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Research

Two Dimensional Near-field Calculations of Radionuclide Releases from the SFL 3 and SFL 5 Repository

António Pereira
Benny Sundström

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SKi

SKI perspective

Background

As part of SKI's own capability to perform radionuclide transport calculations a need to develop a two-dimensional (2D) near-field model of the SFL 3-5 repository was identified. A 2D near-field model of the SFR 1 repository has already been developed and tested (Pereira and Sundström 2003).

Purpose of the project

The purpose of this project is to investigate the possibility to develop a useful two-dimensional radionuclide transport near-field model of the SFL 3 and SFL 5 vaults in the SFL 3-5 repository. The results from the 2D model are compared with the calculated radionuclide release from the SFL 3 and SFL 5 vaults done by SKB in their preliminary safety assessment for the deep repository for long-lived low- and intermediate-level waste.

Results

For most of the studied calculations for the reference case the results agree within a factor of ten with SKB results and for some radionuclides even more. There may be several explanations for this discrepancy. However, to solve this a thorough investigation is needed. In spite of the obtained disagreement in the calculation results, the 2D model concept developed in this project is on the whole applicable to the vaults of the SFL 3-5 repository.

Project information

Responsible at SKI has been Benny Sundström.

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Research

Two Dimensional Near-field Calculations of Radionuclide Releases from the SFL 3 and SFL 5 Repository

António Pereira[1]
Benny Sundström[2]

[1]Department of Physics
AlbaNova University Center
Stockholm Center of Physics, Astronomy and Biotechnology
SE-106 91 Stockholm
Sweden

[2]Swedish Nuclear Power Inspectorate
SE-106 58 Stockholm
Sweden

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Contents

Abstract

A two dimensional finite-element model is developed for this work which aim is to simulate the near-field performance of the SFL 3 and the SFL 5 vaults of the planned repository for long-lived, low- and intermediate level waste, SFL 3-5.

The model represents a 2D section of the vault's geometry. One of the new features in this model is that it allows the study of the migration of solubility limited radionuclides. In respect to the SFL 5 results the breakthrough curves obtained show peak releases and respective time of occurrences in relative good agreement with those obtained by SKB. The shape of those curves is different from those obtained by SKB and can be explained from the fact that we are using different models, which highlights the influence of conceptual uncertainties. The calculations for the SFL 3 vault show systematically higher values, with the exception of tritium, than those reported by SKB, which are due to the fact that we could not take into account the sorption capacity of the concrete in the cubic boxes of SFL 3. The reason is that the SKB reports do not explicitly give the information needed to calculate the amount of concrete in the cubic boxes containing the 80 litre drums for the LILW waste of SFL 3. That information is needed to include an "equivalent barrier" to the concrete barrier in our model.

It is also concluded that the distribution of the different types of waste along the vaults is needed to be able to develop a 3D model that more closely can represent the conceptual approach used by the SKB model. It is expected that such a 3D model could deliver more realistic results.

Sammanfattning

En tvådimensionell finita-elementmodell har utvecklats för att används för simulering av närområdet kring förvarstunnlarna SFL 3 och SFL 5, som är en del av det planerade förvaret för låg- och medelaktivt långlivat avfall, SFL 3-5.

Modellen representerar ett 2D tvärsnitt av förvarstunnlarnas geometri. Den tillåter simulering av migration av radionuklider som är löslighetsbegränsade. De uppnådda resultaten för SFL 5 visar att utsläppskurvornas värden för maximumutsläpp och motsvarande tidpunkter är i relativt god överensstämmelse med SKB:s resultat. Utsläppskurvorna skiljer sig i sin form från SKB:s på grund av att vi inte har använt samma modell som SKB, något som illustrerar påverkan av de ingående konceptuella osäkerheterna. Resultaten av SFL 3 beräkningarna visar värden som är systematiskt högre, än SKB:s, med undantag för tritium. Anledningen är att vi inte har kunnat ta hänsyn till sorptionsförmågan av betongen som finns inuti SFL 3:s kubiska avfallsboxar avsedda för det LILW avfallet. Detta beror på att vi inte känner till mängden betong i boxarna som innehåller 80 liters fat. Denna information är nödvändig för att kunna inkludera en barriär ekvivalent till betongens effekt i vår modell.

Den rumsliga distributionen av olika typer av avfall längst förvarstunnlarna är också nödvändig för att kunna utveckla en 3D modell som bättre representerar SKB:s konceptuella modell. Vi förväntar oss att en sådan modell ska kunna ge mer realistiska resultat.

1 Introduction

The Swedish long-lived low- and intermediate-level waste will according to Swedish Nuclear Fuel and Waste Management Co (SKB), be placed in a deep repository, SFL 3-5. In a preliminary assessment report (SKB, 1999a), the SFL 3-5 repository is placed in the same region as the repository for spent nuclear fuel, (SFL 2), although to a certain respect distance (1 km) from it. The main reason for locating SFL 3-5 there was to facilitate the preliminary assessment by using much of the hydrogeological data available in the SR-97 project (SKB, 1999).

In this work we present calculations on the near-field performance of SFL 3 and SFL 5, which are the vaults in which waste from Studsvik, CLAB, the future encapsulation plant and decommissioning waste from the nuclear power plants will be placed.

The figure below is taken from (SKB, 1999a) and shows the information scheme for the SKB preliminary analysis of SFL 3-5. In Figure1.1 we have enclosed by the dotted line, the part of it that respects to the information necessary for the calculations presented in this work.

