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Flow and solute transport in backfilled tunnel and collapsed backfill – possible extension of Comp32

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Abstract

This report explores the mechanisms and the rate of radionuclide migration up into the backfill and the further transport of the nuclide with the water seeping in the backfill. The consequences of a partly collapsed backfill are also addressed. Simple analytical expressions as well as finite difference models are used for exploratory calculations. A proposal is made of how these processes could be included in the computer program Comp32 for use in PA calculations.

Sammanfattning

Denna korta rapport undersöker de mekanismer som får radionuklider att sprida sig upp till tunnelns återfyllnadsmaterial och med vilken hastighet de sedan transporteras längs tunnel med vattnet som sipprar genom återfyllnaden. Konsekvenserna av en partiell kollaps av återfyllnaden utreds också. Enkla analytiska modeller samt en numerisk finit elementmodell används för beräkningar av några representativa exempel. Ett förslag framförs om hur dessa processer skulle kunna föras in i beräkningsprogrammet Comp32 för att användas för beräkningar i säkerhetsanalysen.

Summary

In the Swedish deep geological final repository for spent fuel the tunnels will be filled with a backfill with low permeability. However, some flow may take place in the backfill. Nuclides released from a leaking canister could diffuse up to the flowing water in the backfill and be transported downstream in the tunnel. At an intersection of the tunnel with a fracture zone the contaminated water might flow out into the zone.

This report addresses the transport mechanisms and rate of transport from a leaking canister up through the buffer and backfill in the deposition hole, further into the backfill in the tunnel and the transport along the tunnel. Spreading by diffusion in the buffer and backfill as well as retardation of sorbing nuclides is accounted for.

The transport mechanisms and rates of transport are described and some simple models with analytical solutions are used to quantify the processes. These simple solutions are used to gain insights into when different transport mechanisms are important. The simple solutions are used to simulate a base case example where a non-sorbing nuclide (iodide) and a sorbing nuclide (radium) move in the backfill by diffusion and by advective flow. The simple sample calculations show that it would take thousands of years for iodide to move 20 m along the tunnel and that a release pulse would spread out considerably over time.

The sorbing nuclide ^{226}Ra with a half life of 1,600 years would be strongly retarded by sorption and would decay to insignificance during its migration along the tunnel.

The consequences of a collapse of backfill leaving a channel above the backfill is also studied by a simple analytical model that accounts for water flowing in the collapsed part of the backfill at the ceiling of the tunnel. A nuclide that diffuses up to the flowing channel will flow with the ("rapidly" flowing) water but will be retarded by diffusion down into the backfill again. This down diffusion retards the nuclide migration considerably and in fact is nearly as effective as if the same water flowrate were to flow in the pores of the backfill and be in direct contact with the sorbing backfill.

A collapsed region at the top of the tunnel thus does not have a detrimental effect on the nuclide movement. In fact, by forming a high conductivity channel on top of the backfill most or practically all water that flows in the tunnels will move there. As a consequence there will be much less flow in the backfill itself. The nuclide will have to diffuse from the canister up to the ceiling of the tunnel before it can move along the tunnel.

Numerical computations are also used to simulate the combined effects of diffusion from a damage at the top of a canister up to and into the backfill and further transport along the tunnel. An intact backfill as well as a collapsed backfill are simulated. The results confirm the analysis based on the simpler models.

The so called Near Field Model Comp32 used in SKB performance assessment modeling could directly be extended to account for flow along the tunnel with or without a collapsed part.

Contents

1 Introduction

The Swedish repository for spent nuclear fuel (SF) is planned to be located at about 500 m depth in crystalline rock. The SF in copper canisters will be emplaced in vertical boreholes from the floor of tunnels. The tunnels will be backfilled with either natural clay or a mixture of bentonite clay and sand. The canisters are surrounded by a buffer consisting of compacted bentonite.

Water flows in fractures in the rock. Some water conducting fractures may intersect the deposition holes and the tunnels. Solutes, e.g. corrosive agents, in the water may enter the buffer and backfill by diffusion and could reach the copper canister and cause corrosion. Radionuclides could escape from a damaged canister, diffuse in the buffer and backfill to water seeping in the fractures in the rock and be carried further in the fracture system in the rock.

The hydraulic conductivity of the buffer is very low and solute transport in the buffer is dominated by molecular diffusion. In the backfill in the tunnels advection may also contribute to solute transport.

This report sets out to study the rate of transport the solute transport paths to and in the backfill in the tunnels and the transfer to the flowing water in fractures and fracture zones that intersect the tunnel.

2 Aims and scope

The aim of this note is to study the radionuclide migration by advective flow along a backfilled tunnel. Advection, molecular diffusion and retardation by sorption in the backfill are to be accounted for. A further aim is to assess whether these processes could readily be included in the near field model Comp32 used in SKB performance assessment modeling.

3 Base case formulation for comparison

The following base case is used for the comparisons. Figure 3-1 shows the dimensions of the region modeled and Table 1 summarizes the data used.

The setting is that there is flow in the backfilled tunnel coming from left to right. The water flow passes the deposition hole from which a solute (nuclide) will diffuse upward and enter the tunnel which is filled with a backfill. The solute is transported by advective flow as well as by molecular diffusion in the backfill. The solute will diffuse upward as well as upstream (left) and downstream (right). Some solute reaches the top of the tunnel where a backfill may have collapsed and where the water flow is faster than in the backfill. There the water may carry the solute faster than in the backfill. However, the solute can also diffuse back into the backfill at locations downstream where the backfill has a lower concentration than that in the flowing water. The solute movement in the collapsed channel will then be retarded.

The system is modeled in two dimensions only, neglecting the third dimension of the tunnel. This is deemed sufficient for the purposes of this report.

Table 3-1. Data for the simulations.

Entity	Meaning	Value
L_{left}	Length of tunnel left of (centre of) deposition hole	20 m
L_{right}	Length of tunnel right of (centre of) deposition hole	20 m
H_{tunnel}	Height of tunnel	5.5 m (including collapsed part)
$H_{collapse}$	Height of collapsed backfill	0.2 m
W_{tunnel}	Width of tunnel	5.5 m
D_{hole}	Diameter of deposition hole	1.75 m
W_{hole}	Equivalent width of deposition hole to have same cross section area as a cylindrical hole	0.44 m
$H_{buffer\ in\ hole}$	Height of buffer in hole	1.5 m
$H_{backfill\ in\ hole}$	Height of backfill above canister	1 m
u_o	Flux in tunnel	0.001 m^3/m^2/year
$q = q_1 + q_2$	Total flowrate through tunnel	0.030 m^3/year
$\varepsilon_{backfill\ anion}$	Porosity of backfill for anions	0.3
$\varepsilon_{backfill\ other}$	Porosity of backfill for cations and uncharged species	0.3
$\varepsilon_{buffer\ anion}$	Porosity of buffer for anions	0.17
$\varepsilon_{buffer\ other}$	Porosity of buffer for cations and uncharged species	0.43
$D_{e\ backfill}$	Effective diffusivity in backfill	1.2 10^{-10} m^2/s
$D_{e\ buffer\ anion}$	Effective diffusivity in buffer for anion	1.0 10^{-11} m^2/s
$D_{e\ buffer\ other}$	Effective diffusivity in buffer for other species	1.0 10^{-10} m^2/s
$K_d\rho_{\ backfill\ Ra}$	Sorption coefficient in backfill Ra	22.8 $m^3/m^3(K_d \cdot \rho \cdot (1-\varepsilon))$
$K_d\rho_{\ buffer\ Ra}$	Sorption coefficient in buffer Ra	7.7 $m^3/m^3(K_d \cdot \rho \cdot (1-\varepsilon))$

