZ in the salt is likely to reduce the permeability; and
- ▲ the build-up of gas pressure in the EDZ is likely to restrict the flow of water into the excavations in the two-phase flow system that will be established.

Gas pressure may restrict the degree to which the excavations creep; for example gas storage caverns in salt must be maintained at a minimum gas or brine pressure to prevent creep closure. It therefore seems likely that one of two situations will develop:

- ▲ the disposal system will self-seal so that very little if any water enters and very little gas is generated once the water that is emplaced with the waste packages has been used up; or
- ▲ a dynamic equilibrium is established between the gas pressure and the inflowing water. If water is able to enter the repository it implies that there will be sufficient permeability for the resulting gas to escape. In this case it may be necessary to consider the implications of the transport of radioactive gases.

The first case does not appear to pose a threat to the repository as the system is essentially static. The second case is self-regulating provided the access tunnel/shaft seals are able to withstand the excess pressure that develops.

In both cases a key parameter is the amount of gas that is generated as a result of the water that is emplaced with the wastes. If there is too much water present at closure for the system to handle, damaging over-pressures may develop. Thus, a key component of the repository design must be to ensure that there is sufficient pore space to accommodate the gas associated with the disposed water, or a means by which any generated gases are allowed to be transported through the repository to a location where any gas build-up can be managed.

Based on the above, sensitivity cases that it would be interesting to run include:

- ▲ A zero geosphere flux case to assess maximal gas generation due to initially disposed water and initial water in the near-package voidage.
- ▲ A slower geosphere flux case in particular to demonstrate the impact on cases that are already water rate limited in the central analysis case (e.g. compactible LILW).
- ▲ A delayed geosphere inflow case for the overpacked waste types to demonstrate the effect of any delays due to consumption of geosphere water in overpack interactions before it can arrive at the package.
- ▲ A case where geosphere flows are reduced/stopped once a limiting gas pressure is reached. Gas will continue to be generated after geosphere flow stops if there is still initially disposed water, or water that has arrived from the geosphere, already in or near the package. This will provide an indication of the engineered pore space that may be required.

These sensitivities are explored in the next section.

# 3 Sensitivity Cases

# 3.1 Zero Geosphere Inflow Results

A sensitivity case has been run in which the inflow rate from the geosphere,  $Q_{geo}$ , in the model is set to zero. Gas generation in this case limited by the amount of water that is initially present, both inside the waste package and in the void space surrounding the waste package (unless the waste contains organic material, in which case radiolysis of the organic material can proceed without requiring water to be present).

The initial amounts of water in the void space surrounding the package are assumed to be the same as in the central analysis case, being based on an assumption of a crushed salt backfill with porosity 0.33 and a water saturation of 0.1 for all cases except the decommissioning and depleted uranium waste groups. Since the KONRAD container is not considered in the analysis, an initial external saturation of zero is assumed for these waste groups to prevent immediate unrealistically high water flows into the waste (Benbow et al., 2023). The chosen backfill porosity and initial saturations are subjective values. In cases where the initial water is consumed without fully corroding the metals, the net gas generation will scale linearly for smaller values of the initial saturation and for larger values of the initial saturation until the limiting saturation required to fully corrode the metals is reached. In cases where the metals are fully corroded without exhausting the initial water inventory, smaller water inventories will lead to identical amounts of gas generation (ignoring contributions from radiolysis) until the limiting saturation is reached. Water saturations outside the package in this case are expected to fall as water is not replenished after being consumed in corrosion reactions with the package exterior or after being transported to the interior of the package. Full water saturation could still be maintained inside the package if there is sufficient water outside the package to resupply it, so this is a conservative assumption as it enables the faster gas generating processes inside the package.

Results for the zero inflow case are shown in Figure 3-1 - Figure 3-10. The plots show the zero inflow case (solid lines) and the corresponding results for the central case (dashed lines). Inventories of metals and organics are shown in the top-left and topright plots respectively. The water saturations inside and outside the package are shown in the bottom-left plot and the generated gas amounts are shown in the bottom-right plot.