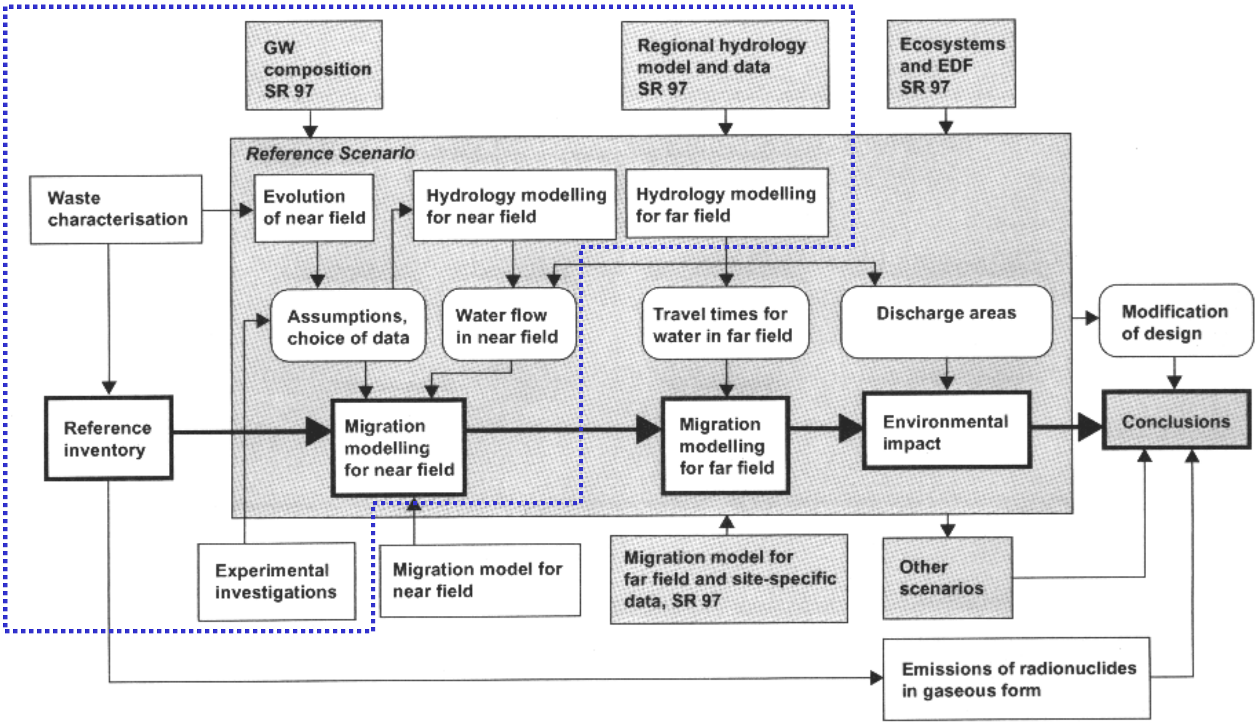

Figure 1.1 The information scheme for the SFL 3-5 repository.

For this work we have developed two-dimensional finite-element codes for the near-field of SFL 3 and SFL 5. For the calculations we use the data chosen by SKB (Skagius et al., 1999) and we expect therefore that the results will agree with those of

SKB. However due to conceptual uncertainties related to the differences between our 2D model and the 3D compartment model of SKB the agreement cannot be complete.

In Section Two we describe briefly the SFL 3-5 system of vaults and we list the radionuclides in the waste examined here, together with their respective inventory at year 2040.

In Section Three the geometry of SFL 3 and SFL 5 are described together with the data on the materials to be used on the different barriers. In Section Four the conceptual model is presented as well as the general assumptions embedded in this model. The reference case is described in Section Five. Section Six presents and discusses the results of the calculations of a reference case. The summary and conclusions are presented in Section Seven, followed by the references and appendixes.

2 The SFL 3-5 system of vaults

A sketch of the SFL 3-5 repository is shown in Figure 2.1. The system is made of three vaults, SFL 3, SFL 4 and SFL 5. In the SR-97 project (SKB, 1999) SKB picked up three alternative places for the safety analysis that are denominated Aberg, Bberg and Cberg. The analysis by SKB is made for one reference scenario. Other scenarios are discussed mainly in a more qualitative way. In this work we do near-field calculations for SKB's reference scenario.

