

Release calculations in a repository of the very long tunnel type

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

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ABSTRACT

The VLH and KBS-3 are two alternative repository designs for high level waste. The repositories differ mainly in the layout and the canister design. In the VLH repository the canisters are placed horizontally in long boreholes. In the KBS-3 repository every canister is placed vertically in repository holes in the tunnel floor. If a small hole forms in the canister wall the nuclides diffuse through this hole into the backfill surrounding the canister. From the backfill the nuclides migrate by different pathways into the mobile water in the fractures in the rock.

A study of comparison of the nuclide release in the two alternative repositories shows releases in the same order in magnitude for a given nuclide. A quantitative assessment of the importance of the different pathways, the influence of the location of the fracture and fracture zone in relation to the damage in the canister wall and the influence of the size of the small hole (damage) is made. The assessment for the VLH-repository shows that the main pathway is that to the disturbed zone and the fracture location in relation to the damage has no large influence in the release.

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SUMMARY

In the VLH-repository for high level wastes, the canisters are placed horizontally in long boreholes. Compacted bentonite will be used to backfill the tunnel. The repository will be located in a uniform rock mass with good properties for storage and tunnelling (Sandstedt et al., 1991). In the disturbed rock zone in the vicinity of the tunnel, the water flows mainly along the tunnel. In fractures and in fracture zones the water flows around the tunnel.

The nuclide releases through different pathways were calculated for several cases. Pu-239 was chosen to study the role played by different pathways for the release. The numerical code used in the calculations is the compartment model (Romero et al., 1991). The results are summarized below.

If one canister is damaged, the nuclides escape through the damage into the bentonite. Some go to the disturbed zone and some into the fractures and fracture zone. Several cases were calculated to quantify the role of the different pathways on the nuclide release into the water. The disturbed zone accounts for 70% of the release into the water. Fractures intersecting the tunnel account for the remainder. The release is quite sensitive to assumptions used to define the boundary conditions in the fracture and in the disturbed zone. The nuclide release is strongly influenced by the size of the damage in the canister wall. The dominant transport resistance is in the small hole (damage) in the canister. For hole sizes larger than 1 cm² area, the resistance of the pathways from the bentonite begins to play a role in the nuclide escape.

The influence of the location of a fracture zone was investigated by varying the distance between the zone and the canister nearest to the zone. For distances larger than 0.5 m, the zone has a minor importance for the release of nuclides. The disturbed zone accounts for most of the release. The influence of the location of fractures along the tunnel was also investigated. This was done for the case when all canisters leak. The location that gives the largest release is when the fracture is opposite to the damage. However, it has no large significance for the total release.

The concentration build up in the disturbed zone was investigated. For the non-sorbing nuclides that have a large decay constant (I-129), the effluent concentration downstream does not change with the travelled distance in the disturbed zone. For some sorbing nuclides (Cs-137, Ra-229, and Pu-239) the relative concentration decreases considerably with the distance downstream of a leaking canister, depending mainly of the sorption coefficient and the decay constant.

The nuclide releases from the VLH and the KBS-3 repositories were compared assuming that the damage in the canister wall is a small hole and only one canister

leaks. The nuclides chosen for the comparison were I-129, Cs-137, and Pu-239. The releases are of the same order of magnitude for a given nuclide. For the sorbing nuclides the uptake in the water is very small compared with the release from the canister. The reason is that for these nuclides the sorption in the bentonite gives the nuclides time to decay. The non-sorbing nuclides with low decay constant (I-129) do not decay much.

Small differences were found for the nuclide escape from the two repositories types. The KBS-3 gives somewhat larger nuclide escape than the VLH-repository. They are mainly due to differences in the thickness of the canister wall, and the larger inventory in the VLH case. The differences are well within uncertainties in the assumptions.

1 INTRODUCTION

In the VLH repository concept (Sandstedt et al., 1991) there are three parallel, 4.5 km long, horizontal tunnels at a depth of 500 m with an investigation tunnel approximately 100 m below the repository. The tunnel diameter is 2.4 m for deployment of canisters with a diameter of 1.6 m. The space between the canister and the rock is totally backfilled with bentonite. Around the tunnel, a disturbed zone forms. Water flows in fractures which intersect the tunnel and in the disturbed zone along the tunnel.

The backfill consists of compacted bentonite with an average density of about 2.0 t/m³ and a hydraulic conductivity between 10^{-14} and 10^{-12} m/s depending of the salt content in the pore water. The slots between the bentonite blocks and the rock are filled with water or a bentonite slurry to ensure an early water saturation. No inflow of water takes place after emplacement of the bentonite.

The canister is a cylinder with a diameter of 1.6 m, length of 5.9 m, and a wall thickness of 161 mm for the steel body covered with a 60 mm layer of copper. The ends are spherical to provide the best possible form to withstand pressure. The canister is designed to contain 24 BWR elements or 6 PWR and 6 BWR elements. The weight of this canister is about 58 tons.

The repository area should be located in a uniform rock mass with good properties for storage and tunnelling. No major fault zones, crushed rock-zones or sections with high fracturing will cross the area. If a major fault zone is to be crossed, the tunnels could be extended and any part of the tunnel near the zone could be sealed off and not be used for storage of radioactive waste.

The VLH and KBS-3 (KBS-3 reports, 1983) are two alternative repositories for high level waste. The repositories differ mainly in the layout. In the VLH repository, the canisters are placed horizontally in long boreholes. In the KBS-3 repository every canister is placed vertically in repository holes in the tunnel floor. There is also another difference which could be important for the environment around the canister, namely the production of oxidants by radiolysis of the water intruding the canister. The iron in the canister in the VLH repository will help to maintain a much lower production rate of oxidants than the KBS-3 repository. The iron in the 161 mm thick steel body will react with the oxidants and ensure that a redox front around the canister does not form.