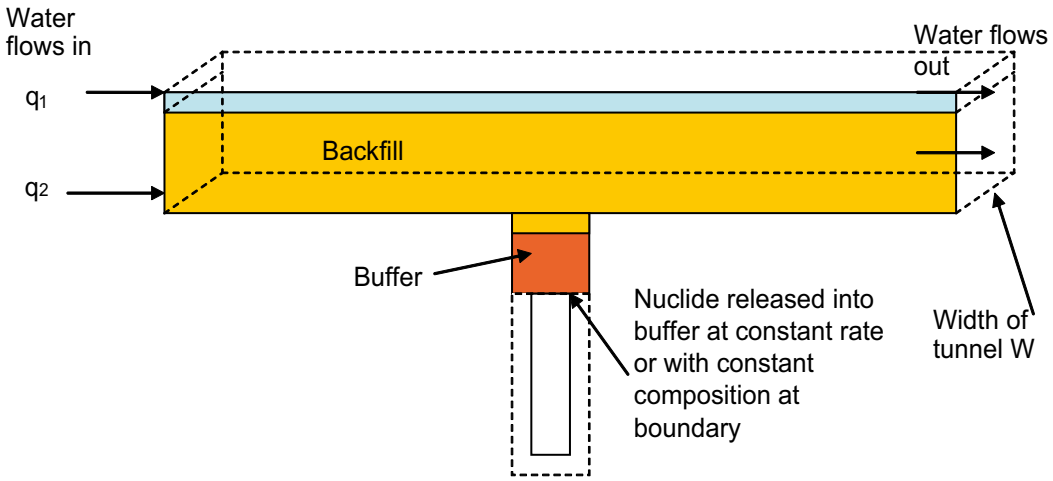

Figure 3-1. *Tunnel system modeled.*

4 Characteristic times

A simple estimate can be made of the times involved for a solute to migrate a distance x by diffusion and by advection. This will be used here to assess the times that need to be considered in the subsequent simulations. These estimates also indicate which processes could be the ones that mainly determine the transport processes from the canister to the outlet from the tunnel. Such simple comparisons often can give insights into the processes which are more difficult to gain from only numerical simulations. Some simple analytical solutions, which although they describing some simple cases (e.g. 1D instead of 2D), can serve the same purpose. They also serve the important purpose of testing the validity of the numerical solutions.

The time for a solute to advance through a porous column by advective flow is simply the ratio of the porous volume divided by the flowrate. For a sorbing solute the retardation due to sorption is accounted for by the retardation factor R. The latter states that the solid has a "holding" capacity R times higher than the same volume of water. Thus for a non sorbing and a sorbing solute alike the residence time of the solute is

$$t_{flow} = \frac{V_{water}}{q_{water}} R = \frac{V_{water}}{q_{water}} (1 + \frac{K_d \rho (1-\varepsilon)}{\varepsilon}) \quad (1)$$

The retardation factor is

$$R = 1 + \frac{K_d \rho (1-\varepsilon)}{\varepsilon} \quad (2)$$

For solute transport by molecular diffusion similar reasoning can be applied. In contrast to advective flow diffusion allows a solute to gradually emerge through the porous volume and increase its concentration slowly over time instead of having a sudden more or less sharp arrival as for flow. Nevertheless, a simple expression is obtained for when the concentration at the outlet end has reached some fraction of that at the inlet. One simple expression for such time is shown, Equation (3).

Figure 4-1 shows the dimensionless concentration profile for one-dimensional diffusion in a plane sheet L thick that has been exposed to concentration 1 since time zero on one side and is closed on the other. Initially it had concentration zero. It is based on the solution to the instationary diffusion equation (Fick's second law) /Crank 1975/. See Appendix 1.

The dimensionless diffusion time $D_a t/L^2$ can be used to illustrate how the concentration of the solute penetrates into the slab. Inspection of Figure 4-1 shows that for $D_a t/L^2 = 1/16$ (= 0.06) the concentration is 0.01 at the far side. We denote the time to reach the concentration 0.01 $t_{diffusion0.01}$.

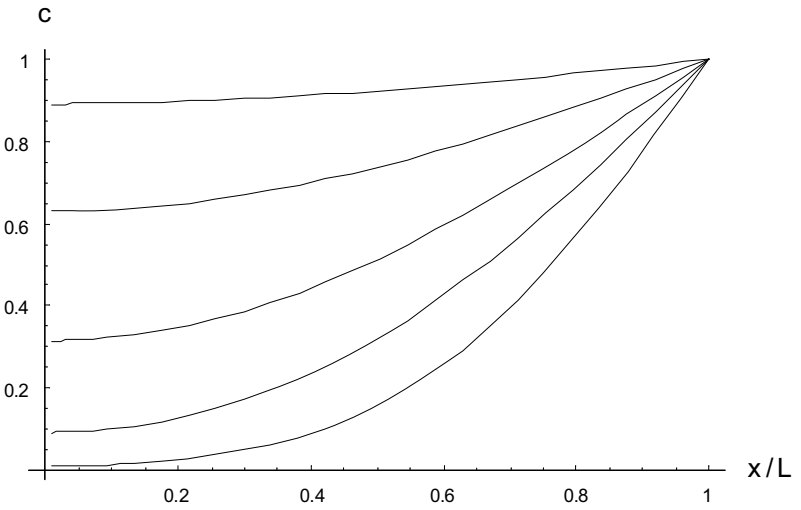

Figure 4-1. *Concentration vs. distance from centre of sheet for $D_a t/L^2$ from bottom and up: 1/16, 1/8, 1/4, 1/2, 1.*

$$t_{diffusion0.01} = \frac{1}{16}\frac{L^2}{D_p}R = \frac{1}{16}\frac{L^2}{D_a} \qquad (3)$$

Here D_p is the pore diffusion coefficient D_e/ε and $D_a = D_p/R$ is the so called apparent diffusion coefficient.

The $t_{diffusion0.01}$ can be used to visualize the time it takes for a diffusing species to reach a small but noticeable concentration at the distance L.