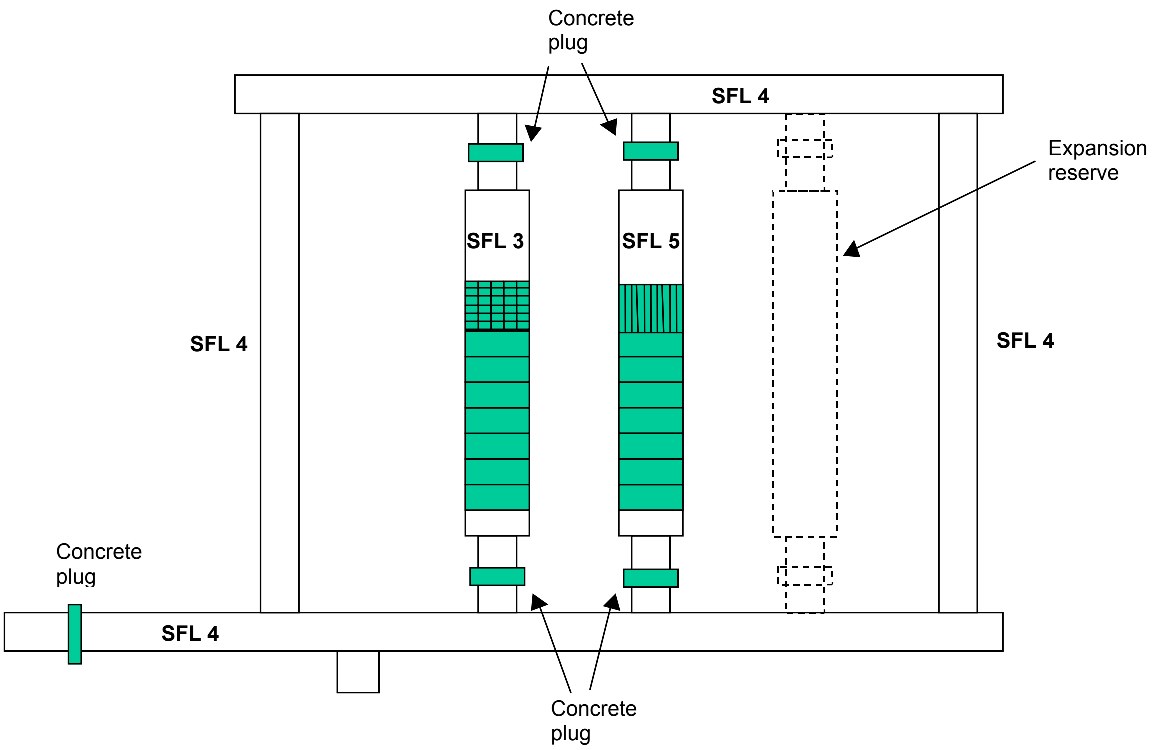

Figure 2.1 *A sketch of the SFL 3-5 repository. To the right of SFL 5 there is space reserved for future expansion if necessary.*

The vaults will be sealed at the ends by concrete or concrete/bentonite plugs with the same "quality" as the intact bedrock The approach of SKB is to provide an hydraulic cage system where the waste will be disposed off. The water will flow mainly around the waste forms and not through them due to the conductivity contrast between the waste forms and the higher conductivity regions involving those forms (the roof of the vaults, the lateral compartments and the bottom region of the vaults). It is also intended to build the vaults so that the water will flow along the direction of the SFL 3 and SFL 5 vaults. The SFL 3 and SFL 5 vaults have the same geometry and dimensions.

2.1 Waste in SFL 3 and SFL 5

The waste in SFL 5 has a high-induced activity and come mainly from operation and decommissioning of the Swedish nuclear power plants (9700 m^3 from reactor internals and core components). That waste is first send to CLAB where the high activity radio-nuclides will decay during 30 to 40 years and simultaneously the temperature of the waste reduced. Some minor quantities come from Studsvik (50 m^3 of decommissioning waste).

The waste in SFL 3 is LILW from Studsvik (1800 m^3) and operational waste from CLAB and from the operation of the encapsulation plant (3800m^3). Waste quantities were taken from Table 2-1 in (SKB, 1999a).

The waste in SFL 5 is placed in boxes of steal, which in turn are placed in concrete boxes (moulds). Porous concrete is injected in the boxes through a hole and will fill the empty space between the solid waste components. Detectors with high activity will first be enclosed in lead boxes. The main part of the SFL 5 waste is made of metal components which activity is due to the near placement to the reactor core, as for instance the moderator tanks. These components may also have their surfaces contaminated if they have been in contact with the primary reactor water.

The SFL 3 waste from Studsvik is placed in 200-litre steel drums or in reinforced concrete moulds (1.2×1.2×1.2 m). The waste from CLAB and the encapsulation plant is placed in concrete moulds of the same dimension as Studsvik's concrete moulds.

Of the total SFL 3-5 waste of 25 000 m^3, 40 % goes to SFL 5. The number of concrete/steel boxes is 1407 and the waste volume is 9750 m^3, Table 2-1 in (SKB, 1999a). The dimensions of the boxes are 1.2×1.2×4.8 m and the walls are 10 cm thick. According to SKB the empty volume that will be filled with porous concrete within the concrete/steel boxes takes up 16% of the total box volume, Figures 2-4 page 2-5 in (SKB, 1999a). The volume of waste that will be placed in SFL 3 represents approximately 20 % of the total waste in SFL 3-5.

2.2 Radionuclides in SFL 3 and SFL 5

The total initial inventory (Figure 2.2) is dominated by the induced activity and is approximately equal to 1.4×10^{17} Bq at year 2040.

Table 2.1 and 2.2 show the inventory (Bq) and half-life (years) of the radionuclides at year 2040 that are examined in this work of SFL 5 and SFL 3 respectively. Values are taken from Table 2-1 in (Pettersson et al., 1999). The uncertainty in the induced activity of the core components and of the internal parts of the reactors in the SFL 5 inventory may be considered uncertain to a factor five to one hundred, page 2-14 in (SKB, 1999a).