2 DESCRIPTION OF THE DIFFERENT CASES

The VLH repository consists of long horizontal tunnels where the canisters are placed horizontally. The space between the canister and rock is backfilled with compacted bentonite. The water flows in fractures and in the disturbed zone along the tunnel (horizontal flow) in the rock immediately adjacent to the tunnel wall. Large water bearing fracture zones will be avoided by sealing off the rock.



Figure 1 Schematic view of the tunnel including the canisters, disturbed zone, fracture zone, and fracture. The arrows show the direction of the water flow.

The system is highly variable in the sense that there may be different modes of damage in the canister. The location of the damage in relation to the fractures can vary, the distance from a canister to the fracture zones can also differ. The disturbed zone properties as well as the transport properties of the fractures and fracture zones can vary considerably. We have elected to approach the problem by defining some cases for which releases are computed. Some variation cases are also investigated. Later, in another report, a sensitivity analysis will be performed to find the influence on the results of the variability of important entities.

When the canister is damaged nuclides will dissolve in the intruding water and leak out through the damage into the bentonite. The damage in the canister wall is assumed to be a small hole. From the bentonite the nuclides may diffuse into fractures intersecting the tunnel, into the disturbed zone around the tunnel, and also into the fracture zones.

In a base case we study only one canister leaking nuclides to the fracture, the disturbed zone, and the fracture zone. In some more complex cases we study the nuclide transport in the disturbed zone influenced by neighbouring canisters which also leak.

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3 BASE CASES, ONE CANISTER LEAKS

The function of the steel wall is to be a mechanical support. If the iron is corroded the copper wall may collapse. A hole may form through which the nuclides can escape. Moreover the properties of the bentonite will be modified by compaction if a canister swells. Another possible perturbation would be if the canister sinks through the bentonite backfill.

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The nuclide release into the fracture may be influenced by various parameters such as the size of the damaged zone in the canister wall, the diffusion coefficient of the nuclide in the bentonite, the nuclide sorption in the bentonite, etc.

The influence of the hole size in the canister wall is studied when the fracture is opposite to the small hole and a disturbed zone surrounds the tunnel, in the central case. The sorption capacity of the bentonite is determined by its volume and the sorption coefficient of the individual nuclide. The volume of the bentonite is varied by including more of the bentonite in the direction of the tunnel axis in the model. The thickness of bentonite between the canister and the tunnel is held constant. The increase of bentonite volume will be important for the nuclides with short half-life.

We start to study a case where only one canister is damaged. The damage in the canister wall is a very small hole through which the nuclides escape into the bentonite and then migrate through different pathways further into the flowing water. Some migrate to the disturbed zone, some to the fractures intersecting the tunnel, and the remainder to the fracture zones.

In a central case a fracture intersects the tunnel opposite to the small hole and a disturbed zone exists around the tunnel. The small hole is at the mid of the canister. We limit the volume of the bentonite to that surrounding the canister. Later, this volume will be increased to study the influence of the sorption capacity of the bentonite on the nuclide release. The influence of the size of the small hole on the release from the canister is also investigated.

Another case is that if a fracture zone intersects the tunnel. This is modelled assuming that the breached canister is located next to the fracture zone and the small hole is at the end of the canister nearest to the fracture zone. The distance between the fracture zone and the canister is varied to investigate the influence of this on the nuclide release.

3.1 Definition of a central case: one fracture and a disturbed zone

The central case is defined by one leaking canister, a disturbed zone around the tunnel, and a fracture intersecting the tunnel. The damage, a small hole of 5 mm^2 area, is at the mid of the canister. The volume of the bentonite is limited to that surrounding the canister. The nuclides escaping through the small hole in the canister diffuse into the bentonite and some of the nuclides diffuse into the disturbed zone where they are carried away by the water. The rest diffuse into the flowing water in the fracture. Figure 2 shows the different pathways by which the nuclides migrate into the water. Water flows in fractures around the tunnel and in the disturbed zone along the tunnel.



Figure 2 Schematic view showing the central case with a fracture, a disturbed zone, and the small hole. The arrows show the paths of nuclides into the water.

To simplify the study it is assumed that the fracture intersects the tunnel perpendicularly. The fracture is opposite to the damage in the canister. If we assume a hydraulic conductivity of 10⁻⁹ m/s, the local equivalent flowrate for the fracture may be calculated (Appendix A2). The same value was assumed in the KBS-3 calculations. The fracture aperture is 0.1 mm. The disturbed rock zone (DRZ) is the zone immediately adjacent to an underground tunnel affected by mechanical, thermal, hydraulic and chemical processes (Winberg A., 1991). A view of the disturbed zone surrounding the tunnel is show in Figure 3.



Figure 3 Cross section of the tunnel, showing the disturbed zone and the small hole in the canister wall.

Zones around excavated drifts have a hydraulic conductivity which differ from that of the undisturbed rock. In general, the conductivity is higher in the axial direction and lower in the radial direction. If there is a hydraulic gradient along the drift the water will preferentially flow in this direction. The flux will be larger than in the undisturbed rock (Push et al., 1991). Assuming a hydraulic gradient, i, equal to the regional gradient $3.0 \cdot 10^{-3}$ m/m and a hydraulic conductivity, K_p, of 10^{-8} m/s in the direction of the tunnel, the flux of water along the tunnel, q, may be calculated.

$$q = K_{p} \cdot i \tag{1}$$

The thickness of the DRZ is 0.3 m. If we assume that the flowing water in the DRZ is directly in contact with the bentonite and thus can take up nuclides which escape through the bentonite, then the water flowrate in the DRZ would be used as the equivalent flowrate Q_{eq} . This is a conservative assumption. The Q_{eq} calculated for the DRZ is 2.3 l/a, its calculation is shown in Appendix A2 in Table-A3 together with the data used to obtain it. It is almost the same as the total water flowrate through the DRZ.