It is also the time for an appreciable amount of the solute through a sheet to start to appear. This is illustrated in Figure 4-2. A noticeable amount of solute through the sheet begins at the dimensionless time $D_a t/L^2 = 0.06$. At $D_a t/L^2 > 0.5$ the flux has essentially reached a steady state.

The time $t_{diffusion0.01}$ can be used to form an impression of the times involved for a nuclide to migrate through the different barriers. It can be used to assess if advection is slower or faster than diffusion to transport the nuclide through a barrier. For advective transport a very simple criterion can be constructed for when a nuclide will have decayed to insignificance. For a residence time equal of 15 half lives a nuclide will decay to $3\ 10^{-5}$ of the original concentration. During 20 half lives it will decay to 10^{-6} and for 30 half lives to 10^{-9}.

For decaying nuclides another simple criterion for when the nuclide can decay to insignificance when diffusing through a medium was suggested by /Neretnieks 1985/ who solved the diffusion equation for a decaying species diffusing through a plane for two different boundary conditions, namely constant influx and constant concentration at the inlet side. The maximum concentration or flux, ever, at the outlet side behaves somewhat differently but for large values of κ, where

$$\kappa = L\sqrt{\frac{\lambda}{D_a}} \qquad (4)$$

the solutions essentially coincide. For large values of κ the nuclide decays significantly. For $\kappa = 10$ the decay is to 10^{-5} and for $\kappa = 30$ it decays to 10^{-15}.

^{129}I has so long half life that it will not be noticeably influenced by migration in the buffer or backfill but ^{226}Ra with a half life of 1,600 years ($\lambda = 4.33\ 10^{-4}$ year^{-1}) will.

Table 4-1 gives the retardation coefficients for an anion (Iodide) and a sorbing nuclide (Ra) in the backfill and in the buffer used in the sample calculations.

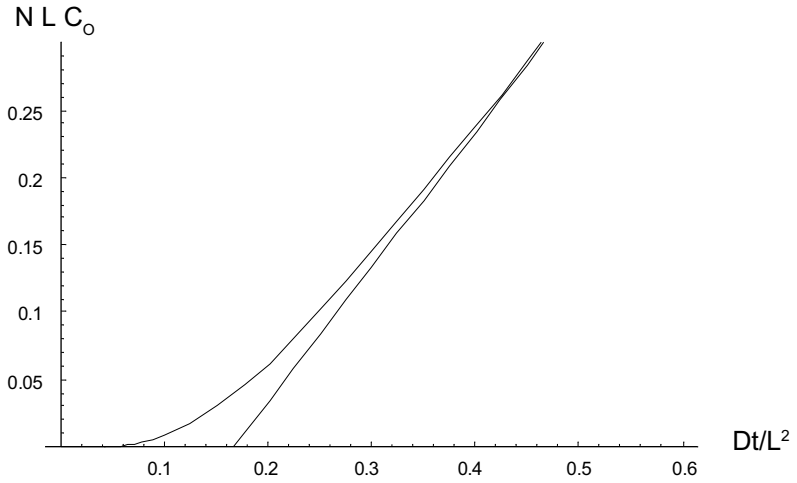

Figure 4-2. *Accumulated amount of solute that has diffused through a sheet as a function of the dimensionless time $D_a t/L^2$.*

Table 4-1. Retardation coefficients in backfill and buffer for iodide and radium.

Material	Species	Retardation coefficient	Pore diffusion coefficient m²/s
Backfill			
	I^-	1	$3.33\ 10^{-10}$
	Ra^{2+}	77.0	$3.33\ 10^{-10}$
Buffer			
	I^-	1	$5.88\ 10^{-11}$
	Ra^{2+}	18.9	$2.79\ 10^{-10}$

Table 4-2. Diffusion and advection times.

Entity	Meaning	Iodide, time years	Radium, time years	Number of half lives and κ for ^{226}Ra
$t_{diffusion0.01}$ buffer	Through 1.5 m buffer	75	304	$\kappa = 1.44$
$t_{diffusion0.01}$ backfill	Through 5.3 backfill + 1 m buffer	200	15,400	$\kappa = 5.1$
$t_{diffusion0.01}$ along backfill	Along 20 m buffer	2,400	183,000	$\kappa = 17.6$
t_{flow} buffer	Through 20 m buffer, all water	6,000	462,000	Number of $t_{1/2}$'s 289
t_{flow} collapse	Through 20 m collapsed buffer, all water	733 No diffusion down into backfill assumed	733 No diffusion down into backfill assumed	Number of $t_{1/2}$'s 0.46

It is seen in Table 4-2 that ^{226}Ra would be expected to decay significantly during its travel along 20 m backfilled tunnel. Some decay may also be expected during its diffusion from the deposition hole up to the ceiling of the transport tunnel with its potential collapsed backfill.

5 Some simulation tools

In this section we explore the movement in the backfilled tunnel with flow as well as diffusion. Furthermore the impact of a collapsed backfill at the top of the transport tunnel is studied. See Figure 3-1. Three tools will be used. The first is an analytical expression for flow in a porous medium with advection, diffusion (dispersion) and retardation due to sorption. This is called the Advection-Diffusion equation. It is shown in Appendix 1.

The second tool is also an analytical expression that shows how the concentration along water flowing in and above the collapsed backfill evolves over time and distance. Account is taken of solute diffusion in and out of the stagnant water in the backfill below the flowing water. The solution by /Sudicky and Frind 1982/ is used. It is summarized in Appendix 1. Nuclide containing water enters at one end of the flowing channel and is followed along the flowpath

The third tool is a numeric technique based on finite element discretisation to account for all the processes depicted in Figure 3-1 simultaneously. Water flows in the collapsed channel past the deposition hole, the nuclide diffuses up from the deposition hole, reaches the seeping water in the backfill, is partly swept along with the water in the backfill and partly it diffuses up to the flowing water above the backfill and is swept downstream. As this water flows past as yet uncontaminated backfill the nuclide can diffuse down into the backfill. The multipurpose numerical program Multiphysics /Comsol 2005/ is used.

The first two cases are simplifications of the third and used to verify the numerical solutions.

5.1 Simple solutions: Advection-Diffusion equation and solution for flow in a channel with solute uptake into a porous matrix contacted by the stream

5.1.1 Advection-Diffusion equation, AD

The Advection-Diffusion equation gives the following results for radium migration along a 20 m length of tunnel with the data given in Tables 3-1 and 4-1.

Figure 5-1 shows that advection dominates the transport although there is a noticeable contribution by the molecular diffusion to the transport of a radium-like substance. Figure 5-2 shows that a substantial decay can be expected for ^{226}Ra for migration along 20 m of the backfilled tunnel. These results agree with the data presented in Table 4-2.

No calculations are made for iodide because it will not decay noticeably. The AD breakthrough curve would be practically identical to that in Figure 5-1 except that the time scale would be 77 times shorter as there is no retardation for this nuclide.