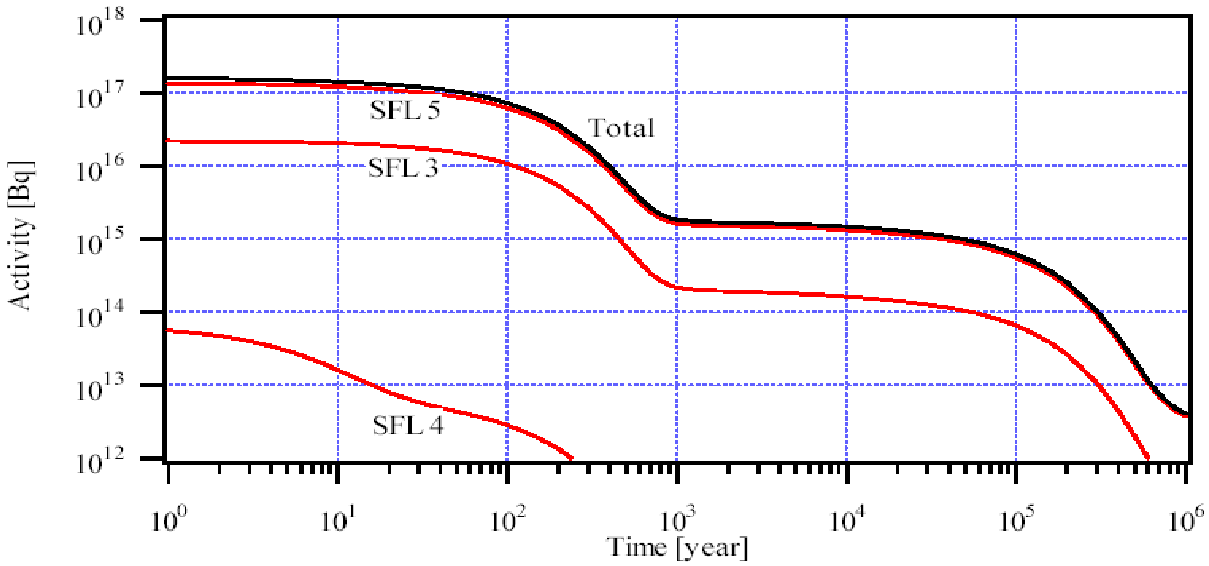

Figure 2.2 *Radioactivity (Bq) as a function of time in SFL 3-5, where time zero corresponds to year 2040. The picture is taken from (Pettersson et al., 1999).*

Table 2.1 *Inventory of the radionuclides, at year 2040, in SFL 5 that are studied in this work. From Pettersson et al. (1999), Table 2-1.*

	Half-life (years)	**Activity** (Bq)
^{14}C (inorganic)	5.7×10^{3}	1.7×10^{14}
^{59}Ni	7.6×10^{4}	1.4×10^{15}

Table 2.2 *Inventory of the radionuclides, at year 2040, in SFL 3 that are studied in this work. From Pettersson et al. (1999), Table 2-1.*

	Half-life (years)	**Activity** (Bq)
^{3}H	1.2×10^{1}	3.2×10^{12}
^{14}C (inorganic)	5.7×10^{3}	3.5×10^{13}
^{36}Cl	3.0×10^{5}	2.1×10^{10}
^{59}Ni	7.6×10^{4}	1.6×10^{14}
^{129}I	1.6×10^{7}	3.4×10^{7}
^{135}Cs	2.3×10^{6}	5.7×10^{8}

3 Geometry and materials

The SFL 3 and the SFL 5 vaults have the same geometry. They are 133 m long, 14 m wide and 19 m in height. The interior of the vaults where the waste is disposed of, is approximately 115×11×11 m. Figure 3.1 shows a vertical cross section perpendicular to the main axis of the vaults.

In the SFL 3 vault a maximum of eight moulds or ten steel drums can be stacked on top of each other in each of the 21 pits that the vault is divided into. There is space for 256 moulds or 1280 steel drums.

The SFL 5 vault is divided into 21 pits and each pit can hold 64 moulds (stacked 8 moulds high) for core components and reactor internals. Totally there is space for 1344 concrete moulds. For details the reader should consult SKB´s compilation of data (SKB, 1999a).

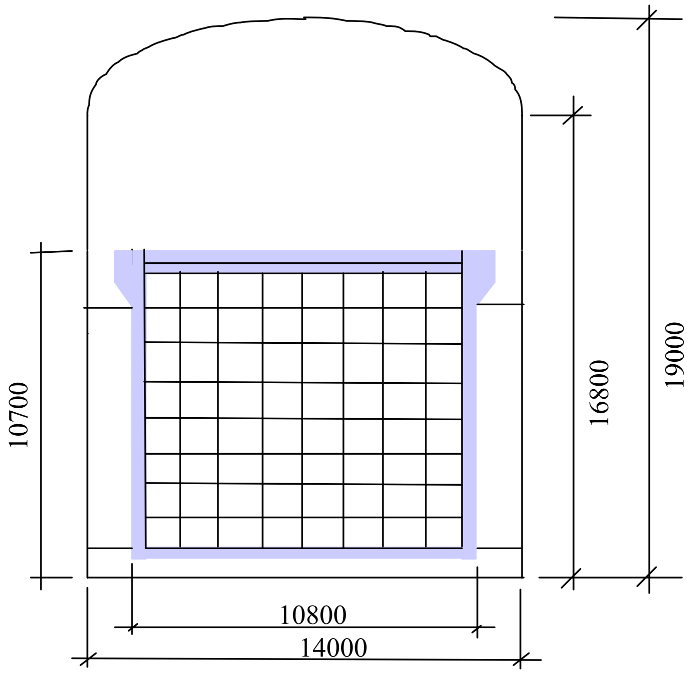

Figure 3.1 *A sketch of the cross section of the SFL 5 vault. The dimensions are given in millimetre.*

3.1. Barrier properties and data

The data on the physical and chemical properties of the different materials used in the construction of SFL 3-5, which are of relevance for our calculations, are given in this section. They are needed as input data to the radionuclide release code developed for use in our calculations. Table 3.1 gives the densities, porosities and diffusivities for the different materials used in the construction of the vaults ; the solid density of the materials is computed from the bulk density. Table 3.2 gives the distribution coefficients (sorption coefficients) of the radionuclides in the host rock. The solubility data respecting solubility limited radionuclides is given in Table 3.3.

Table 3.1 *Densities, porosities and diffusivities for the materials used in SFL 3 and SFL 5. From SKB (1999), Table 8-2.*

Material	**Bulk density** [a)] ρ_b (Kg/m^3)	**Porosity** ε (m^3/ m^3)	**Effective diffusivity** D_e (m^2/s)
Structural Concrete	2295	0.15	1×10^{-11}
Porous concrete	1890	0.30	1×10^{-10}
Gravel/sand	1890	0.30	6×10^{-10}
Pure water [b)]	-	-	2×10^{-9}

[a)] The bulk density is given by $\rho_b = \rho_s (1- \varepsilon)$ where ρ_s is the solid density.
[b)] The diffusivity data for water (all ions) is included here for the sake of completeness.