The vitrified, research reactor spent fuel, uranium collection filters and reprocessing wastes (Figure 3-1 - Figure 3-4) show no difference in rates and amounts of corrosion when compared to the central analysis case because the initial water inventory assumed outside the package is sufficient to corrode the packaging and then the waste metals without requiring an additional flux of water from the geosphere. The only noticeable difference between the zero inflow and the central case is in the calculated gas amounts

for the vitrified waste (Figure 3-1). For the central case the continuing supply of water leads to continuing radiolysis at late times and therefore a continually increasing amount of generated gas. For the zero geosphere inflow case, the remaining water initially outside the package becomes available to the inside after the package is corroded, but this is eventually consumed by radiolysis at around  $2 \times 10^5$  y, after which time gas generation ceases, resulting in~23% as much gas being generated as for the central case. The final gas amount would be lower if a smaller initial saturation outside the package was assumed.

The decommissioning and legacy wastes (revised from the OPERA HLW technical waste) are shown in Figure 3-5 and Figure 3-6 respectively. As noted in Section 2.5, in the decommissioning waste case it is assumed that there is initially no water in the void space outside the package to avoid an unrealistic influx of water when the package is emplaced. Therefore, for this case, the zero flux case results in no water being available to the package and so no gas generation occurs. Sensitivity to the initial amount of water that is assumed could be investigated, but since only a small amount of gas is generated in the central case for this waste group this calculation has not been done.

The legacy waste (Figure 3-6) shows some more interesting variation from the central case. For this waste group, corrosion of the packaging is delayed in the zero geosphere flux case. This is because the interior of the package is initially dry. In the central case, since the package is vented, a fraction of the water from the geosphere flows directly to the interior of the package, allowing the waste packaging to be corroded from both sides. The waste metal corrodes simultaneously. In the zero flux case, the waste packaging can only corrode from the outside and the waste metal cannot corrode until the packaging corrosively fails. Corrosion of the packaging therefore takes approximately twice as long in the zero flux case and complete corrosion of the waste metal occurs at close to 10<sup>6</sup> y. The waste contains organics. In the central case, water is always available in the package interior allowing organic hydrolysis reactions to proceed. In the zero flux case water is not available until the package is corroded, which allows the reactive and stopped phases to approach equilibrium, while being degraded by radiolysis. After the package is corroded the hydrolysis reactions can commence and the organics are quickly depleted. Net amounts of gas produced by the central and zero flux cases are approximately the same, being mostly determined by the initial metal and organics inventories, which are eventually depleted in both cases. However, since the corrosion and package failure is delayed in the zero flux case the generation of gas is similarly delayed. The final gas amounts differ slightly due to the differing amounts of gas that are produced as a consequence of radiolysis between the cases.

Results for the depleted uranium waste group are shown in Figure 3-7. All gas generation for this case is a consequence of radiolysis of  $H_2O$  (Section 0) and so amounts of gas generated are considerably reduced for the zero flux case, being around 2% of the

amount generated in the central case. If the initial amount of water outside the package was assumed to be smaller, the final gas amounts would be scaled by the same amount.

The molybdenum waste group results are shown in Figure 3-8. Since there is sufficient water available initially (inside and outside the package), the metals corrode at the same rate for the zero flux case as for the central case. The water inventory inside the package is reduced as a consequence of the corrosion, but not depleted. The amount of gas generated is therefore identical for both cases.

The non-compactible LILW (Figure 3-9) behaves similarly to the molybdenum case, with amounts of gas generated again identical for the zero flux and central cases.

The compactible LILW waste group results are shown in Figure 3-10. For this case the results differ considerably from the central case. The initial water inventory inside the package is consumed during storage in both cases. Once placed in the repository, the initial water outside the package is quickly consumed while fully corroding the galvanised steel packaging and partially corroding the aluminium in the waste. After this time no more water is available in the zero flux case and so the metal amounts remain constant for the remainder of the evolution. The only gas generating process in the zero flux case is then radiolysis of organics, which contributes a small amount of additional gas to that produced through corrosion of the metals. The final amount of gas generated is ~13% of that generated in the central case.



Figure 3-1 Vitrified waste: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-2 Research reactor spent fuel: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-3 Uranium collection filters: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-4 Reprocessing waste: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.

56



Figure 3-5 Decommissioning waste (revised OPERA HLW Technical Waste): metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-6 Legacy waste (revised OPERA HLW Technical Waste): metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-7 Depleted uranium: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-8 Molybdenum waste: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-9 Non-compactible LILW: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.



Figure 3-10 Compactible LILW: metals (top-left); organics (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – zero geosphere inflow case; dashed lines – central case.