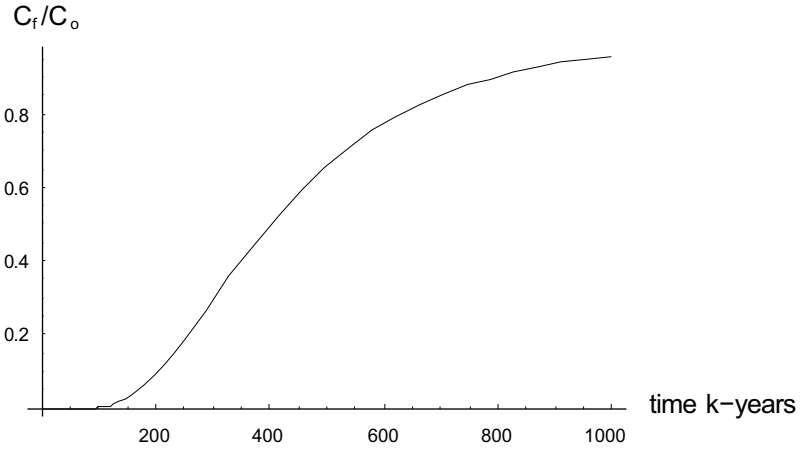

Figure 5-1. *Break through curve for a Radium like substance that does not decay.*

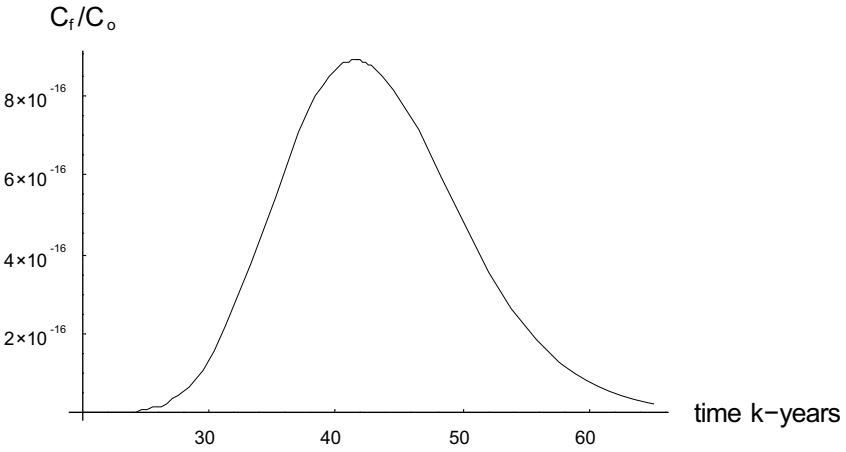

Figure 5-2. *Break through curve for ^{226}Ra when the inlet of the tunnel is fed by a decaying band release, Coe-λt.*

5.1.2 Flow in a collapsed region with solute uptake into a porous matrix contacted by the stream

In these simulations all the water that would flow in an intact backfill with a flux of 0.001 m^3/m^2/ year over the 30 m^2 cross section of the tunnel (0.03 m^3/year) now flows only in the collapsed upper section of the tunnel. The collapsed region is taken to be 0.2 m high. However, it should be noted that the results would be essentially the same for any value smaller than this. The water velocity as such has a marginal impact provided the total flowrate is the same.

It is seen from Figure 5-3 that the solute in the flowing water is very strongly influenced by diffusion in and out of the buffer the water passes. Should this not have been accounted for, all the Iodide would have arrived after 733 years.

Figure 5-4 shows the same simulation for a radium-like substance (without decay).

It is seen in Figure 5-4 that the diffusion to and from the buffer from the flowing water is very effective to retard the radium movement. Should there be no exchange between the flowing water and the stagnant water in the backfill the radium would not be retarded. It would arrive after 733 years as a sharp front. The diffusion exchange allows a very effective retardation of the radium. The mean residence becomes as large as if the water had flown through the backfill instead of above it.

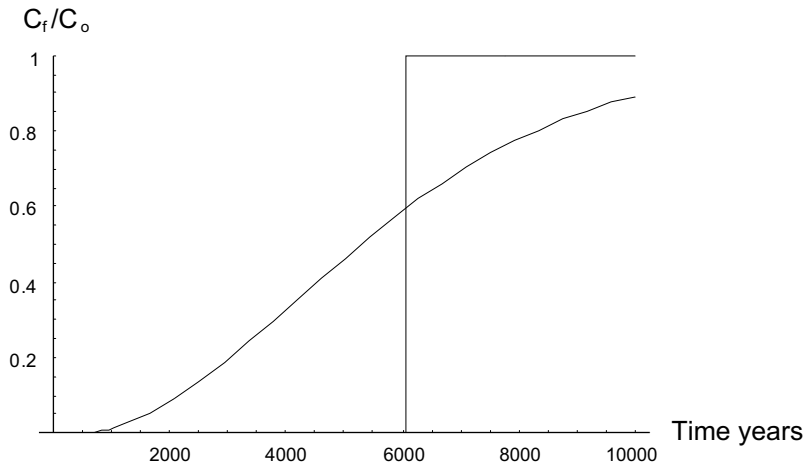

Figure 5-3. *Breakthrough curve for iodide for flow in collapsed part with diffusion in and out of the backfill it passes. The sharp curve shows the break through curve for only advection in the backfill for comparison.*

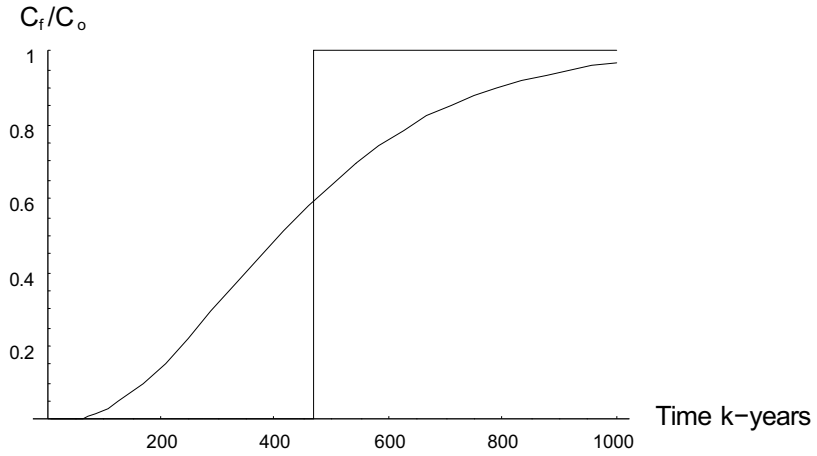

Figure 5-4. *Breakthrough curve for ^{226}Ra for flow in collapsed part with diffusion in and out of the backfill it passes. The sharp curve shows the break trough curve for advection in the backfill for comparison. Note the time scale in thousands of years.*

A similar effect can be expected for all nuclides because they have similar diffusion coefficients in water as radium. For all practical purposes therefore the presence of a collapsed backfill above at the top will cause marginal increase of the nuclide transport, provided the total flowrate in the tunnels is the same. The mean residence time for nuclide *i* will be $t_i = t_w R_i$.