Table 3.2 *Sorption coefficients (m^3/kg). From Skagius et al. (1999), Table 7-5.*

Ox. State [a)]	**Nuclide**	**Rock / gravel in saline groundwater**
M(I)	H	0
	Cs	0.05
M(II)	Ni	0.02
M(IV)	C (inorganic)	0.001
M(-I)	Cl, I	0

[a)] At reducing Eh and pH 7-9.

Table 3.3 *Upper bounds for solubility in concrete pore water. From Skagius et al. (1999), Table 7-6.*

Nuclide	**Solubility** *(mol/ℓ)*
H	Unlimited
C	Unlimited
Cl	Unlimited
Ni	10^{-7}
I	Unlimited
Cs	Unlimited

In Table 1 and 2 in Appendix II we list the sorption coefficients in the different regions of the engineered barriers. That Table summarises also the densities, porosities and diffusivities for each one of the regions of the FEM model.

3.2 Hydrology and host rock data

The three alternative locations used by SKB in their preliminary assessment (SKB, 1999) are Aberg, Bberg and Cberg. The hydrogeological data needed for our near-field calculations is taken from the SKB modelling of future hydrogeological conditions at the Aberg site (SKB, 1999a). In this location the SFL 3-5 repository crosses a regional zone. The transit times are lower than in Bberg and Cberg and the water path lengths are shorter, see Table 7-3 in (SKB, 1999a). The transit time data and path lengths are not used in our calculations because we focus on the near-field performance of the repository. Table 3.4 gives the total water flow rate and the specific flow rate for the barriers of SFL 5 and SFL 3.

Table 3.4 *Total and specific water flow through the near-field barriers at Aberg of the SFL 3 and SFL 5 repository, for a horizontal regional water flow along the vaults. From SKB (1999a), Table 7-3.*

	Encapsulation (concrete)	**Backfill (gravel)**
SFL 5		
Total	10^{-2} m^3/year	62 m^3/year
Specific	10^{-4} m/year	0.32 m/year
SFL 3		
Total	10^{-2} m^3/year	60 m^3/year
Specific	10^{-4} m/year	0.31 m/year

4 Vault modelling

4.1 The conceptual model

It is assumed in the conceptual model that the radionuclide release from the vault is controlled by advection and diffusion. The rates of diffusion through the different parts of a vault are expressed by the diffusivities of the respective materials and may differ from each other (for instance porous concrete and gravel have different effective diffusivities for the same radionuclide). The conductivities of the barriers are different and therefore also the water flow through those barriers. The vaults are modelled by a system of partial differential equations. The dimensions of the 2D cross sections of the barriers in the model are the same as the corresponding physical barriers. By avoiding "equivalent" barriers as much as possible makes the 2D modelling reasonably transparent. However we will need one equivalent barrier to simulate the retardation in the porous concrete that is spread inside the steal/concrete containers filling the empty spaces between the metal components (SFL 5) or the retardation due to the agglomeration of 16 boxes in a single "equivalent box" (SFL 3 and SFL 5).

The radionuclides leaving the waste boxes will migrate to the top of the vault and subsequently penetrate into the adjacent rock from which they will be transported up to the surface by the groundwater circulating in the repository region. The model takes into account that fissures will develop in the concrete of the tanks and walls by using the equivalent values of the conductivity in the concrete. This hydraulic conductivity corresponds to the existence of a certain number of fractures per metre (one fracture with aperture 10 -100 µm each tenth metre (Höglund and Bengtsson, 1991).

Most of the SFL 5 radionuclides in the metal components are released at a rate that depends on the corrosion rate of the metal. There are also radionuclides that are solubility limited. The solubility limit is introduced in the model through a reaction term $A(t) = k_f C - k_b$. In that reaction $A(aq) \Leftrightarrow A(s)$ the reaction rate constants are high and can therefore be approximated by the equilibrium situation. However for the mass balance we do not need to make that approximation and we can therefore write in general terms,

$$\partial C / \partial t + \nabla.(D\nabla C + C\mathbf{u}) + (k_f C - k_b).(switch\_function) = 0$$

and where:

C - is the radionuclide concentration in pore water, (Bq/m^3).
t - is the time, (years).
u - is the Darcy velocity, (m/year).
k_f - forward reaction constant.
k_b - backward reaction constant.

The switch function has zero value from to A(aq) approximates the solubility limit. The values of the forward and backward reaction constants (k_f and k_b respectively) can be chosen arbitrarily as far as they "almost" fulfil the equilibrium condition.

The near-field release is modelled in two dimensions considering a vertical section perpendicular to the longitudinal axis of the vault. The model simulates two-dimensional advective-diffusive-reactive processes and the radioactive decay (Eq.3.1 and 3.2).

$$\begin{cases} \frac{\partial}{\partial t}(R_i c_i) + \nabla .(-D_i \nabla c_i + c_i \mathbf{u}_i) + A = -\lambda_i R_i c_i \qquad (i=1...n) \\ \\ A(t) = k_f\, c - k_b \end{cases} \tag{3.1}$$

with:

$$R_i = 1 + \frac{K_{d,i} \rho_i (1-\varepsilon_i)}{\varepsilon_i} \tag{3.2}$$

and where:

i - is the label of a zone or region in the 2D integration domain, Ω.
n - number of zones in the domain Ω.
$c_i\,(x,y,t)$ - is the radionuclide concentration in pore water in zone i, (Bq/m^3).
R_i - is the retardation coefficient in zone i, (-).
ρ_i - is the density in zone i, (kg/ m^3).
ε_i - is the porosity in zone i, (-).
$K_{d,i}$ - is the distribution coefficient in zone i, (m^3/kg).
D_i - is the effective diffusivity in zone i, (m^2/year).
t - is the time (years).
λ - is the radioactive decay constant, (year)$^{-1}$.
$u_i\,(x,y,t)$ - is the Darcy velocity in zone i, (m/year).
$A(t)$ - is the reaction term expressing the solubility limitation.
k_f - forward reaction rate.
k_b - backward reaction rate.