## 3.2 Slower Non-Zero Geosphere Inflows

The effect of geosphere fluxes that are slower than that considered in the central case would be bounded by the zero flux results and the central case results and can be qualitatively predicted to be as follows:

- ▲ Vitrified waste an intermediate flux would lead to gas generation between 23% and 100% of that seen in the central case, depending on the degree to which the supply of water allows radiolysis to occur. The generation rate due to radiolysis attains a maximum when the package volume is saturated. Any additional flux that is greater than the rate of consumption due to radiolysis will have no effect.
- ▲ Research reactor spent fuel an intermediate flux would lead to the same amount of gas generation as the zero flux and central cases.
- ▲ Uranium collection filters an intermediate flux would lead to the same amount of gas generation as the zero flux and central cases.
- ▲ Reprocessing waste an intermediate flux would lead to the same amount of gas generation as the zero flux and central cases.
- ▲ Decommissioning waste (revised OPERA HLW Technical Waste) an intermediate flux would lead to gas generation between 0% and 100% of that seen in the central case. The final amount will depend on whether the cumulative supply of water is able to fully corrode the metals. While metals are present, rates of gas generation from corrosion will dominate. After the metals are corroded, the gas generation is determined by radiolysis, with a rate that only reduces by a factor of ~4 between 10<sup>3</sup> and 10<sup>6</sup> y due to the long-lived radionuclide inventory.
- ▲ Legacy waste (revised OPERA HLW Technical Waste) an intermediate flux would lead to the same amount of gas generated as the zero flux and central cases, with the timing being between that of the two cases.
- ▲ Depleted uranium an intermediate flux would lead to generation of gas in excess of that seen in the zero flux case. The excess above this will be bounded by the maximum rate of gas production that is possible from radiolysis of H<sub>2</sub>O, which attains a maximum when the package volume is saturated. Any additional flux that is greater than the rate of consumption due to radiolysis will have no effect.
- ▲ Molybdenum waste an intermediate flux would lead to the same gas generation as the zero flux and central cases.
- ▲ Non-compactible LILW an intermediate flux would lead to the same gas generation as the zero flux and central cases.
- ▲ Compactible LILW an intermediate flux would lead to gas generation between 13% and 100% of that seen in the central case. Compared with the zero flux case,

the additional flux of water would be mostly consumed in corrosion reactions with the waste metals.

The effect of varying the initial amount of water inside and outside the package can be similarly qualitatively assessed by considering whether for wet packages the initial water inside the package is sufficient to fully corrode the packaging and waste, whether for dry packages the initial water outside the package is sufficient to corrode the packaging and then the waste. If contributions from radiolysis and organics are ignored, smaller initial amounts of water will lead to similar amounts of gas generation until a critical amount is reached that is insufficient to fully corrode the package and waste. The final amount of gas generated would then scale linearly with the initial amount of water for initial amounts that are less than the critical value.

# 3.3 Delayed Inflow Due to Overpack

The following waste groups contributed the most significant amounts of gas in the central case (see Section 2.11):

- ▲ Vitrified waste, ~91% of gas in lower level;
- ▲ Depleted uranium, ~84% of gas in upper level;
- ▲ Compactible LILW, ~16% of gas in upper level;
- ▲ Molybdenum, ~0.5% of gas in upper level, but potentially more significant given emplacement geometry and pessimisms in depleted uranium model;
- ▲ Non-compactible LILW, ~0.3%% of gas in upper level, but potentially more significant given emplacement geometry and pessimisms in depleted uranium model.

Of these cases, the vitrified waste will be emplaced in an overpack that would be expected to provide some resistance to the geosphere flux. Although corrosion of the overpack is not explicitly modelled (it is not included in the scope of the current study) its presence can be represented by assuming that it leads to a delay in the arrival of water from the geosphere. A notional time of 1,000 y is assumed to be required to corrode the overpack once it is placed in the repository. Before this time, it is assumed that the geosphere flux cannot access the package and the initial water in the void space outside the package is also isolated from the package. After failure of the overpack, water is assumed to flow towards the package at a rate equal to that in the central case (1 g/m/day). The instant availability of the initial water in the void volume surrounding the package is not applied in this case.

Figure 3-11 shows the results for the vitrified waste case (solid lines) compared with those from the central case (dashed lines). The onset of corrosion of the steel packaging can be seen to be delayed. However, the 1,000 y delay is insignificant in the overall

corrosive failure time of  $\sim 5 \times 10^4$  y, and since the major contribution to gas generation is radiolysis of H<sub>2</sub>O inside the package after corrosive failure, the overall rate of gas generation is largely unaffected.