6 Numerical simulations

Figure 6-1 shows the modeled region. Water flows into the system from left to right. The water flows only in the backfill in this case. There is no collapsed region. The canister leaks at its top and maintains a concentration of 1 mol/m^3 of a solute with the diffusion and sorption properties of radium. The solute diffuses up through the buffer and into the backfill with the flowing water, which has a velocity of 0.0033 m/year that sweeps the nuclide downstream. Figure 6-2 shows the effluent concentration over time at 20 m distance from the deposition hole. The concentration in the water stabilizes at slightly more than 0.1 mol/m^3. The total outflow of the solute with the water is 0.0018 mol/year at 1 million years.

In another simulation the backfill has collapsed leaving a 0.2 m high channel with the same width as the tunnel. All the water flows in this channel. The solute diffuses up through the backfill both up- and downstream. The nuclide enters the flowing water in the collapsed section and flows downstream. Underway it diffuses down into the backfill and is retarded by sorption. This is illustrated by the particle tracks in Figure 6-3, which also shows the concentration distribution after 1 million years. Figure 6-4 shows the concentration over time in the out flowing water. Note that the time goes to 10 million years in this figure whereas Figure 6-2 ended at 2 million years. The concentration rises much more slowly in the collapsed case. At 10 million years the total outflow of the solute with the water is 0.0015 mol/year.

Note that the concentration in Figure 6-4 has been scaled by the porosity in order to be comparable to Figure 6-2.

The presence of a collapsed zone above the backfill is advantageous when the total water flowrate through the tunnel is the same. This is because the solute first has to diffuse more than 5 m up through the backfill before it can reach the mobile water.

An increase of the total flowrate by a factor of 10 in the collapse case does not add to the total release rate of the solute but the breakthrough comes earlier. This is shown in Figure 6-5. However, the buildup of the release over time is comparable to that in the no collapse case shown in Figure 6-2.

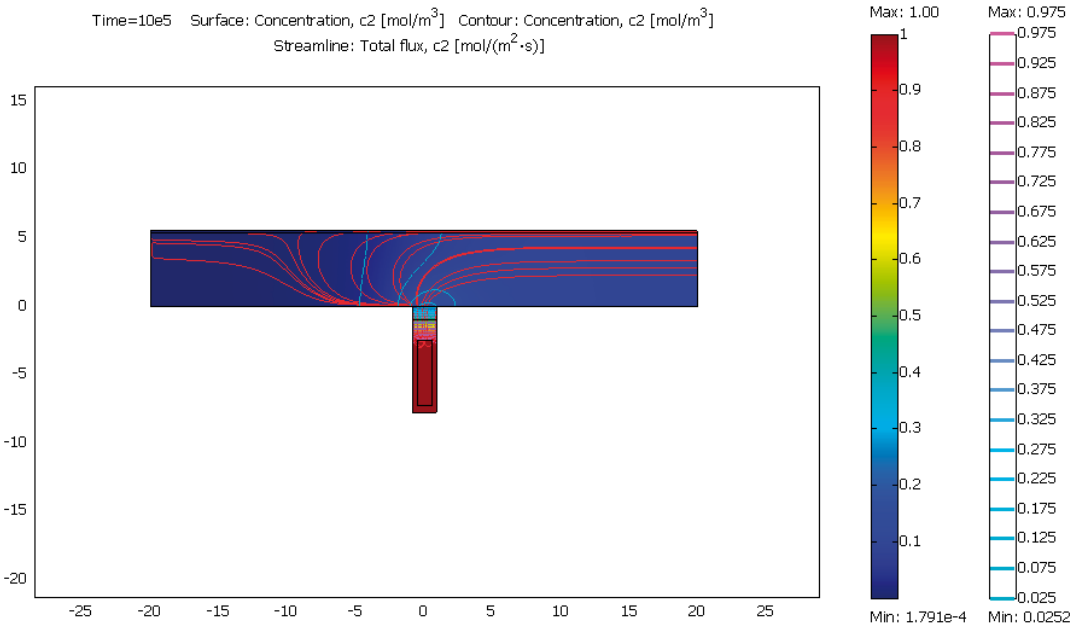

Figure 6-1. *Concentration (colour), potential(blue lines) and steam line (red lines) plot at time 1 million years. Flow in Backfill.*

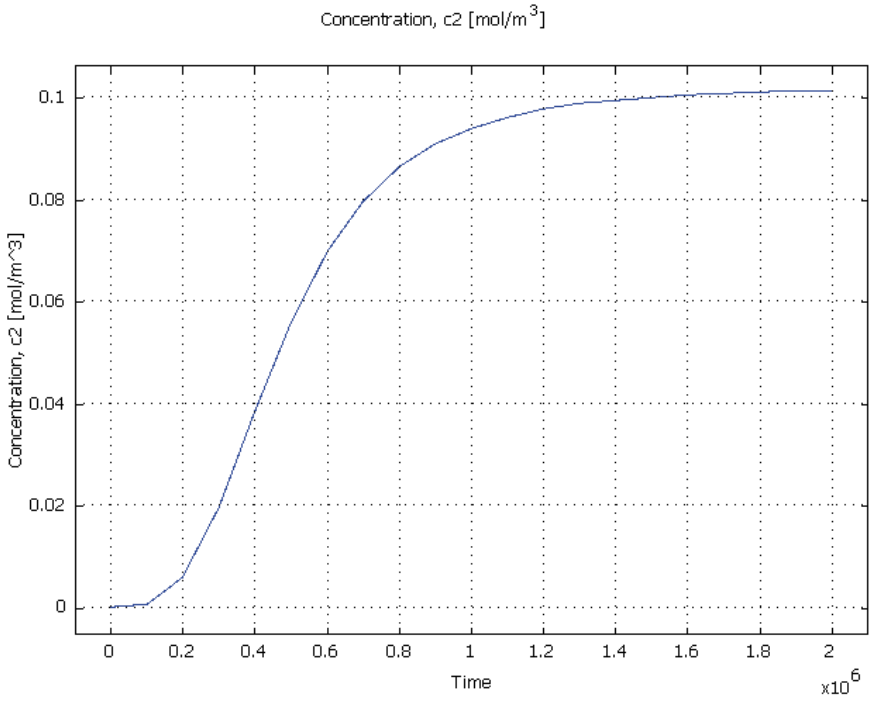

Figure 6-2. *Breakthrough curve for a radium like solute at end of tunnel (20 m). Flow in tunnel.*