3.2 Addition of a fracture zone intersecting the tunnel

If a fracture zone intersects the tunnel, a certain distance to the nearest canister is required. A part of the tunnel near the zone could be sealed off and not be used for storage of radioactive waste (Push et al., 1991).

As a particular case, the release of nuclides into the water in a fracture zone (FZ) intersecting the tunnel is investigated. The case is shown in Figure 4. The water flows in the FZ around the tunnel. Only one canister is damaged and is located next to the FZ. The small hole in the canister wall is at the end of the canister, next to the FZ. The release into the water either in the FZ or DRZ is calculated by varying the distance between the FZ and the small hole, distance x in Figure 4. The thickness of the FZ is assumed to be 0.5 m. This zone is formed by fractures of second and third order with a typical hydraulic conductivity ranging in 10^{-7} - 10^{-8} m/s (Pusch et al., 1991). The local equivalent flowrate of water for this zone is calculated and given in Table A3, in Appendix A2.



Figure 4 Schematic view showing the fracture zone, the disturbed zone, and the small hole at the end of the canister. The distance between the hole and the fracture zone is denoted by x.

3.3 Release rates of some nuclides over time

Here we use the central case to calculate the nuclide release into the water of the nuclides Pu-239, I-129, Cs-137. These calculations are compared with those for the KBS-3 repository.

The central case (see Figure 2) for the VLH-concept was already defined by that one canister leaks, the water flows along the tunnel in the DRZ and around the tunnel in the fracture intersecting the tunnel, and the damage in the canister wall is a small hole (5 mm^2) of the same size as the small hole assumed in the KBS-3 concept. The fracture is opposite to the damage.

The KBS-3 calculations are described in detail in an earlier report (Romero et al., 1991). A brief description of the repository and data are given in Appendix A1. The canisters are deposited in repository holes in the floor of a tunnel, one fracture intersects the repository hole, a DRZ exists below the tunnel and around the repository hole, one fracture intersects the tunnel, and a fracture zone is present below the repository hole.

4 COMPLEX CASES, SEVERAL CANISTERS LEAK

If several canisters leak simultaneously the situation is more complex because the water in the disturbed zone has already a nuclide concentration profile as it approaches the next canister. Several cases are studied. The influence of the location of the fracture, the uptake in the damaged zone, and the number of canisters damaged are studied.

4.1 Location of the fracture intersecting the tunnel

It is assumed that all the canisters have a small hole and the tunnel is intersected by fractures every 6 metres (\approx canister length). To simplify the study it is assumed that the fractures intersect the tunnel perpendicularly to the tunnel. The water in the fracture flows around the tunnel. All nuclides escaping from the damaged canisters diffuse through the bentonite into the fractures intersecting the tunnel and into the disturbed zone.

The influence of the fracture location along the tunnel and of the water flowrate in the fracture on the nuclide release is studied. Figure 5 shows a view of fractures intersecting the tunnel and the dashed lines show a different location of the fractures. The damage is placed both at the center and at the end of the canister. The fractures are located both opposite to the damage and far away from it.



Figure 5 Schematic view of the tunnel, showing the small hole in the canister wall and two different possible locations of the fracture.

4.2 Disturbed zone

To study the release into the disturbed zone, the previous nuclide uptake upstream must be considered. We study cases where all canisters and where a few canisters are damaged. For the case of a few damaged canisters, we consider if they are located adjacent to each other or not.

The assumptions in the calculations for all damaged canisters and few damaged canisters are otherwise the same. The calculation of the local equivalent water flowrate is used to estimate the diffusional transport into the water in the zone. The local equivalent flowrate of water (Q_{eq}) is calculated by a simple relation, see Section 5.2.

$$Q_{eq} = \sqrt{n} \cdot Q_{eq,1} \tag{2}$$

Where n is the number of damaged canisters and $Q_{eq,1}$ is the local equivalent flowrate of water in the DRZ when the water along the tunnel passes the first damaged canister.

The concentration in the DRZ, downstream the damaged canister, may decrease due to diffusion into the rock matrix and sorption within it. If sorption is important, the nuclide residence time in the DRZ along the tunnel can be long and allow some decay. Analytical solution will be used to investigate this effect.

5 APPROACHES TO CALCULATIONS

After the canister is breached the nuclides dissolved in the water volume within the canister escape through the small hole into the bentonite by diffusion. The water inside the canister is assumed to be well mixed. The transport resistance of the canister itself is thus reduced to the resistance of the small hole which depends on its size. In the bentonite in the tunnel there is no flow of water. The solute transport through the bentonite is by diffusion only. The transport into the bentonite and into the mouth of the fractures is approximated using earlier derived analytical solutions (Romero et al., 1991).

5.1 Compartment description

The basic idea behind the compartment model (Romero et al., 1991) is to subdivide a complex geometry into a number of compartments. In our model we also use analytical solution in zones where the solute transport calculation would otherwise require a very fine discretization in compartments.



Figure 6 A first discretization of the VLH-repository in compartments when there is only one breached canister. The arrows show the direction of the flowing water.

Figure 6 shows a first subdivision into compartments of the VLH-repository. The hole is represented by two compartments and the bentonite by one compartment. To approximate the transport into the bentonite from the small hole and from the bentonite

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into the fracture, two additional compartments are introduced at the outlet of the small hole and at the inlet of the fracture. Each of these compartments represents the resistance of the bentonite to the transport of solute. These compartments are obtained using exact analytical solutions at steady state.

5.2 Notion of the equivalent flowrate, Qeq

The equivalent flowrate Q_{eq} is a fictitious flowrate of water which carries with it a concentration equal to that at the compartment interface. It has been derived by solving the equations for diffusional transport to the passing water (Neretnieks, 1979).