The advective and diffusive processes included by the model are illustrated by Figure 4.1. The initial and boundary conditions are described in the section 5.2.

The radionuclides are collected in the top filling and lateral zones of the vault and the concentration obtained there (Bq/m^3) is multiplied by the total water flow (m^3/yr) to give the final release rate to the near-field (Bq/year). The conceptual model described here is implemented into the two-dimensional commercial 2D program FlexPDE (version 2.1). An example of the script code used in FlexPDE for the SFL 5 vault is described in appendix I.

4.2 Assumptions and model simplifications

The assumption made is that the 2D representation of the vault is a sufficient one, which implies that we avoid CPU-intensive 3D-finite element calculations. In fact, the 2D calculations can be by themselves quite demanding in terms of computer time, depending on the parameters used as input data. Another assumption is that the flow in each vault is horizontal (se Figure 4.1 where the advection has the direction of the longitudinal axis of the vault). Therefore the y-component and z-component of the ground water velocity are zero, resulting in a diffusion controlled model.

The SFL 3 and SFL 5 vaults have 64 sections of waste concrete boxes (se Figure 3.1) in an 8x8 pattern. To simplify the model we agglomerate 16 boxes in a single box and therefore the cross section of Figure 4.1 and 5.1 show four equivalent boxes. This simplification results in a "lost" of concrete walls from the original smaller boxes. But this is compensated in the thickness of the four larger boxes, i.e. the same quantity of concrete is used in the modelling as if there was 64 waste boxes.

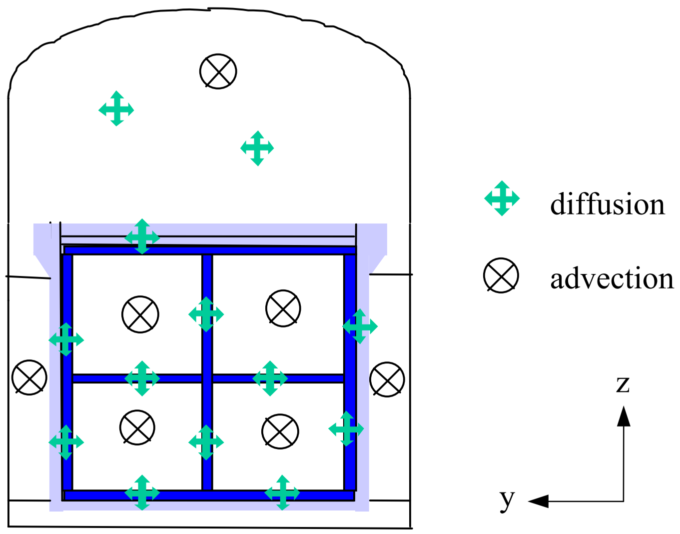

Figure 4.1 *The advection and diffusion processes as included by the conceptual model of the SFL 3 and 5 vaults with waste. The advective water flow is along the vault main axis.*

5 Reference case

5.1 Introduction

The scope of the present work is limited to the development of models of the SFL 3 and SFL 5 vaults and to study of the migration of some important radionuclides. We have based our calculation cases on SKB's reference scenario. The case study addresses a situation with intact barriers; the barriers are chemically not degraded but physically it is assumed that there exist a certain number of fissures in the concrete. The inner part (made of steel boxes) of the concrete boxes, that are placed in SFL 5, are not considered as a barrier.

This reference case follows the SKB approach although the mathematical model is different. This allows us therefore accessing the conceptual (model) uncertainty by comparing our results with those of the SKB preliminary assessment for the radio-nuclides here selected.

5.2 Description of the barriers

To model the deposition vaults using the two-dimensional code FEM_SFL we divide the geometry of the deposition vault's cross section in regions shown in Figure 5.1; these regions correspond to distinct barriers. The input data corresponding to each region of the integration domain are labelled with the respective zone (region) number. For instance the porosity of the bottom plate (zone 1) is ε_1, its density is ρ_1, etc.

Initial conditions:

The source term is given by an initial concentration of the radionuclides in the concrete tanks of the deposition vault. . The radionuclide inventories (activities) are given in Table 2.1 and Table 2.2. It is assumed that the inventory is evenly distributed in the boxes. Except for the inner part of the concrete boxes (zone 9 in Figure 5.1), the initial concentration in all zones is zero. The pore water in the walls of the each box will penetrate to its interior, dissolve the radionuclides (no solubility limitations are assumed by SKB other than for the radionuclides given in Table 3.3) transporting the radio-nuclides in solution outwards by diffusion. It is assumed in the model that the radio-nuclides are dissolved in a certain amount in the pore water from the very beginning. The initial concentration and the source term are controlled by the rate at which radionuclides are released from the metals due to corrosion and by solubility limitations.

Boundary conditions:

It is assumed that the concentration of radionuclides in the rock at a reasonable distance from the walls of the deposition vault, roof and bottom plates is zero. Mass balance is controlled by mixed boundary conditions between the different regions.

