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Flow and solute transport in a zone damaged due to spalling

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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 and do not necessarily coincide with those of the client.

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Abstract

This short report addresses the consequences of the presence of a damaged zone in the rock adjacent to the deposition hole due to spalling. The possible increase of water flow rate through the zone is studied by simple scoping modelling and calculations. The impact of the increased flowrate on the release of nuclides or transport of other solutes to and from the canister is also studied by simple model calculations.

Sammanfattning

Denna korta rapport studerar hur närvaron av en uppsprucken zon i berget runt deponeringshålet skulle kunna påverka vattenflödet. Enkla modeller och överslagsmässiga beräkning presenteras. Ett ökat vattenflöde kan också leda till en ökning av uttransport av radionuklider från och andra lösta ämnen till och från kapseln. Även detta behandlas i rapporten.

Summary

There may be a damaged zone due to spalling in the rock wall in the deposition hole for waste canisters. The zone can have higher conductivity and porosity than the intact rock. Water will be drawn into the damaged zone from fractures that intersect the deposition hole. The water can attain a longer residence time in contact with the buffer in the hole than would otherwise be the case when only the thin fracture contacts the buffer. This may lead to a higher exchange of solutes between the flowing water and the pore water in the buffer. This short report explores the possible increase in water flowrate in the damaged zone and the resulting increase in mass transfer. The latter is illustrated by the equivalent flowrate that will equilibrate with the pore water on the buffer surface in contact with the flowing water.

The flowrate of water will increase due to the presence of the damaged zone. However, only a fraction of that water will exchange solutes with the buffer. Nevertheless, the equivalent flowrate *QeqDZ* due to the presence of a damaged zone could be considerably larger than when there is no damage. Scoping calculations indicate that the increase can be on the order of up to ten times depending on the angle at which the deposition hole is intersected. For very high flowrates the solute exchange between canister and flowing water will be determined and limited by the diffusion resistance in the buffer. The overall equivalent flowrate, Q_{eq} , for solute transfer will not exceed some tens of litres per year.

Contents

1 Introduction

The rock nearest to the surface of the deposition hole for the waste canisters can be damaged due to natural stress distribution in the rock and due to stresses induced due to heating by the waste in the canister. This is called spalling.

A wedge formed region of fractured rock on both sides of the deposition hole may form. This is illustrated in Figure 3-1 where the hole is seen from above. The damaged zone is envisaged to extend some 10 cm into the rock and be 15 to 20 cm wide. The zone will contain several small fractures that form a connected network for flow. The porosity and hydraulic transmissivity of the damaged zone is assumed to be higher than that of the surrounding rock. A water conducting fracture that intersects the deposition hole will also intersect the zone with the damaged rock and allow water to flow through it.

Water that enters the zone from the upstream side of a fracture will spread out in the zone both upward and downward before it again leaves at the downstream side. Because the hydraulic conductivity of the damaged zone is higher than the undamaged rock it may allow more water to be drawn in from the flowing fracture.

The water in the porous damaged rock will have a longer residence time in contact with the buffer and may therefore have more time to equilibrate with pore water of the backfill.

Thus the spalled zone can increase the nuclide uptake due to

- 1. Larger water flow to the canister.
- 2. Longer residence time and larger contact area with the buffer.

We will first estimate the increase in water flowrate to the canister and then assess the increase of solute exchange rate between the water and the backfill.

2 Aims and scope

The aim of this short report to explore the potential consequences of the presence of a damaged zone in the rock nearest the deposition hole on flow and solute transport to and from a canister for spent nuclear fuel. The damage is assumed to be caused by spalling. The approach is to use simple modelling tools that may give insights into which processes may be important and may point to where furhter information may be needed if more refined analyses are to be made.

3 Water flowrate in the damaged zone

Neither the exact form of the damaged zone nor its properties are known in detail. The problem is therefore approached by determining how much increase in water flowrate can be expected *in a worst case*. For illustrative purposes the width of the zone is taken to be $W_{zone} = 0.2$ m and the depth to be $d_{zone} = 0.1$ m.

As a basis for this analysis it is assumed that a zone with very high *(infinite) hydraulic conductivity* forms adjacent to the deposition hole. An upper bound of the increase in flowrate can then be assessed. This exaggerated assumption will be revisited later in the report.