Figure 7 Schematic picture, which describes the definition of the local equivalent flowrate of water, Q_{eq}.

We assume that the nuclide concentration of the approaching water is constant, e.g., zero. Then during its slow passage past the length of bentonite the nuclides will diffuse into the mobile water. When this water leaves the vicinity of the bentonite, the water will have picked up nuclides to a certain distance (penetration of the solute by diffusion) from the interface. If the concentration at the interface between the bentonite and the mobile water is c_w , the flowrate of nuclide (N) from the bentonite to the water is

$$N = q \cdot W \cdot \overline{\eta} \cdot c_w \tag{3}$$

where q is the flux of water passing the bentonite, W is the width of the bentonite area in contact with the fracture, fracture zone or damage zone. $\overline{\eta}$ is the mean penetration thickness into the water by diffusion from the bentonite. These entities are defined in Figure 7.

The mean penetration, $\overline{\eta}$, can be obtained by integrating the solution to the diffusion equation for the case of a solute diffusing into the passing water (Bird et al., 1960), for a time equal to its residence time, t_w. This was obtained by Neretnieks (1980).

$$\overline{\eta} = \sqrt{\frac{4 \cdot D_{w} \cdot t_{w}}{\pi}}$$
(4)

The residence time, t_w , is the time that the water is in contact with the bentonite. This is obtained from the flux of water (q), flow porosity (ε_f), and the length of the pathway in contact with the water (L):

$$t_{w} = \frac{L}{q/\varepsilon_{f}}$$
(5)

Replacing Equation (4) in Equation (3), we get,

$$N = q \cdot W \cdot \sqrt{\frac{4 \cdot D_w \cdot t_w}{\pi}} \cdot c_w$$
(6)

The equivalent flowrate of water is defined by

$$N = Q_{eq} c_w \tag{7}$$

Then combining the Equations (6) and (7), we obtain the definition of the equivalent flowrate Q_{eq} expressed as

$$Q_{eq} = q \cdot W \cdot \sqrt{\frac{4 \cdot D_w \cdot t_w}{\pi}}$$
(8)

Combining the Equations (5) and (6), we obtain the equivalent flowrate expressed in another form where $A = L \cdot W$ is the contact area of the bentonite with the rock.

$$Q_{eq} = A \cdot \varepsilon_{f'} \sqrt{\frac{4 \cdot D_w}{\pi \cdot t_w}}$$
(9)

If n canisters after each other are damaged the situation will resemble a case where the contaminated clay is n*L meters long. The mean penetration thickness for canister "i" may be calculated by using Equations (4) and (5). The cross section area which carries water with a concentration c_w , added by canister "i" becomes

$$A_{i} = W \cdot (\overline{\eta}_{i} - \overline{\eta}_{i-1})$$
(10)

and the flowrate of nuclides transported from any canister "i" is

$$N_{i} = q \cdot W \cdot (\overline{\eta}_{i} - \overline{\eta}_{i-1}) \Delta c_{w}$$
(11)

Thus for an arbitrary canister the equivalent flowrate is defined by the following equation:

$$Q_{eq, i} = q \cdot W \cdot \left(\overline{\eta}_i - \overline{\eta}_{i-1}\right)$$
(12)

If we are interested in the local equivalent flowrate of n successively breached canisters the calculation is simpler. It may be obtained directly from Equation (8) by setting $t_w = n \cdot t_{w,i}$. Where $t_{w,i}$ is the residence time for one canister.

$$Q_{eq} = q \cdot W \cdot \sqrt{\frac{4 \cdot D_{w} \cdot n \cdot t_{w,i}}{\pi}}$$
(13)

This equation may be simplified. We obtain the equivalent flowrate for n successive canisters as a function of the first canister of a succession of damaged canisters.

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$$Q_{eq} = \sqrt{n} \cdot Q_{eq,1} \tag{14}$$

So far no account has been taken of decay and uptake into the rock matrix along the flow path. If the flow path from a damaged canister is long in the disturbed zone, the nuclides in the mobile water may diffuse into and sorb in the porous matrix of the rock. Sorbing nuclides will then be retarded during their transport in the zone. This process gives the nuclides more time to decay during their transport already in the near field. If the half-life of the nuclides is short it is possible that the water passing the next canister already is noticeably depleted of nuclides. This will be investigated further by using the equation for flow and transport in fractured rock, the ADD-model.

6 MATHEMATICAL MODELS

The main model used in the calculations is the compartment model (Romero et al., 1991). The advection - dispersion with matrix diffusion, ADD-model (Neretnieks et al., 1980) will be used to investigate the concentration downstream in the disturbed zone.

6.1 Compartment model

The core of this model is the compartment with its in and outflows and accumulation of nuclides. Special compartments are introduced at the mouths of the small in and outflow locations at the damage in the canister and at the fracture mouths. They are designed so that they have the correct transport resistance at steady state. The capacity of these compartments for holding solute is negligible. The transport into flowing water is formulated as a compartment but with no capacity of accumulation because the water flows away. The special compartment is that of the fuel itself. This compartment acts as a single well-mixed compartment with a volume equal to the volume of water within the canister.

The system of equations describing the radionuclide release of a single nuclide was developed by Romero et al. (1991). The system of equations is summarized in a matrix form:

$$\frac{d\bar{c}}{dt} = \overline{\bar{F}} \cdot \bar{c} + \overline{B}$$
(15)

where the term $(d\overline{c}/dt)$ accounts for the change of concentration with time. It is a vector of dimension m where m is the number of compartments by which the repository is subdivided. The term $(\overline{\overline{F}} \cdot \overline{c})$ accounts for the transport by diffusion. $\overline{\overline{F}}$ is a matrix of dimension mxm and \overline{c} is a vector of dimension m. The term (\overline{B}) accounts for the boundary conditions. It is a vector of dimension m.