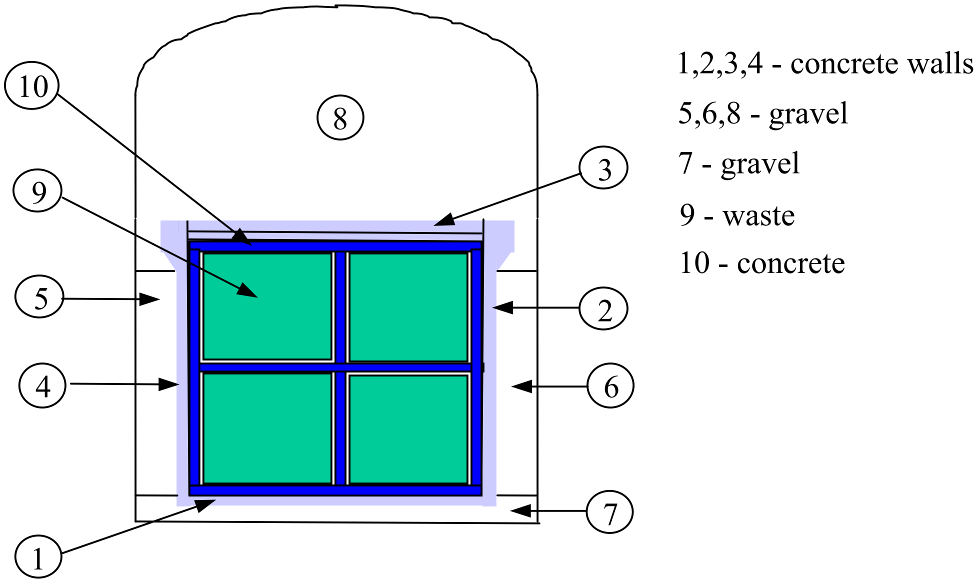

Figure 5.1 *In the FEM_SFL model the different barriers (zones) can have different porosities, densities, etc. These properties are assigned according to the zone numbers given in the picture.*

The model domain is divided in the following zones (Figure 5.1) corresponding to the different barriers:

- Zone 1 is the bottom plate
- Zone 2 is a lateral wall
- Zone 3 is the top plate and the radiation protection lid together
- Zone 4 is a second lateral wall
- Zone 5 is a draining lateral zone
- Zone 6 is a second draining lateral zone
- Zone 7 is the bottom floor
- Zone 8 is the roof of the vault (top filling)
- Zone 9 is the source term (interior of the concrete boxes)
- Zone 10 is a multiple zone consisting of concrete from the walls of the boxes and also of concrete filling between the tanks.

The cement that fills the empty space in the boxes is assumed to have the same porosity as the cement from the tanks. Initially all radionuclides are found in the zones assigned by number 9 (the concrete tanks), the activity being nil in the other zones. After diffusion and advection through the different barriers, the radionuclides either enter in the roof of the vault or leave that vault through the side walls and bottom plate and enter in the rock adjacent to those regions. In the first case the radionuclides are transported by water moving along the longitudinal direction of the vault before they penetrate into the roof and later into the adjacent rock. In both cases the radionuclides are finally transported by the groundwater circulating in the rock fractures, reaching soon or later the biosphere recipients.

6 Calculation results – reference case

6.1 SFL 5 vault

In this section we present the near-field releases of the two test radionuclides dissolved in the water living the SFL 5 vault. The contribution to those releases comes from the radionuclides in the water passing through the roof of the deposition vault and from the lateral zones (regions number 8, 5 and 6 in Figure 5.1). The results are shown in Figure 6.1 and Table 6.1 shows the maximum release rate regardless of time. The results are discussed in section 6.3.

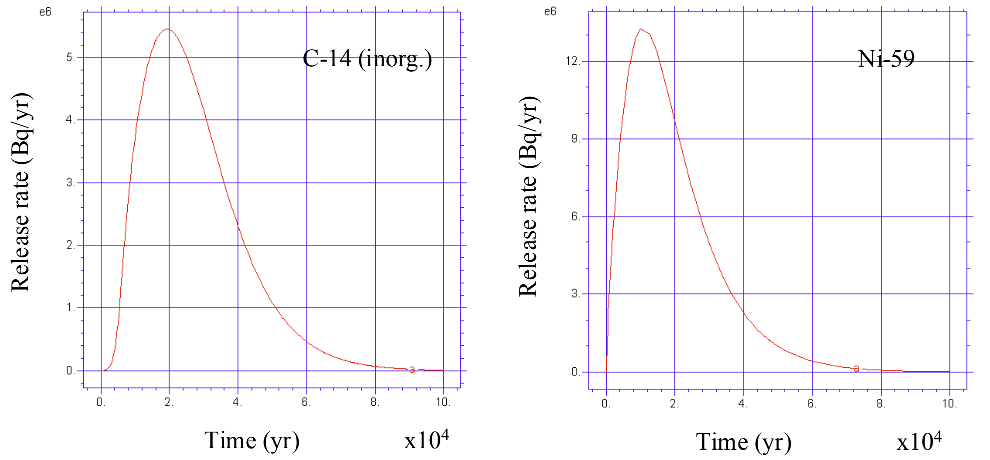

Figure 6.1 *The breakthrough curve of C-14 (inorganic) from SFL 5.*

Table 6.1 *SFL 5 peak release rates and their time of occurrence for the reference case at Aberg. SKB results in parentheses, from SKB (1999a), Table 8-5.*

Nuclide	**Peak release** (Bq/year)	**Time of occurrence** (years)
C-14 (inorganic)	5.13×10^{6} (1.0×10^{6})	1.8×10^{4} (8.0×10^{3})
Ni-59	1.32×10^{7} (3.0×10^{7})	1.0×10^{4} (3.0×10^{5})

6.2 SFL 3 vault

The radionuclides released from SFL 3 that we have considered in this work were: ^{14}C (inorganic), ^{36}Cl, ^{135}Cs, ^{3}H, ^{129}I, and ^{59}Ni. The results are shown in Figure 6.2 and Table 6.2 and discussed in the next section.