Assume that the deposition hole is intersected by a fracture with known hydraulic transmissivity and that the fracture properties outside the zone are not influenced by the spalling. Thus the fracture will have the same properties as before. Now, however, the flowing water in the fracture will not be diverted around the low conductivity buffer as it is when there is no damaged zone. Instead the water will be drawn into the high permeability zone.

The maximum flowrate of water that can flow through the width of the damaged zone only increases by about a factor of two due to the damage compared to the water flowrate through the fracture if there were no damage. This is illustrated in Figure 3-2.

Consider a damage like the wedge in Figure 3-1. The damage is much more conductive than the fracture that intersects it. Water will be drawn into the irregular damage from the fracture and the capture width will be approximately twice the largest extent to the cross section of the damage. Of peripheral interest for the present problem but worth mentioning is that studies have also been performed on draw-in of water to low permeability regions for 3-dimensional flow in a porous medium /Bengtsson et al. 1991, Jackson 1992/. They have been used to study flow on tunnel and repository scales where the fractured rock is approximated as a porous medium.

Figure 3-1. Deposition hole with buffer and backfill. The rock has been spalled in some regions.

Figure 3-2. Streamlines drawn into a high conductivity zone from twice the extent of the zone.

For example a fracture that intersects the deposition hole at right angles will have a total capture width W_{capture} (two zones)

$$
W_{\textit{capture}} = 4d_{\textit{zone}} \tag{1}
$$

For other intersection angles the capture width can be larger.

Figure 3-3 shows that fractures can intersect the deposition hole and the damaged zones at different angles. The projected area of the intersection with the damaged zone will vary with the angle. Also the largest length of the projected area will vary with the intersection area.

Figure 3-3. Fractures intersecting the deposition hole at different angles.

It has not been deemed worthwhile at this stage to account in detail for the variation of these entities with the intersection angle because of the inherent uncertainty of the shape, extent and properties of the damaged zone. Instead two extremes are studied. In the first case the fracture intersects the hole at right angles. In the second it is parallel to the hole and intersects both zones along their entire length.

The fracture that intersects the hole at right angles will have two separate zones that can draw in water. The longest part of the projected area will be the width W_{zone} in the case we study. Each of the zones will draw in water from a capture width $W_{\text{capture}} = 2 W_{\text{zone}}$. A fracture that intersects the hole at an angle will further increase the capture length by up to $1/Cos(\alpha)$ depending on the orientation in space. This is not further analysed.

The other extreme case with the vertical fracture and where the hydraulic gradient is near vertical is not expected to be very common. Such a fracture would be aligned perpendicularly to the direction of the highest stress and be expected to be subject to closing stresses. Nevertheless, in this note it is presented as an extreme case with the highest flowrates and the largest exposed area for mass transfer between water and buffer.

A vertical fracture that intersects the damaged zone around the deposition hole will then have a capture width equal to twice the length of the deposition hole which is about 8 meters. Another angle of intersection will have a length which depends on the locus of intersection, the angle and the shape of the zone.

The length of intersection can thus vary between W_{zone} and L_{hole} i.e. about 0.2 m to 8 m. The capture width *Wcapture* will then vary between *2Wzone* on both sides of the canister giving in total *4Wzone* and *2Lzone* for the vertical case*.* In the latter case the zones are so near each other that they will seem to be only one for the capture width. See Figure 3-4.

In summary it can be expected that the capture width will vary between about 0.8 m and 16 m.

The flowrates (q) through the zone are obtained from Equation (2) and are summarized in Table 3-1 for a hydraulic gradient $i = 0.01$.

$$
q = T \cdot i \cdot W_{\text{capture}} \tag{2}
$$

The reader is reminded that the spalled zone has been assumed to have a very high (infinite) hydraulic conductivity. The vertical fracture is likely to be compressed due to the rock stresses, which is not accounted for. The figures in the table are thus absolute upper bounds.

Fracture transmissivity m^2/s	Flowrate q litre/year Horizontal fracture $W_{\text{capture}} = 0.8 \text{ m}$	Flowrate q litre/year Vertical fracture W_{capture} = 16 m
10^{-9}	0.25	5
10^{-8}	2.5	50
10^{-7}	25	500
10^{-6}	250	5.000

Table 3-1. Flowrates for different transmissivities.