The basic system of equations expressed above is solved by using standard numerical techniques. We use the stiff solver based on Gear's method. This solves a problem of "m" ordinary differential equations of the form dY(I)/dt = F(Y(I), t), given the initial conditions Y(I) = YI (Kahaner et al., 1988). The solution is straightforward once the initial and boundary conditions have been defined. These are defined by the uptake in the flowing water on one hand and on the release from the fuel on the other hand.

6.2 Advection - dispersion with matrix diffusion, ADD-Model

In the disturbed rock zone around the tunnel, the water flows in the direction along and parallel to the tunnel. The DRZ is formed by a great number of fractures distributed on the cross section to the water as it is shown in Figure 8. Most of the water flow is in a few channels. To simplify the study of this zone we assume that the water flows in one channel. The width of this channel is the sum of the widths of all channels with large flowrates. Then the width of this preferential channel is assumed to be 2 m and its aperture 0.1 mm, see Figure 8. With these data, the effluent concentration from the channel may be investigated.



Figure 8 Cross section of the disturbed zone, DRZ, with different channels.

In a channel where water flows a nuclide is assumed to be introduced at a certain location with concentration $c_0 e^{-\lambda \cdot t}$. The effluent concentration from the channel including the diffusion into and sorption on the micropores was modelled by Neretnieks, 1980. The solution to this problem is

$$\frac{c}{c_o} = e^{-\lambda \cdot t} \cdot \operatorname{erfc}\left(\frac{L \cdot W}{Q} \sqrt{\frac{D_e \cdot K_d \cdot \rho_p}{t - t_w}}\right)$$
(16)

 K_d is the mass sorption coefficient, ρ_p is the rock matrix density, D_e is the effective diffusivity of the nuclide in the rock matrix, λ is the decay constant, Q is the water flowrate in the channel, and W is the width of the channel. These entities are depicted in the Figure 9.



Figure 9 Channel carrying with it all the water flowing in the disturbed zone. The width of the channel W is approximated to be 2 m and the aperture δ is 0.1 mm.

In the calculation of the effluent concentration c, the length of the channel L will be varied in multiples of the length of the canister.

7 RESULTS AND DISCUSSION

Several cases have been calculated. The results are presented for one leaking canister in the base cases and for more than one leaking canister in the complex cases. Pu-239 is used in all cases described in Sections 3 and 4. For the case when one canister leaks, the release of Cs-137 and I-129 is also calculated.

The bentonite volume surrounding the canister (see Figure 6) is divided into several compartments to improve the accuracy in the calculations. The local Q_{eq} to approximate the diffusional transport into the water in the DRZ is calculated using Equation (8) or (12). A flow porosity of 10^{-4} is used to calculate the residence time (Equation (5)) for the water in the DRZ. The basic data on chemical and physical properties for Pu-239 and other nuclides are given in Table 1. The volume of water within the canister is assumed to be 100 liters in the VLH-canister and 20 liters in the KBS-3 canister. In the VLH-canister, the nuclide inventory is assumed to be three times larger because the mass of fuel in the canister is approximately three times larger than in the KBS-3 case. Other data required is given in Table A1, Appendix A1.

	water	bentonite	rock	hole
Porosity [-]	1.0	0.25	0.005	1.0
Density [kg/m	n ³] 1000	2000	2700	1000
Diffusivity [m ² /s	a]			
Pu-239	0.123	3.15·10 ⁻³	3.15·10 ⁻⁶	0.123
I-129	0.123	7.9·10 ^{- 5}	3.15·10 ⁻⁶	0.123
Cs-137	0.123	0.79	3.15·10 ⁻³	0.123
Sorption [m ³ /k	g]			
Pu-239	0	5	3	0
I-129	0	0	0	0
Cs-137	0	0.05	0.05	0
Solubili	ity, $[mol/m^3]$	Half-life, [a]	Inventory, [moles]	
			KBS-3	VLH
Pu-239 2.	0·10 ^{- 5}	24 100	28.1	84.3
I-129	High	1.6·10 ⁷	2.2	6.6
Cs-137	High	30	6.2	18.6

Table 1Physical properties of some nuclides used in the calculations.

7.1 Results for the base cases

The description of the cases for the results presented here, have been presented in previous sections. The central case is for one breached canister in the tunnel, a disturbed zone (DRZ) around the tunnel, and a fracture intersecting the tunnel. The damage is a small hole (5 mm²) in the canister wall at the center of the canister and opposite the fracture. The length of the canister is approximated to 6 m. Then, the volume of the clay surrounding the canister is ≈ 15 m³. To simplify the definition of some geometric parameters, the ends of the canister are assumed to be flat.

Figure 10 shows the mass flowrate of nuclides through the different pathways for the central case. The figure shows that the nuclide transport in the pathway to the disturbed zone is dominant compared to that going to the fracture.

The release to the DRZ is approximately 2.5 times larger than to the fracture. This factor is very sensitive to the location of the fracture along the tunnel and the estimation of the local equivalent flowrate of water to define the boundary conditions in the flowing water in the fracture and in the DRZ. The ratio of transport to the fracture and to the DRZ is quite sensitivity to assumptions underlying the determination of Q_{eq} . With this approximate model it can only be stated that the rates of transport in the two pathways are comparable but it cannot be determined which are actually dominates. The fracture location is investigated later in this report and the analysis of sensitivity of the parameters involved in the calculation of Q_{eq} will be done in a later report.



Figure 10 Central case, one canister leaks. Mass flowrate of Pu-239 through the different pathways over time.

The influence of the bentonite volume was also investigated. The volume variation was made in relation to the base case ($\approx 15 \text{ m}^3$) by extending the volume of the clay sideways in the direction of the canister length. The results are shown in Figure 11. This figure shows the maximum nuclide flowrate into the water via the different pathways as a function of the volume and as a function of the length of the bentonite compartment. The entities are correlated because the cross section area is constant. A variation in volume is equivalent to a variation in length. The figure shows very small changes for the DRZ and not any change for the nuclides transported to the fracture. The overall release rate of nuclides from the canister (input) does not change.