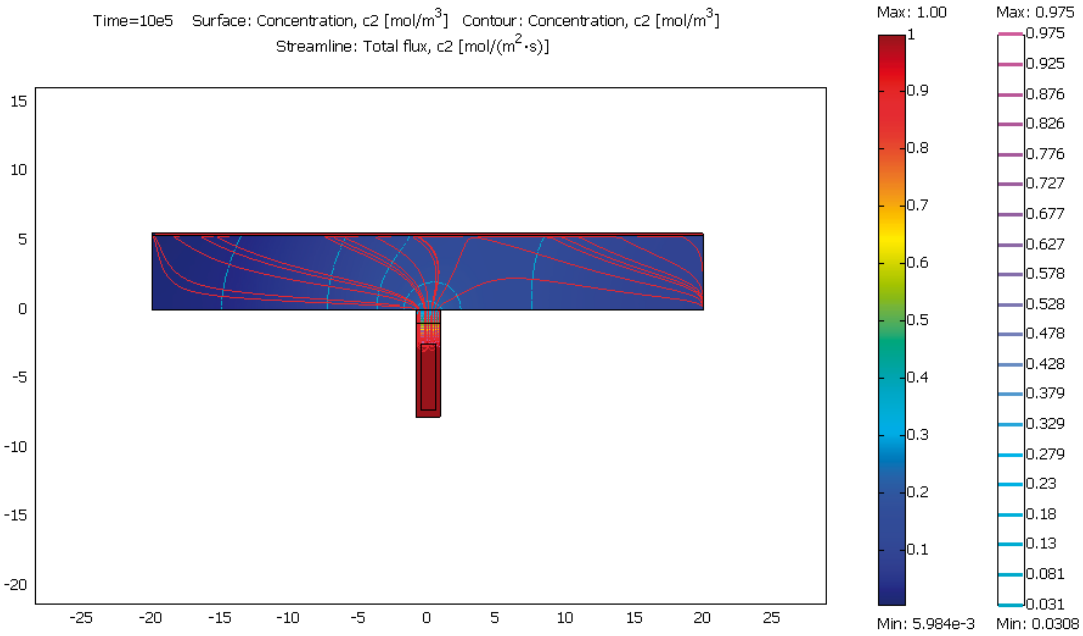

Figure 6-3. *Concentration (colour), potential(blue lines) and steam line (red lines) plot at time 1 million years. All flow in collapsed zone.*

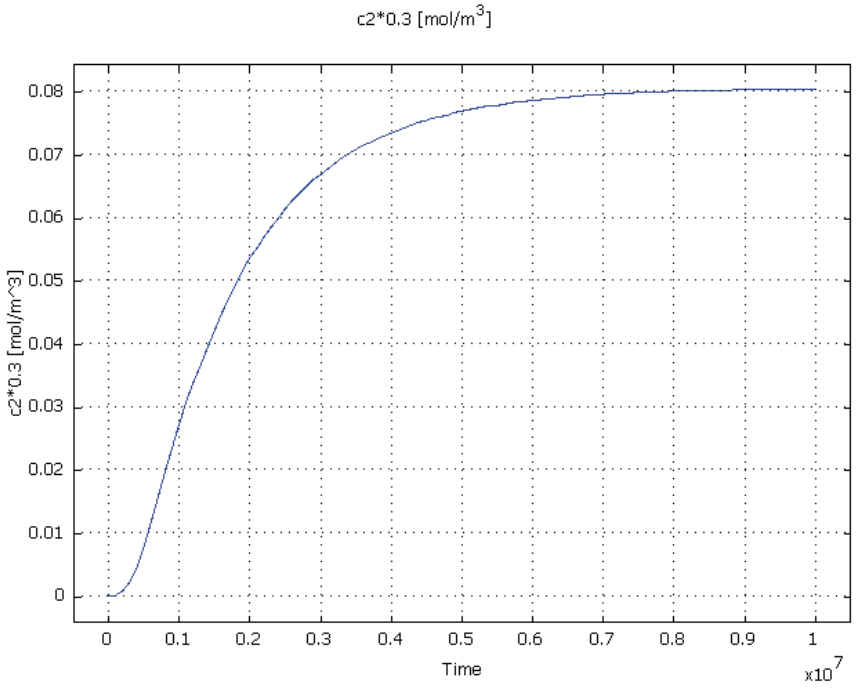

Figure 6-4. *Breakthrough curve at end of tunnel (20 m). All flow in collapsed zone.* ***Note that scale is*** *10 million years.*

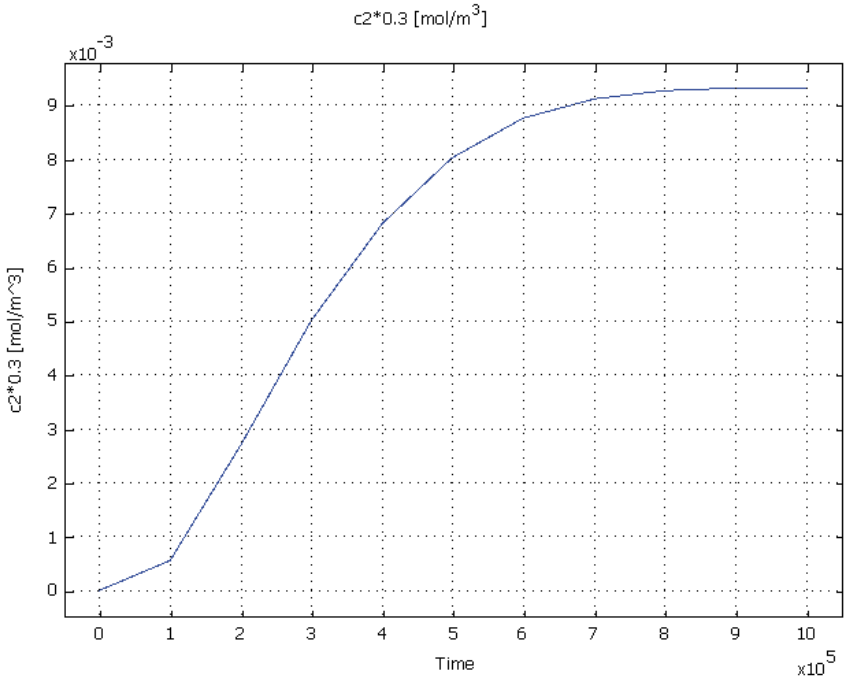

Figure 6-5. *Breakthrough curve at end of tunnel (20 m). All flow in collapsed zone.* ***10 times higher*** *flowrate than in the central case.*

7 Some thoughts on extension of Comp32 to account for advection along the tunnel

Comp32 uses a compartment model which is based on an integrated finite volume discretisation of the buffer and backfill around the canister. It uses imbedded analytical solutions to describe the release of nuclides from a small damage in the canister and also for the entrance of the diffusing nuclide into the water seeping in the fractures intersecting the deposition hole. The basic ideas have been described by /Romero et al. 1995ab/.