Figure 3-4. View in the plane of the fracture. Streamlines in a fracture that intersects the deposition hole along its length.

4 Solute transport by the water

The details of the number of fractures, their aperture and the resulting porosity and diffusion properties in the damage are not known. A worst case assumption would be that all the flowing water would be available to solute exchange. However, this may be too pessimistic and we estimate the fraction of the flowing water that can be affected. We use a method very similar to that what is was used to derive the equivalent flowrate for transfer to and from water flowing in a fracture. Such a model was presented earlier for flow in a fracture in contact with the buffer using diffusion theory /Neretnieks 1979/. The model is used in the near field computational scheme, Comp32. It is adapted here to the conditions in the damaged zone.

Below an analysis of the diffusion rate of a solute to the water flowing in the damaged zone is presented. It is based on modelling the rate of diffusion from the buffer to the water that flows past it in the damaged zone. The penetration depth of the diffusing solute during the time the water is in contact with the buffer determines the total uptake of solute is estimated below. The residence time of the water in the damaged zones is determined by its pore volume of mobile water and the flowrate.

$$
t_{res} = 2 \frac{\varepsilon_{zone} L_{zone}}{q} \frac{W_{zone}}{2} f \tag{3}
$$

An essentially triangular shape of the zone and that the flowing water can access a fraction "*f*" of the volume is assumed. The factor *f* will be discussed later. It will be nearly 1 for flow in the length direction of the hole and smaller in the other directions. ε*zone* is the porosity of the zone. The entities in the equations are explained in Table 4-1.

From diffusion theory we have that the mean penetration depth of the solute can be determined by integrating the concentration profile from the surface $(z = 0)$ to infinity /Bird et al. 2002, p 621/. That will be the distance which the solute has penetrated from the buffer into the flowing water and will have attained the concentration at the surface of the buffer. It is

$$
\eta_{\text{mean}} = 1.13 \sqrt{D_p} t_{\text{res}} \tag{4}
$$

The equivalent flowrate of "contaminated" water in the zone is

$$
Q_{\text{edDZ}} = q \frac{\eta_{\text{mean}}}{d_{\text{zone}}} = 1.13 \sqrt{\frac{D_p q W_{\text{zone}} L_{\text{zone}} \varepsilon_{\text{zone}} f}{d_{\text{zone}}}}
$$
(5)

This is a fair approximation when η*mean* is less than about 2 times smaller than the thickness of the zone d_{zone} . Otherwise it is approximately equal to the thickness and $Q_{eapZ} \cong q$. For simplicity the zone is depicted and modelled as rectangular instead of triangular for these calculations. This simplification is deemed acceptable because there are many uncertainties regarding the geometry and the properties of the zone.

 D_n is the diffusion coefficient of the solute in the fractures in the damaged zone. It can be estimated from the diffusivity of the solute in unconfined water D_w and the tortuosity of the diffusion paths τ^2 . The former is on the order of 10^{-9} m²/s for the nuclides and τ^2 can be expected to be in the range 1 to 10 or more depending on how tortuous the fractures and the fracture network is in the damaged zone.

$$
D_p = \frac{D_w}{\tau^2} \tag{6}
$$

If all the water in the damaged zone is equilibrated, in addition, the water flowing in the fracture just outside the damaged zone will take up nuclides as they diffuse out to the water as it passes the deposition hole.

The equivalent flowrate contaminated due to this effect can be obtained from (the 2 is for both sides of the hole)

$$
Q_{eq,fracture} = u_{\text{fracture}} \delta \cdot 2\eta_{\text{mean}.\text{fracture}} \tag{7}
$$

where

$$
\eta_{\text{mean}.\text{frature}} = 1.13 \sqrt{D_{w} t_{\text{res},\text{fract}}}
$$
(8)

and

$$
t_{res,fract} = \frac{W_{zone}}{u_{fracture} Cos(\alpha)} \text{ or } t_{res,fract} = \frac{L_{zone}}{u_{fracture}}
$$
(9a)

depending on whether the fracture intersects the hole at an angle α , or is vertical. α is zero for a horizontal intersection and may be up to the angle that intersects the hole or the spalling zone diagonally, about 78 and 89 degrees respectively.