The results suggest that the overpack will not greatly affect the amount of gas that can be generated from the vitrified waste package unless it can be engineered to isolate the waste package from any available water for timescales much greater than 1,000 y. The same effect would be expected if the overpack was represented in the same way for the other overpacked packages in the lower repository level.

Like the central case, this delayed geosphere flux case does assume a constant flux of water from the geosphere (after the delay), which is noted to be an unrealistic assumption. This is investigated further in Section 0



Figure 3-11 Vitrified waste: metals inventory (top-left); organics inventory (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – delayed geosphere inflow case; dashed lines – central case.

# 3.4 Limiting Inflow with Pressure

As noted in Section 2.11, it might be expected that the rate of inflow of water from the geosphere would be slowed by the gradual build-up of pressure in and around the waste packages. Such a case can be approximated in the model by setting the geosphere flux,  $Q_{geo}$  (kg/y), to be function of the gas pressure outside the package,  $P_{g,out}$  (Pa). If  $Q_{geo,0}$  (kg/y) is the initial geosphere flux before any gas is produced, then the pressure-dependent (and therefore time-dependent) geosphere flux can be defined to be

$$Q_{geo}(t) = Q_{geo,0} \left( \frac{P_{\rm lim} - P_{g,out}(t)}{P_{lim}} \right).$$
(3.1)

Here,  $P_{\text{lim}}$  (Pa) is a limiting gas pressure at which the geosphere inflow is assumed to halt. For the calculations,  $P_{\text{lim}} = 10.78$  MPa has been chosen, which is approximately lithostatic pressure at 500 m depth in halite, or alternatively is approximately hydrostatic pressure at 900 m depth. To perform the calculations, it is necessary to calculate  $P_{g,out}(t)$ . This can only be approximated in the current model, given the simplistic treatment of the void space and the disposition of water and gas in it.

In the model, gas is produced inside and outside the package through degradation of the waste form and the outer packaging. Gas produced inside the package will remain in the package if it is sealed, until such time that the package fully corrodes or fails mechanically, when the gases produced inside /outside of the package can begin to migrate out of / into the package and mix. For open/vented packages, this mixing can take place immediately.

It is assumed that the gas outside the package can migrate directly into open pore and void space that is directly connected to the pore and void space outside the package. This assumes that the gas can easily migrate into the void space surrounding the package and so implicitly assumes that the pores represented by this volume are large, in some sense. Additionally, if the gas pressure is sufficiently large it may exceed the air entry pressure for tighter regions of the pore space and gas may begin to penetrate deeper into the salt, but this is currently ignored.

To approximate  $P_{g,out}(t)$  it is necessary to define the volume in which the generated gas can reside. It will be assumed that:

- ▲ The void space in and around the package that can potentially accommodate gas is unchanged from the initial emplacement conditions; in particular, reduction of void space due to salt creep is neglected; and
- ▲ The total void space will be assumed when calculating gas pressures; any water in the void space will be ignored for the purposes of calculating the gas pressure.

These assumptions will tend to over-estimate the volume available to accommodate gas, and hence under-estimate the gas pressure. This in turn will tend to over-estimate the inflow, by (3.1).

For closed packages, prior to corrosive or mechanical failure of the outer packaging the separate gas pressures inside and outside of the package,  $P_{g,in}$  and  $P_{g,out}$  (Pa), can be approximated by

$$P_{g,k} = \frac{R_{GAS}T}{V_k^P} \sum_{i \in \{Gases\}} G_{i,k}, \quad \forall \ k \in \{in, out\}.$$
(3.2)

Here,  $R_{GAS}$  (J K<sup>-1</sup> mol<sup>-1</sup>) is the gas constant and T (K) is the temperature. The other terms on the right-hand-side use the same notation as Benbow et al. (2023), so that  $V_k^P$  (m<sup>3</sup>) is the available pore space/void volume inside and outside the package and  $G_{i,k}$  (mol) is the cumulative amount of gas of type *i* generated inside and outside the package. While the package is closed, with the above assumptions  $P_{g,out}$  is an approximation to the tunnel gas pressure from the model that should be used in (3.1). The approximation assumes that all packages of the same type evolve identically.