The model is readily extended to include flow along the tunnels and also a collapsed zone, if needed. The characteristic times and the simulations presented above suggest that an upstream region on the order of 5 to 10 metres should be sufficient to account for any upstream diffusion. Downstream the distance could be chosen to be equal to that where there is a major fracture or fracture zone where the water flowing in the tunnel is noticeably diverted. Should the zone be closer to the deposition hole than about 10 m a longer tunnel could be modeled to allow the nuclide to diffuse further downstream along the tunnel. In the model this would decrease the nuclide release to the water in the fracture.

Considering that the total nuclide release and transport is strongly limited by the resistances in the immediate near field of the canister and its damage a coarse discretisation of the tunnel suffices. The increase in computation effort will be marginal by adding some tens of metres of tunnel with advective flow. A geometrical progression of the size to the compartments further away from the deposition hole will decrease the computational demand.

The release by diffusion to the flowing water in the fracture intersecting the tunnel could be handled by introducing a sink Q_{eq3} in the compartment with the fracture. See Figure 7-1 below. Nuclide transport between compartments is handled in the usual way but with advection added. In the compartment that is intersected by the fracture the nuclide leaves by advection with a rate $q_3 c_3$ as well as by diffusion to the flowing water in the fracture, $Q_{eq3} c_3$. The remaining nuclide mass moves further downstream into the next compartment. If one wishes to include diffusion downstream of the Q_{eq3} compartment then more compartments can be added. Alternatively such compartments could be omitted and only convective flow allowed from the Q_{eq3} compartment. This can be defended because the further downstream from the source the Q_{eq3} compartment is, the less will be transported by diffusion compared to that by advection.

The above can be used also when the advective flow is negligible. Then the procedure automatically reverts to the conventional Comp32 without advection.

A further simplification could be made by entirely closing the outlet of the Q_{eq3} compartment and forcing all water flow out into the fracture. This would be a conservative assumption.

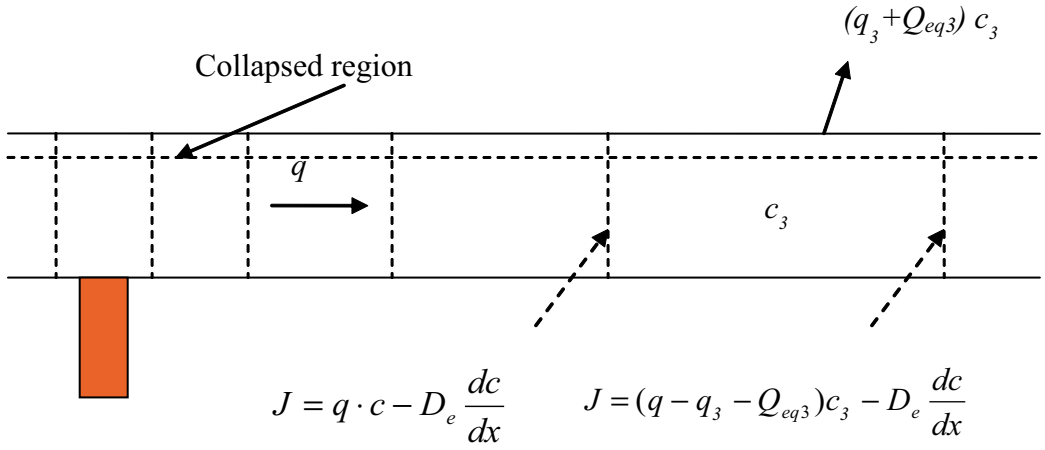

Figure 7-1. *Advective flow and nuclide transport in tunnel. Some nuclide leaves by advection (q_3) and some by diffusion (Q_{eq3}) to water in the fracture. Remaining nuclide flows and diffuses further down along tunnel.*

8 Discussion and conclusions

The simple models and the analysis of the characteristic times for diffusion and advection show that the transport of non sorbing nuclides will spread a release pulse considerably over time and that advection and diffusion times on the order thousands of years can be expected to move the nuclide 20 m along the backfilled tunnel.

A sorbing nuclide such as radium would be considerably retarded. Transport times on the order of hundreds of thousands of years to millions of years could be expected. This would give sufficient time for ^{226}Ra to decay to insignificance.

A collapsed zone above the backfill has little influence on nuclide release and can even be beneficial if the total water flowrate does not increase. Even a considerable increase in water flowrate in a collapsed zone would not add much to the rate of transport along a 20 m distance of the tunnel.

For longer times the total flowrate of the nuclides will be limited by the release rate from the very near field adjacent to the canister.

The numerical model simulations suggest that SKB's near field model can be readily extended to account for flow along the tunnel using advective flux boundary conditions at some distance downstream of the tunnel where the water could be assumed to be diverted into a fracture zone. A distance of 20 m downstream from a leaking canister should be sufficient because already this distance gives rise to very long transport times for sorbing nuclides.

9 Notation

See also Table 3-1.

b	Height of collapsed zone	m
C_f	Concentration in flowing water	mol/m^3
C_o	Concentration at inlet	mol/m^3
C_p	Concentration in pore water	mol/m^3
D_a	Apparent diffusion coefficient	m^2/s
D_e	Effective diffusion coefficient	m^2/s
D_p	Pore diffusion coefficient	m^2/s
J	Solute flux	mol/m^2/s
K_d	Sorption coefficient	m^3/kg
L	Thickness of sheet	m
N	Amount of solute passed through sheet	mol/m^2
q	Flowrate of water	m^3/s
R	Retardation factor	–
t	Time	s
t_w	Water residence time	s
$t_{1/2}$	Half life	s
u_o	Flux (Darcy velocity) of water	m^3/m^2/s
u	Water velocity	m/s
V	Volume	m^3
W	Width of collapsed zone	m
x	Distance along flowpath	m
z	Distance into backfill	m
ε	Porosity	–
λ	Decay constant	s^{-1}
ρ	Density	kg/m^3

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Appendix 1

A1 Diffusion into a sheet from one side of a sheet closed at the other side

Fick's second law (Mass balance for diffusing solute)

$$\frac{\partial C_p}{\partial t} = D_a \frac{\partial^2 C_p}{\partial z^2} \tag{1}$$

Initial condition states that there is no solute in the sheet at time zero

$$C_p(z, t = 0) = 0 \tag{2}$$

Boundary conditions state that at the surface of the sheet the concentration is kept constant at C_o

$$C_p(z = 0, t) = C_o \tag{3}$$

At distance L there is no solute flux. The surface of the sheet is closed to diffusion

$$\frac{\partial C_p}{\partial x}(z = L, t) = 0 \tag{4}$$

The solution to these equations is /Crank 1975, p 47/

$$\frac{C_p}{C_o} = 1 - \frac{4}{\pi} \sum_0^\infty \frac{(-1)^n}{2n+1} e^{-\frac{D_a t (2n+1)^2 \pi^2}{L^2 \quad 4}} Cos(\frac{(2n+1)\pi z}{2L} \tag{5}$$

The group $\frac{D_a t}{L^2}$ can be seen as dimensionless time. It occurs in many equations that describe diffusion in solids and liquids that are stagnant or subject to laminar flow.