For an undamaged hole the water flows around the buffer and the residence time is

$$
t_{res,fract} = \frac{2r_{hole}}{u_{fracture} Cos(\alpha)}
$$
(9b)

This will be used when comparing solute transfer for an undamaged hole with a damaged hole

$$
u_{\text{fracture}} = \frac{T \cdot i}{\delta} \tag{10}
$$

4.1 Comparison of Qeq in fracture and Qeq in damaged zone

When the penetration depth in the spalling zone is less than its thickness a simple relation can be obtained between *QeqDZ* and *Qeq*. Combining Equations (5) and (7) with (9b) for the water residence time to obtain the ratio between *QeqDz* and *Qeq* gives for an intersection with angle α.

$$
RatioW = \sqrt{\frac{\varepsilon_{zone} L_{zone} W_{zone} f Cos(\alpha)}{\tau^2 \delta 2r_{hole}}}
$$
\n(11a)

and for the vertical intersection

$$
RatioL = \sqrt{\frac{\varepsilon_{zone} L_{zone} W_{zone} f}{2\tau^2 \delta d_{zone}}}
$$
\n(11b)

It is interesting to note that an increased intersection angle α will tend to decrease the ratio because the *Qeq* for the non-damaged case will increase due to the longer contact time for the water in the fracture with the hole as the angle increases. This will, however be more than compensated by increasing *f*.

4.1.1 An example

An example with data that are within the expected range is given below. Table 4-1 shows the data used and table 3 the resulting equivalent flowrates for different transmissivities of the fracture

For this example it is seen in Table 4-2 that for all cases the penetration depth is smaller than the thickness of the damaged zone. Thus only a fraction of the total flowrate in the zone will be "contaminated". Further, there is no need to account for diffusion into the water flowing in the fracture in the rock.

With the data in Table 4-1 *RatioW* is 0.96 for $\alpha = 0$ and increases to a maximum of *RatioL* = 9 for the vertical fracture. This is caused by a combination of increasing f and $\cos(\alpha)$. Thus the presence of a spalling zone with infinite conductivity can cause a considerable increase in the equivalent flowrate.

However, this is also sensitive to the assumption of the actual fracture aperture. A larger fracture aperture will not influence the conditions in the spalling zone but will increase the traditional *Qeq* for an undamaged hole. For example a 1 mm fracture (instead of 0.1 mm) will change the ratios to 0.3 and 2.8 times for the horizontal and vertical fracture respectively.

Table 4-1. Data for the example.

5 Transport resistance in the buffer

The transport resistance for a solute in the damaged zone can be expressed as the inverse to the *Qeq*. A solute will have to pass the buffer also on its way to or from the canister. The resistances are coupled in series and can be added. The inverse of the sum of the resistances will make up the overall equivalent flowrate. The largest resistance (smallest Q_{eq}) will dominate the transport.

The rate of transport trough the buffer can be described by Fick's first law. The area for diffusion is taken to be the whole length of the hole times the width of the spalling zone on both sides of the canister.

$$
N = D_{buffer} A \frac{\Delta c_{buffer}}{\Delta x_{buffer}} = D_{buffer} 2W_{zone} L_{zone} \frac{\Delta c_{buffer}}{\Delta x_{buffer}} = Q_{eq,bulfer} \Delta c_{buffer}
$$
(12)

With typical values for the buffer ($D_{\text{buffer}} = 10^{-10} \text{ m}^2/\text{s}$, $\Delta x_{\text{buffer}} = 0.35 \text{ m}$).

 $Q_{eq,buffer}$ is 29 litres/year for both the horizontal fracture and the vertical fracture.

This will be the limiting equivalent flowrate even when those due to diffusion in the water in the zone would permit a higher value.

6 Some further questions

Here we explore some questions and revisit some assumptions. They are:

- 1. When can the hydraulic conductivity of the damaged zone be assumed to be so large that it may be considered to be infinite for the purposes of the draw in?
- 2. How large part of the damaged zone can be effectively accessed by the drawn in water- the factor "*f*"?
- 3. How to estimate the tortuosity in the damaged zone?