For open/vented packages or for closed packages after corrosive or mechanical failure of the outer packaging, the gas pressures inside and outside the package are assumed to be equal, and can be approximated by

$$P_{g,in} = P_{g,out} = \frac{R_{GAS}T}{V_{in}^P + V_{out}^P} \sum_{i \in \{Gases\}} G_{i,in} + G_{i,out}.$$
(3.3)

Again,  $P_{g,out}$  is then the approximation the tunnel gas pressure that should be used in (3.1), which assumes that all packages of the same type evolve identically.

These estimates are clearly only a very approximate measure of the possible gas pressure in the disposal tunnels. A more detailed coupling of gas generation and gas migration in the near field and geosphere would be required to provide a more realistic estimate. (Similar coupled models have previously been simulated using QPAC in Watson et al., 2012.) The effect on each of the waste groups of limiting the geosphere inflow as a function of gas pressure is summarised below. In several cases the limiting of the flux has little or no effect. The cases for which the effect is more significant are discussed further below.

- ▲ Vitrified waste no difference to the calculated gas generation, but the effect on the water saturation can be seen. The case is discussed further below.
- ▲ Research reactor spent fuel the limiting pressure is not reached so almost identical gas generation to the central case is seen.
- ▲ Uranium collection filters – the limiting pressure is not reached so almost identical gas generation to the central case is seen.
- ▲ Reprocessing waste – the limiting pressure is not reached so almost identical gas generation to the central case is seen.

- ▲ Decommissioning waste – the limiting pressure is not reached so almost identical gas generation to the central case is seen.
- ▲ Legacy waste – the limiting pressure is not reached so almost identical gas generation to the central case is seen.
- ▲ Depleted uranium a significantly smaller amount of gas is generated. The case is discussed further below.
- ▲ Molybdenum waste no difference to the calculated gas generation. The case is discussed further below.
- ▲ Non-compactible LILW same as molybdenum
- ▲ Compactible LILW a significantly smaller amount of gas is generated. The case is discussed further below.

The results for the vitrified waste when the geosphere flux is pressure-limited are compared with those from the central case in Figure 3-12. The pressure-limited case is shown by the solid lines and the central case is shown by the dashed lines. Gas generation is identical to the central case because by the time that the pressure-limitation begins to significantly reduce the inflow (as seen in the water saturation outside the package in the bottom-left plot) the interior of the package is fully saturated and so radiolysis of  $H_2O$ , which is the only gas generating process, can continue at the maximal rate. If the flux had been halted much sooner it is possible that the water inventory inside the package could become exhausted by radiolysis, but for the central case parameterisation and simplistic pressure model described above the exterior of the package does not become dry in the  $10^6$  y period that is simulated, which allows the inside of the package to remain fully saturated (since water outside the package is still conservatively assumed to be rapidly transferred to the interior of the package when space is available).

The results for depleted uranium when the geosphere flux is pressure-limited are compared with those from the central case in Figure 3-13. The pressure-limited case is shown by the solid lines and the central case is shown by the dashed lines. The pressure-limitation halts the geosphere inflow at  $\sim 2 \times 10^4$  y, as seen in the water saturation outside the package in the bottom-left plot. At the same time, water in the inside the package continues to be consumed by radiolysis. The remaining water is drawn from the outside into the interior of the package (to maintain full saturation inside the package) until  $\sim 10^5$  y when the water outside the package becomes exhausted. After this time, the water saturation inside the package begins to fall until it is completely consumed by  $\sim 2 \times 10^5$  y. At this point, gas generation stops. The final amount of gas generated is  $\sim 7\%$  of that seen in the central case. The resulting amount of gas generation would be lower if a slower initial geosphere flux had been assumed.

The results for the molybdenum waste when the geosphere flux is pressure-limited are compared with those from the central case in Figure 3-14. The pressure-limited case is shown by the solid lines and the central case is shown by the dashed lines. An identical amount of gas is generated as for the central case because at the time that the pressurelimitation causes the geosphere inflow to halt (at  $\sim 1.6 \times 10^4$  y, as seen in the water saturation outside the package in the bottom-left plot) there is sufficient water outside the package to continue to supply the interior of the package to fully corrode the waste metals. The result for non-compactible LILW is similar.