Figure 11 Maximum mass flowrate of Pu-239 into the disturbed zone and into the fracture as a function of the bentonite volume (left figure) and the length (right figure).

An analysis at steady state of the transport resistances in the different pathways shows that the resistance of the small hole in the canister governs the escape rate of the nuclides from the canister. Any change in volume of the bentonite does not change the release from the canister, see figure 11. The maximum mass flowrate of the nuclides transported into the water and from the canister were calculated for different areas of the small hole. Figure 12 shows that an increase in the size (area) of the small hole increases the release of nuclides. For a size in area of 100 mm² the transport resistance in the hole is one order in magnitude larger than in the other pathways. The flowrate of nuclides from the canister is still dominated by the resistances in the hole. For holes larger than 100 mm² the resistances in the other pathways begin to play a role.



Figure 12 Maximum mass flowrate of Pu-239 into the disturbed zone and into the fracture as a function of the area of the damage of the canister.

As a particular case, we have investigated the release of nuclides into a fracture zone intersecting the tunnel. The water flows around the tunnel and we assume that this zone has not been sealed off. The small hole is at the end of the canister nearest to the fracture zone. Figure 12 shows the results obtained for this case under the influence of the DRZ. The maximum nuclide flowrate into the fracture zone is presented for different distances between the fracture zone and the nearest canister to this zone, distance "x" in Figure 4. The thickness was assumed to be 0.5 m. The Qeq of the fracture zone is 2.4 l/a, Table A3 in Appendix A2.

The release of the nuclides to the water is more influenced by the disturbed zone than by the fracture zone. The uptake in the disturbed zone dominates and is not influenced by the distance between the hole and the fracture zone as much as the uptake in the fracture zone is influenced. Figure 13 shows that the maximum release into the fracture zone decreases several orders of magnitude with an increase of the distance between the hole and the fracture zone. This in practice has not importance for the total release into the water. The release into the DRZ dominates.



Figure 13 Maximum mass flowrate of Pu-239 into the disturbed zone and into the fracture zone (FZ) as a function of the distance between the canister and FZ.

7.2 Results for the complex cases

The calculations are based on the assumption that a few or all canisters are damaged. These cases have been described previously. A complication in the calculations arises when a few canisters are damaged. The problem is that if they are located sparsely in the tunnel, the water passing the next breached canister already carries nuclides. This concentration must be accounted for. This effect has been investigated for some nuclides as a particular case of the analysis of the effluent concentration in the DRZ. The location of the fracture on the nuclide release has also been investigated for a case when all the canisters are damaged.

7.2.1 All canisters are breached

The nuclide release into the water has been calculated for two locations of the fracture. In the first the fractures are opposite to the small hole in the canisters and in the second the fractures are at the ends of the canisters. See Figure 5 in the section where these cases have been described. The results are shown in Figure 14. When the fracture is opposite the damage, the fracture accounts for 30% of the release. When the distance between the damage and the fracture is larger the significance of this pathway decreases further.



Figure 14 Two different locations of the fracture. Mass flowrate of Pu-239 through the different pathways. In the left figure, the fractures are opposite to the small hole and in the right figure they are at the ends of the canisters.

7.2.2 Analysis of the concentration downstream in the DRZ

The water coming to the next breached canister has travelled a certain distance downstream. During the time the water travels this distance, some sorbing nuclides may be retarded by sorption in the rock in the DRZ. Some decay may take place. The concentration of nuclides when the water comes to the next damaged canister may have decreased. This case was described previously in Section 6.2. This effect has been investigated for some nuclides using the ADD-model. The downstream concentration in the DRZ has been calculated by varying the distance in the water downstream of the canister.

In those calculations the flowrate along the DRZ is 2.4 l/a and it is assumed to be all in one fracture of width 2.0 m. We assume that there is not dispersion. The results in Figure 15 show that for those non-sorbing nuclides having a large decay constant the effluent concentration does not change with the distance (I-129). This means that the local Q_{eq} for the few canisters can be approximated using the equation for n-breached canisters, Equation (14). For the other considered nuclides the relative concentration decreases considerably with the travelled distance. For nuclides with very large decay constant (Cs-137), the concentration of nuclides in the water coming to the breached canister is approximately zero. For Ra-226 which has the same sorption coefficient as Cs-137, the concentration is much larger. The reason for this is the smaller decay constant (53 times shorter), see Table 1. For Pu-239 which has the smallest decay constant and the largest sorption coefficient (Table 1) of the sorbing nuclides considered, the relative concentration is very low.



Figure 15 Relative effluent concentration (c/c_0) over a certain travelled distance in the disturbed zone, for different nuclides.

From Figure 15, we can deduce that the concentration of Ra-226, Pu-239, and Cs-137 in the water is very low (practically zero) when it comes to the next breached canister. Thus Q_{eq} for the next breached canister may be calculated as if the water contains no nuclide.

7.3 Release rates for some nuclides in two different repositories

Calculations to compare the nuclide release from two different repository concepts, VLH and KBS-3, have been made for the central cases. These cases were described in Section 5 and mainly consider the case with only one damaged canister. The nuclides chosen are Pu-239, I-129, and Cs-137. The damaged zone in the canister wall is a small hole (5 mm²) in both repository concepts.

It should be noted that the comparison is valid only when one canister is damaged. Because if n successive canisters are damaged in the VLH-repository the release into the water from any canister is influenced by the preceding damaged canister. The comparison when several canisters are damaged will be reported in a later study. The results are shown in Figures 16 and 17 for the VLH and KBS-3 repositories respectively. The figures show the mass flowrate escaping from the canister and the release of nuclides into the water flowing around the repositories.