A2 The flux J through a sheet

The same equations as above (1), (2) and (3) but with the boundary condition (4) changed to state that at $z = L$ the concentration is 0.

$$C_p(z = L, t) = 0 \tag{6}$$

The solution for the accumulated amount (N) of the solute that has passed through the sheet per unit area is given by Equation (7). The flux J is obtained by division with the time t.

$$\frac{N}{C_0 L} = \frac{D_a t}{L^2} - \frac{1}{6} - \frac{2}{\pi^2} \sum_1^\infty \frac{(-1)^n}{n^2} e^{-\frac{D_a t}{L^2} \pi^2 n^2} \tag{7}$$

A3 Flow in a porous medium with equilibrium sorption and diffusion- the Advection-Dispersion model

We model an infinitely long porous column where water flows in the x direction with velocity u, carrying a solute with retardation coefficient R and a solute diffusivity in the pore water D_p. Initially the water has no solute. From time zero the concentration at $x = 0$ is maintained at C_o.

The differential mass balance is written

$$R\frac{\partial C_f}{\partial t} + u\frac{\partial C_f}{\partial x} = D_p\frac{\partial^2 C_f}{\partial x^2} \tag{8}$$

The initial condition is

$$C_f(x, t = 0) = 0 \tag{9}$$

Boundary conditions state that at the inlet of the column the concentration is kept constant at C_o

$$C_f(x = 0, t) = C_o \tag{10}$$

The column is infinitely long and the concentration when x– > infinity is zero

$$C_f(x- > \infty, t) = 0 \tag{11}$$

The solution is /Carslaw and Jaeger 1959, p 388/

$$\frac{C_f}{C_o} = \frac{1}{2}\left(Erfc\left(\frac{x - tu/R}{2\sqrt{D_p t/R}}\right) + e^{\frac{ux}{D_p}} Erfc\left(\frac{x + tu/R}{2\sqrt{D_p t/R}}\right)\right) \tag{12}$$

For a decaying nuclide where the column is fed by a decaying band release the above solution is multiplied by $e^{-\lambda t}$.

A4 Flow in a channel and diffusion into a plane sheet (backfill) in contact with the channel

A differential mass balance is used to describe the advective transport of the solute in the channel similar to that for the Advection-Dispersion model described earlier, Equation (8). In this case diffusion in the flowing water is taken to be negligible compared to the effects of diffusion in and out of stagnant water in the backfill. This is accounted for as well as the linear sorption in the backfill. The mass balance is:

$$\frac{\partial C_f}{\partial t} = -\frac{q}{Wb}\frac{\partial C_f}{\partial x} + \frac{D_e}{b}\frac{\partial C_p}{\partial z}\bigg|_{z=0} \tag{13}$$

Here, C_f is the aqueous concentration in the channel, C_p is the pore-water concentration in the pore water in the backfill, W is the channel width and b the height of the channel. D_e is the effective diffusivity, and q is the advective flowrate in the channel. The term on the left-hand side of the equation is the accumulation term describing the rate of change of concentration in the water in the channel. On the right-hand side of the equation are the advective flux term and the pore water diffusive flux terms, respectively.

A similar mass balance is used to describe the diffusive transport and linear sorption within the pore water in the backfill.

$$\frac{\partial C_p}{\partial t} = D_a \frac{\partial^2 C_p}{\partial z^2} \tag{14}$$

where,

$$D_a = \frac{D_p}{R} = \frac{D_p}{1 + \frac{(1-\varepsilon_p)}{\varepsilon_p} K_d \rho_s} \tag{15}$$

ε_p is the porosity of the backfill. The initial conditions are:

$$C_f(x, t=0) = 0 \qquad C_p(x, z, t=0) = 0 \tag{16}$$

The boundary conditions are.

$$C_f(x=0, t) = C_0 \qquad C_f(x \to \infty, t) = 0$$
$$C_p(x, z=0, t) = C_f(x, t) \qquad \frac{\partial C_p(x, z=B, t)}{\partial z} = 0 \tag{17}$$

B is the thickness (height) of the backfill. The analytical solution by /Sudicky and Frind 1982/ is used. The solution for no dispersion (diffusion) in the channel in the flow direction and no radioactive decay is

$$\frac{C}{C_0} = 0 \quad \text{for t < x/u} \tag{18}$$

$$\frac{C}{C_o} = \frac{2}{\pi} \cdot \int_0^\infty \frac{1}{\varepsilon} \cdot Exp\left(\varepsilon_R^o\right) \cdot \left[\sin\left(\varepsilon_l^o\right) + \sin\left(\Omega^o\right)\right] \cdot d\varepsilon \quad \text{for t > x/u} \tag{19}$$

$$T^o = t - \frac{z}{u} = t - t_w \tag{20}$$

$$\varepsilon_R^o = -\frac{\omega\varepsilon}{2} \cdot \left(\frac{\sinh(\sigma\varepsilon) - \sin(\sigma\varepsilon)}{\cosh(\sigma\varepsilon) + \cos(\sigma\varepsilon)} \right) \tag{21}$$

$$\varepsilon_l^o = \frac{\varepsilon^2 \cdot T^o}{2} - \frac{\omega\varepsilon}{2} \cdot \left(\frac{\sinh(\sigma\varepsilon) + \sin(\sigma\varepsilon)}{\cosh(\sigma\varepsilon) + \cos(\sigma\varepsilon)} \right) \tag{22}$$

$$\Omega^o = \frac{\omega\varepsilon}{2} \cdot \left(\frac{\sinh(\sigma\varepsilon) + \sin(\sigma\varepsilon)}{\cosh(\sigma\varepsilon) + \cos(\sigma\varepsilon)} \right) \tag{23}$$

$$\omega = \frac{LW}{q} \sqrt{D_e(\varepsilon_{Backfill} + K_d \rho)} \tag{24}$$

$$\sigma = \left(\frac{K_d \cdot \rho_p}{D_e} \right)^{0.5} \cdot B \tag{25}$$

As may be seen from the equations above, the breakthrough curves are determined by three parameters, namely t_w, ω and σ . The first parameter is the residence time of the water in the channel. The parameter ω accounts for the diffusion and sorption in the backfill and the contact surface LW between backfill and the flowrate q. The parameter σ takes into account the effect of a limited diffusion depth into the backfill. For σ sufficiently large compared to ω, the breakthrough curve would be similar to that for infinitely thick backfill. On the other hand, for a small value of σ (small depth B or large diffusion coefficient) the backfill will be equilibrated with the water in the channel.