The results for the compactible LILW waste when the geosphere flux is pressure-limited are compared with those from the central case in Figure 3-15. The pressure-limited case is shown by the solid lines and the central case is shown by the dashed lines. The results are significantly different to those of the central case. As for the central case, after the package is placed in the repository there is a period of rapid corrosion of the galvanised steel packaging followed by some aluminium corrosion. The corrosion reactions are sufficiently rapid that a zero saturation is effectively maintained, the rate of corrosion is therefore limited by the rate at which water is supplied by the geosphere flux. Before the aluminium is fully corroded, the pressure limit is reached and inflows from the geosphere are halted. The package and its surroundings then remain dry for the remainder of the evolution. The only gas generation process that can continue to occur is radiolysis of the organic waste, as seen in the top-right plot. Due to the decay and ingrowth pattern (Figure 2-51) the decay power is greater at later times, causing greater amounts of gas generation towards the end of the simulated period. The final amount of gas generated is ~13% of that seen in the central case.



Figure 3-12 Vitrified waste: metals inventory (top-left); organics inventory (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – pressure-limited geosphere inflow case; dashed lines – central case.



Figure 3-13 Depleted uranium: metals inventory (top-left); organics inventory (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – pressure-limited geosphere inflow case; dashed lines – central case.
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Figure 3-14 Molybdenum waste: metals inventory (top-left); organics inventory (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – pressure-limited geosphere inflow case; dashed lines – central case.



Figure 3-15 Compactible LILW: metals inventory (top-left); organics inventory (top-right); water saturation (bottom-left); and gas generated inside and outside (bottom-right). Pink shading – storage period; grey shading – period after disposal. Solid lines – pressure-limited geosphere inflow case; dashed lines – central case.

## 3.5 Discussion

Each of the sensitivity cases that have been analysed limit the supply of water from the geosphere in different ways. Delaying the inflow for  $10^3$  y, which could be associated with a minimum time that it might take to corrode the overpacks of the packages in the lower level of the repository, was seen to have little effect on total amount of gas generated. The delay would need to be made to be significantly longer by suitably engineering the overpack to have a noticeable effect of overall gas generation in the  $10^6$  y simulation period. Assuming no inflow or a pressure-limited inflow from the geosphere only led to differences in a small number of the cases, since for most cases the amount of gas generation was determined by the water that was initially disposed in the waste and in the void space around it. Combining the pressure-limited inflow with the corrosion of the overpacks of the packages in the lower repository level may be interesting, since it is possible that overpack corrosion itself may lead to sufficiently elevated pressures that inflow may cease before the overpack is corroded, which would effectively isolate the waste indefinitely.

The effect on the final amount of gas generated of applying the alternative assumptions in the sensitivity cases is shown in Table 3-1.

Table 3-1 Percentage of gas generated in 10 <sup>6</sup> y in sensitivity calculations compared
to the central case. Cases where there is a significant reduction in the amount of gas
generated are shown in bold. Cases corresponding to blank entries were not simulated.

Waste Group	Zero Flux	Delayed Inflow	<b>Pressure-Limited</b>
Vitrified waste	23.2%	99.9%	100%
Research reactor spent fuel	99.9%		
Uranium collection filters	100%		
Reprocessing waste	100%		
Decommissioning waste	0%(*)		
Legacy waste	94.7%		
Depleted uranium	1.6%		6.8%
Molybdenum	100%		100%
Non-compactible LILW	100%		100%
Compactible LILW	12.6%		12.9%

(\*) As noted in Section 2.5, in the decommissioning waste case it is assumed that there is initially no water in the void space outside the package to avoid an unrealistic influx of water when the package is emplaced. Therefore, for this case, the zero flux case results in no water being available to the package and so no gas generation occurs.

The results suggest that the most significant factor for reducing the amount of gas generated in most cases would be to reduce the amount of water initially in and around the waste, combined with limiting the water supply, since limiting the water supply alone cannot achieve that aim in most cases.

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Other sensitivity cases were considered in the process of the analysis, in particular the effects of higher temperatures. Higher temperatures were found to have little effect, with the majority of the gas generation occurring over timescales that are longer than the  $\sim 10^4$  y timescale over which temperatures might be expected to remain elevated. In those cases in which corrosion occurs over shorter timescales (e.g. the compactible LILW waste), the increase in temperature may cause some corrosion reactions to be accelerated, but this would only shorten the (already short) timescale over which gas is generated and not affect the total amount of gas that is generated.