6.1 When is the hydraulic conductivity "high"?

This question is addressed using the solution to flow from a thin fracture into a large volume of porous material.

Figure 6-1 below illustrates the situation.

The flow in the porous body can be approximately described by a 2- dimensional partial differential equation. This has been done and the solution for this case can be found in /Neretnieks 1986/. The solution was obtained for diffusion but it can be directly applied for flow. It was shown that the entire resistance to transport in the porous body can be visualised and expressed in terms of the resistance in a short plug with the hydraulic properties of the porous medium. The plug has the thickness of the fracture aperture δ and the length of 3–8 times the aperture, depending on the geometry of the porous body. This in the present case is the geometry of the damaged zone. We chose a factor 5 for this example.

The water flow in the fracture is driven by a gradient *i*. We simplify the geometry for his analysis to be linear flow over a distance equal to the width of the spalled zone. The entire pressure drop takes place over one plug at the upstream side and one at the downstream side of the (square) hole. The plug with hydraulic conductivity *K* has a transmissivity $T_{plug} = K^* \delta$.

Figure 6-1. Water flowing in a fracture expands out into a large porous body.

The gradient over the plug is larger by a factor $W_{zone}/(2d_{blue})$. This is because the pressure drop that would have taken place over a distance equal to the width of the spalled zone now will occur over the length of two plugs. As the flow through the fracture and the plug is equal the following relation is obtained

$$
q = Tid_{zone} = K\delta d_{zone}i \frac{W_{zone}}{10\delta}
$$
\n(13)

From the second and third term we obtain

$$
K = \frac{10T}{W_{zone}} = 50T\tag{14}
$$

Thus when $K>>50T$ the porous medium can be taken to have infinite conductivity for the purpose of the draw in of water. When $K = 50T$ there will be no extra draw in of water and when $K < 50T$ the water in the fracture will flow around the damaged zone as if it is impervious.

This analysis is highly idealized. Nevertheless, a hydraulic conductivity larger than 10^{-6} m/s in the spalling zone does not seem reasonable, considering that it is confined by the rock on two sides and by the bentonite buffer that has a strong swelling pressure and will counteract the movement of the rock pieces in the spalled zone. However, it must be recognised that there are no experimental data available.

6.2 How large part of the spalled zone is passed by the water?

Below we address the second point of how large a cross section of the damaged zone most of the water will pass through. The model is set as a 2.5 m long 0.1 m high zone. Due to symmetry only half the length of the canister region is modelled and the fracture intersects in the middle. See Figure 6-2. An inlet point (the intersection with the inlet of the fracture) is located at the lower left hand corner and an exit point at the upper left hand corner. The figure thus is turned 90 degrees compared to the deposition hole. Darcy's equation is solved for the two dimensional region. The computational tool /Comsol Multiphysics 2005/ was used to obtain the numerical solutions. The solution also verified that the plug length discussed above is on the order of 3–5.

Figure 6-2 shows the head distribution and the streamlines through the damaged zone from the fracture intersecting the zone, through the zone, and out through the fracture at the other side. The horizontal direction in the figure should be seen as either upward or downward in the zone.

Fracture transmissivity m^2/s	Zone conductivity $K = 50T m/s$
10^{-9}	5.10^{-8}
10^{-8}	510^{-7}
10^{-7}	510^{-6}
10^{-6}	510^{-5}

Table 6-1. Lowest conductivity of spalling zone which would cause water to be drawn in to the zone.

Figure 6-2. Pressure head distribution and streamlines in the lower or uppermost 0.25 m of the damaged zone.

Figure 6-3 shows how the flowrate through the zone is distributed as a function of the distance below or above the fracture. It is seen from the figures that practically all flow will pass through 5–10 % of the length of the damaged zone. For practical purposes in this note an "*f*" of 0.1 is used for intersection angles not very near the vertical. For a vertical fracture all the zone will be accessed by the water and $f = 1$.

Figure 6-3. Pressure head gradient (or flowrate) at mid line of damaged zone. The fracture intersects at arc length 0. Arc-length 0.2 is 0.2 m below or above the fracture.