Release results through the different pathways are not shown here for the nuclides considered. Calculations show that they follow the same tendency as the results shown in the preceding section for Pu-239 in the VLH-repository. These showed that most of the nuclide release into the water occurs through the pathway going to the DRZ. For the KBS-3 repository the pathway, which plays the largest role in the release is that going to the fracture intersecting the repository hole (Romero et al., 1991).

An analysis of the transport resistances shows that for nuclides with high diffusion coefficients (Cs-137 and Pu-239), the largest and dominant resistance is in the small hole in both repositories. The resistance for the VLH is approximately 3 times larger than for the KBS-3. For I-129 the dominant resistances are in the small hole and in the bentonite nearest the hole in both repositories. The resistance in the bentonite adjacent to the hole is larger because of the very low diffusion coefficient of the I-129 in the bentonite in comparison to the other nuclides, see Table 1.

The results show that the release into the water is of the same order in magnitude for both repository concepts. For that sorbing nuclides, Pu-239 and Cs-137 the releases are almost the same. The releases into the flowing water are much lower in comparison with the nuclide escape from the canister. This is due to the decay and the sorption of the nuclides in the bentonite. For the long lived and nonsorbing I-129, the maximum release into the water is slightly less than the release from the canister.

The release from the canister is dominated by the small hole in both cases. The dissolution rate plays a role for that nuclides which are completely dissolved in the water volume within the canister. For Pu-239 which is limited by solubility, the

nuclide escape depends only on the relation of the resistances in the hole (the relation in resistance VLH/KBS is about 3). Then, the escape of Pu-239 in the KBS-3 is expected to be 3 times larger than in the VLH. For Cs-137 which is not limited by solubility, the nuclide escape depends on both parameters (the relation VLH/KBS in resistance and initial concentration within the canister are 3.5 and 0.6 respectively). Then, for Cs-137 the expected escape is approximately 3.5/0.6 times larger. These expected relations are seen in the figures below.

For I-129, a non sorbing nuclide, Figures 16 and 17 show a clear difference in the depletion time in the canister. The KBS-3 has a shorter depletion time than the VLH repository. This may be explained by simplifying the system to those compartments that really play a role in the transport of nuclides from the canister. These are the small hole and the bentonite at the mouth of the small hole. Then, the depletion time may be determined calculating the time constant (volume*resistance) for the canister in both repositories. The time constant for the KBS-canister is 5 times less than for the VLH-canister.



Figure 16 Nuclide release for the VLH-repository. The figure to the left shows the nuclide escape from the canister and the figure to the right shows the release into the water.



Figure 17 Nuclide release for the KBS-3-repository. The figure to the left shows the nuclide escape from the canister and the figure to the right shows the release into the water.

NOTATION

Α	Contact area	m^2
Aw	Wetted area	m ²
с	Concentration	moles/m ³
co	Initial concentration	moles/m ³
Cw	Interface concentration	moles/m ³
De	Effective diffusion coefficient	m²/a
D_w	Diffusion coefficient in water	m²/a
i	Hydraulic gradient	m/m
kd	Mass sorption coefficient	kg/m ³
Kp	Hydraulic conductivity	m/a
L	Length of pathway	m
n	Number of breached canisters	-
Ν	Mass flowrate of nuclides	moles/a
m	Number of compartments	-
q	Flux of water	m ³ /m ² ·a
Q	Flowrate of water	m ³ /a
Q _{eq}	Equivalent flowrate of water	m ³ /a
Qfrac	Local equivalent flowrate in fracture	m ³ /a
Q _{DRZ}	Local equivalent flowrate in disturbed zone	m ³ /a
r	Radius	m
t	Time	а
tw	Residence time	а
W	Width	m
x	Distance to the fracture zone	m
ε _f	Flow porosity	-
η	Penetration thickness into the water	m
ρ _p	Rock matrix density	kg/m ³
λ.	Decay constant	a ⁻¹

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APPENDIX A1

Description of the KBS-3 repository

In the Swedish KBS-3 design of a nuclear waste repository for spent fuel copper canisters containing the fuel are deposited in vertical holes in tunnel floors. The canisters are surrounded by compacted bentonite and the tunnels are backfilled with a mixture of bentonite and sand. The rock is fractured with water bearing fractures at typical distances of several meters. In the immediate proximity of the tunnels, within a few meters, the rock is more fractured due to blasting damage and rock stress changes.

Once water penetrates into the canister the nuclides dissolve and diffuse out through the damage in the canister wall and further out through the bentonite. Some species diffuse into the fracture that intersects the repository hole, some into a fracture zone below the repository hole and some up to the disturbed zone around the tunnel at the top of the repository hole. From the pathway that goes to the top of the repository hole, a part diffuses into the disturbed zone at the bottom of the tunnel. The other part diffuses up into the backfill in the tunnel, along this and into fractures that intersect the tunnel. The region adjacent to a repository hole including the tunnel and its disturbed zone, the damage in the canister wall, and the different paths are illustrated in Figure A1.

In the figure, the different regions such as the damage in the canister, the different parts of the backfill in the repository hole and the tunnel, the rock, fractures and fracture zones are modelled as a number of compartments. Only transport by diffusion is considered in the clay and in the rock matrix because the advective transport is negligible compared to the transport by diffusion. Analytical "exact" solutions are used to define the proper sizes and shapes of fictitious compartments at sensitive zones. These are at the mouths of the damage in the canister wall, at the mouth of the fractures, and in the flowing water in the fractures and fracture zones.

Because of the low permeability of the rock matrix and backfill, the transport by flow of solute is negligible compared to that by molecular diffusion. Every compartment can thus only exchange solute with adjacent compartments by diffusion except for the flowing water in the fractures and fracture zones where transport by advective flow also takes place. These zones are denoted by $Q_1 - Q_4$ in Figure A1. The data used in the calculations is tabulated in the Table A1.