## 4 Summary

The gas generation model described in Benbow et al. (2023) has been run for the central analysis case described in the report and for a selection of sensitivity cases in which the availability of water is varied. A summary of the resulting evolution of the waste form and resulting gas generation for the central case is given in Section 2.11. The following waste groups were found to lead to the major contributions to gas generation in the lower and upper levels of the repository when gas generation from all disposed packages is considered:

- ▲ Vitrified waste, 90% of potential lower repository level gas.
- ▲ Depleted uranium, 84% of potential upper repository level gas.
- ▲ Compactible LILW, 16% of potential upper repository level gas.
- ▲ Molybdenum, 0.5% of potential upper repository level gas, but potentially a larger contribution if depleted uranium model conservatisms were addressed.
- ▲ Non-compactible LILW, 0.3% of potential upper repository level gas, but potentially a larger contribution if depleted uranium model conservatisms were addressed.

For the vitrified waste and depleted uranium waste groups, gas generation is primarily a consequence of radiolysis of H<sub>2</sub>O inside the package after failure, which is likely to be over-estimated in the model due to the assumption that water can intimately mix with the radionuclide inventory, whereas in reality the glass and cement grout matrices would probably absorb a significant proportion of the alpha decay energy. Other than accounting for this inhibition of alpha decay energy, with the modelling assumptions a reduction in the amount of gas generation can only be achieved by limiting the amount of water initially in and around the package and limiting the geosphere flux. Comparing the zero flux and central case results for the depleted uranium case, it is seen that radiolysis from water due to the geosphere flux, rather than the water initially surrounding the package, hugely dominates the rate of gas generation. Several waste groups include a cement grout. The role of grout in the depleted uranium case is complicated. It introduces initially disposed water which leads to gas generation but would also be expected to restrict access of water to the waste and reduce radiolysis. In the current model direct conclusions cannot be drawn regarding its effectiveness at limiting gas generation.

For the molybdenum and non-compactible LILW waste groups, metal corrosion dominates the gas production. The zero-flux sensitivity case showed that the water assumed to be initially inside and outside the packages was sufficient to fully corrode the metals without requiring an additional source of water from the geosphere and so gas generation can only be reduced by reducing the amount of water initially in and around the package. The waste groups account for less than one percent of the simulated gas production in the upper level of the repository, but since these waste packages are packaged relatively tightly in the repository and have small internal voidage to contain any produced gas, their overall effect may be more significant than indicated by the amount of gas produced.

The compactible LILW waste group shows the most complex gas generation behaviour, due to the mixture of metals and organics in the waste, with corrosion/degradation of both significantly contributing to the overall amount of gas produced. Like the depleted uranium case, corrosion due to the geosphere flux, rather than the water initially available to the package, hugely dominates the overall gas generation. This waste group has the greatest number waste packages in the repository by far, they are packed the most tightly and they therefore have the smallest voidage per package of all of the waste groups in the upper level of the repository. Given that gas generation from the depleted uranium waste group is likely over-estimated in the model, as was noted above, compactible LILW is likely to be the most significant source of gas in the upper level of the repository.

Gas generation in all the above cases is sensitive to both the initial amount of water in and around the package and the geosphere flux. The estimation of the amount of water initially surrounding each package is highly uncertain. Gas generation in the central analysis may be reduced in some cases if data were available that allowed a more realistic estimate to be made. A more realistic representation of the coupled effect of salt creep on water availability in the model could lead to a significant reduction in gas produced in each of the cases. This would however reduce the void space in which gas can reside, which would ultimately have an inverse effect on the gas pressure.

The model also does not account for potential 'sharing' of void space between the waste groups if gas is allowed to migrate through the facility. This would affect the calculated gas pressure in the sensitivity case in which inflow is pressure-limited, since void space around packages exhibiting little gas generation may potentially provide a 'buffer' for more highly gas-generating waste groups.

The effect of the overpack is ignored in the current models since this is being investigated in separate studies by COVRA, but it could be added in a future update to the model.

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Overpack corrosion will be an additional source of gas in the system but, if watertight, the overpack will provide additional isolation of the waste packages from sources of water until it fails corrosively. The effect of the isolation provided by the overpack was investigated in the delayed inflow case. This was seen to have little effect unless the delay can be made to be very long by suitably engineering the overpack. A delay of 1,000 y was seen to lead to negligible differences, with its most significant effect being on the timing, but not the magnitude, of gas generation. It is possible that, in the context of the pressure-limited inflow sensitivity case, gas generation from corrosion of the overpack may raise pressures to a level where water availability becomes pressure limited. If this occurs before the overpack is corroded, then the waste may be isolated indefinitely.

# References

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