6.3 Tortuosity of the spalled zone

The third point on tortuosity is now addressed briefly. There are no readily accessible data for the tortuosity of rock that has been subjected to spalling. Tortuosity is caused by lengthening the transport pathways as the solute has to move at slanted angles in the fractures. Also in the term tortuosity generally effects of constrictivity of the narrow fractures is included. Relations between porosity and tortuosity have been proposed such as the so called Archie's "law" which suggests that approximately the following relation could be used

$$
\tau^2 \cong \varepsilon_{zone}^{\quad \text{0.6}} \tag{15}
$$

A porosity of 0.01 would give a tortuosity of about 16. As neither the porosity of the zone nor the alignment or frequency of the fractures is known a tortuosity of 10 is tentatively suggested.

7 Discussion and conclusions

7.1 General

The simple models and examples show that there may be a considerable flowrate through a zone damaged by spalling if the transmissivity of the fracture in the rock that intersects it is large. However, for this to happen also the hydraulic conductivity of the damaged zone must be large. No data are available for this at present.

The solute transport to or from the water in the zone is limited by the rate of diffusion in the flowing water during its passage of the zone. By far not all the water flowing through the zone will exchange solutes with the buffer. A considerable increase of the flowrate of water that can take up solutes from a leaking canister can be expected if the hydraulic conductivity of the zone is large. In the sample calculations, where data that are in the range of possible values have been used, the increase in the equivalent flowrate was found to be about a factor of 1.4 compared to when there is no damaged zone for not very steep fractures. In the extreme case with a vertical fracture intersecting the damaged zones on both sides of the deposition hole an increase of up to a factor 9 was found. However, for a larger fracture aperture of 1 mm instead of the 0.1 mm in the above example the ratios change to 0.4 and 2.8 respectively. No constant ratio between the *Qeq* for the non-damaged and the damaged case can therefore be found.

Note that in addition to the $Q_{\text{e}qDZ}$ in the spalling zone also the $Q_{\text{e}q}$ in the fracture intersecting the hole outside the zone must be accounted for. These values are additive, neglecting the somewhat decreased fracture intersection length along the undamaged part of the hole and the changes in flow pattern caused by the zone.

Equivalent flowrates up to several tens of litres per year could result when a very high transmissivity fracture intersects the deposition hole.

However at very high flowrates the diffusion resistance in the buffer will put an upper bound on the rate of solute exchange between the flowing water and the copper canister. At most about 30 litres per year of water could be fully depleted of a solute e.g. a corrosive solute or take up a nuclide to the concentration at the canister surface.

It should be stressed that the hydraulic properties of the damaged zone have not been measured. Therefore it has been assumed as an extreme that the conductivity is very large and does not contribute to limit the water flow in the zone. Also the diffusion properties of the zone are only roughly estimated. The data that have been used in the sample calculations have been chosen to be as realistic as possible but on the conservative side.

7.2 Application in PA

Assume that for every canister position the flowrate *q* in the fracture that intersects the deposition hole has been determined from hydraulic calculations. To the Q_{eq} for a deposition hole without spalling should be added a Q_{e0Z} caused by the presence of the damage.

A straightforward approach would be to use Equation (5) directly. All geometric entities, W_{zone} , \overline{L}_{zone} and d_{zone} , are known. The pore diffusion coefficient D_p is obtained from Equation (6) with the tortuosity τ^2 from Equation (15) if the porosity of the spalling zone is known. I would, however, suggest that a constant D_p of 10^{-10} m²/s be used because the data are quite uncertain and this value would probably be on the conservative side.

The remaining question is how to assess *f*. If the location and orientation of the fracture that intersects the deposition hole is known then it would in principle be possible to determine how long the intersection with the spalling zone(s) is. This length would be substituted for W_{zone} . The factor *f* could also be increased proportionally until it becomes 1. For a fracture intersecting the hole at right angles *f* could be taken to be 0.1.

However, considering the uncertainties involved I feel that such refinements are not warranted. A simple approach could be to take $f = 0.5$ for all holes irrespective of orientation. This would account for both an increase in *Wzone* and *f* for all intersection angles and be on the conservative side.

Furthermore, account should be taken of the diffusion resistance in the buffer. This would limit the total to some 30 litres/year even for extremely high flowrates in the spalling zone.

8 Notation

9 References

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