Figure A1 Schematic view of the entire system showing its geometry. To the right, the subdivision in compartments of the system described in the figure to the left. Numbers in the figure denote compartment numbers.

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Symbol Description	Units	Range	KBS-3	VLH
Diameter of canister	m	-	0.8	1.2
Diameter of repository hole	m	-	1.5	-
Hole diameter in canister wall (Dh)	m	10 ⁻³ - 10 ⁻¹	0.0025 (5 mm ²)
Tunnel height	m	-	4.5	-
Tunnel width	m	-	3	-
Tunnel diameter	m		-	2.4
Length of canister	m	-	4.5	6
Thickness of canister (Fe)	m	-	-	0.161
Thickness of canister (Cu)	m	-	0.06	0.06
Length between the top of the canister				
and the disturbed zone (L_5)	m	-	1.5	-
Thickness of the disturbed zone (L_6)	m	-	1.0	0.3
Partial length of the tunnel $(L_7+L_8+L_9)$	m	-	6.5	-
Length between the bottom of the caniste	r and			
the bottom of the repository hole (L_{11}) Length between the repository hole and	m	-	0.5	-
the fracture zone (L_{12})	m	0-10	3	-
δ_1 Aperture (channel)	m	10 ⁻⁵ - 10 ⁻³	10 ⁻⁴	10-4
δ_2 Thickness (disturbed zone)	m		1	0.3
δ_3 Aperture (channel)	m	10 ⁻⁵ - 10 ⁻³	10-4	-
δ_4 Thickness (fracture zone)	m	0.2 - 2		0.5
Local equivalent flowrates for the central	case			
Q ₁ channel (repository hole)	l/a	0.03 - 3	0.1	-
Q ₂ disturbed zone, Q _{DRZ}	l/a	0.03 - 3	0.5	2.3
Q_3 channel (tunnel), Q_{frac}	l/a	0.03 - 3	0.1	0.1
Q ₄ fracture zone	l∕a	0.03 - 100	100	2.4
Equivalent diffusion length for the compa	urtment a	t the mouth of	fractures	
in repository hole (plug)	m	(3 - 8)·δ	5*δ	-
in tunnel (Plug)	m	(3 - 8)·δ	5*δ	5*δ

Table A1Parameter values required for the release calculations for the KBS-3
and VLH repositories. For symbol description see Figures A1 and 6.

APPENDIX A2

Estimation of Q_{eq}

In the release calculations, the equivalent flowrate, Q_{eq} , is used to define the boundary conditions in the model by calculating the diffusional nuclide transport into the flowing water. This entity is a fictitious flowrate of water which carries with it a concentration equal to that at the interface between the solid and the flowing water. The equations described in Section 5.2 are used to obtain the Qeq.

$$Q_{eq} = q \cdot W \cdot \overline{\eta}$$
 or $Q_{eq} = A \cdot \varepsilon_{f} \sqrt{\frac{4 \cdot D_{w}}{\pi \cdot t_{w}}}$

where the wetted area is $A_w = A \cdot \varepsilon_f$. A is the contact area of bentonite with rock and ε_f is the flow porosity. W is the width of the bentonite area in contact with the fracture, fracture zone or damaged zone. $\overline{\eta}$ is the mean penetration thickness into the water by diffusion from the bentonite, see Figure 7. The residence time, t_w , is the time that the water is in contact with the bentonite. This time is obtained from the flux of water (q), flow porosity (ε_f), and the length of the pathway in contact with the water (L):

$$t_w = \frac{L}{q/\epsilon_f}$$

If the flow is along the drift, L is the length of drift which has "contaminated" bentonite. If the flow is perpendicular to the drift L is half the circumference of the drift.

units	Fracture zone	Fracture	Disturbed zone
		<u> </u>	
m	1.2	1.2	1.2
m	0.5	6	7.54
m	3.77	3.77	6.0
m²/s	3.9·10 ⁻⁹	3.9·10 ⁻⁹	3.9·10 ⁻⁹
-	10 ⁻³	1.67.10 ⁻⁵	10-4
m/s	10-7	10 ⁻⁹	10 ⁻⁸
m/m	3·10 ⁻³	3·10 ⁻³	3.10-3
	units m m m ² /s - m/s m/m	units Fracture zone m 1.2 m 0.5 m 3.77 m ² /s 3.9·10 ⁻⁹ - 10 ⁻³ m/s 10 ⁻⁷ m/m 3·10 ⁻³	unitsFracture zoneFracturem 1.2 1.2 m 0.5 6 m 3.77 3.77 m²/s $3.9 \cdot 10^{-9}$ $3.9 \cdot 10^{-9}$ - 10^{-3} $1.67.10^{-5}$ m/s 10^{-7} 10^{-9} m/m $3 \cdot 10^{-3}$ $3 \cdot 10^{-3}$

Table A2Data used in the calculations of the Qeq

Table A3	Local eq	uivalent	flowrate,	Qeq
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units	Fracture zone	Fracture	Disturbed zone
l∕m²∙a	9.46	0.0946	0.946
a	0.398	0.664	0.634
m	0.25	0.32	0.32
m ²	0.0038	0.000754	0.0045
l/a	2.36	0.366	2.25
	units 1/m ² ·a a m m ² 1/a	units Fracture zone $1/m^2 \cdot a$ 9.46 a 0.398 m 0.25 m ² 0.0038 $1/a$ 2.36	unitsFracture zoneFracture $1/m^2 \cdot a$ 9.460.0946a0.3980.664m0.250.32m^20.00380.000754 $1/a$ 2.360.366

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A rock mechanics study of Fracture Zone 2 at the Finnsjön site

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