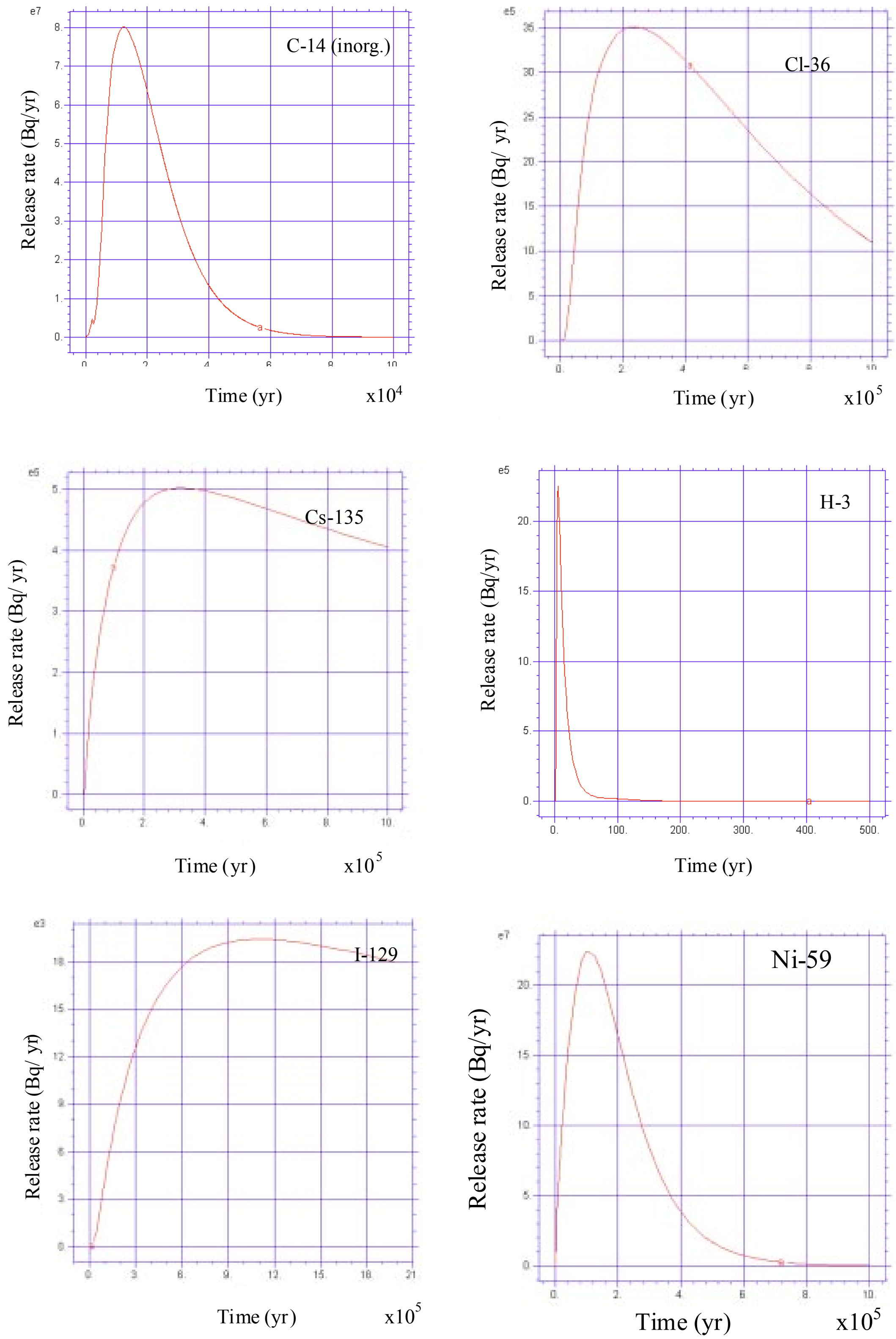

Figure 6.2 *The breakthrough curve of the release of six radionuclides from SFL 3.*

Table 6.2 *SFL 3 peak release rates and their time of occurrence for the base case at Aberg. SKB results in parentheses, a) from SKB (1999a), Table 8-8 and b) from Pettersson et al. (1999), Table 7-1.*

Nuclide	**Peak release** (Bq/year)	**Time of occurrence** (years)
C-14 (inorganic)	8.0×10^{7} (1.0×10^{6}) a)	1.2×10^{4} (2.0×10^{4}) a)
Cl-36	3.5×10^{6} (3.0×10^{6}) a)	2.0×10^{5} (1.0×10^{4}) a)
Cs-135	5.0×10^{5} (2.0×10^{4}) b)	4.0×10^{5} (2.0×10^{4}) b)
H-3	2.2×10^{6} (8.0×10^{8}) a)	5.0×10^{0} (4.0×10^{1}) a)
I-129	1.9×10^{4} (1.0×10^{3}) b)	1.0×10^{6} (4.0×10^{3}) b)
Ni-59	2.2×10^{8} (4.0×10^{7}) a)	1.0×10^{5} (1.0×10^{5}) a)

6.3 Discussion

The differences between our results and SKB results in respect to SFL 5 are in contrast with the agreement obtained for the SFL 3 calculations. We see three reasons for the discrepancy, with the following one as possibly the main reason of the discrepancy:

a) It is not possible to compute the amount of concrete inside the moulds with 80 litres drums, see Figure 2-1 in (SKB, 1999a), because it is not known how many of such moulds will exist in SFL 3. Table 2.1 of the same report gives a total of 4500 packages of LILW but not the proportion between drums and moulds. Therefore the retention of the concrete in those moulds was not taken into account. This explains the systematically higher release rates (one exception is the release of tritium), although it is not possible to quantify the conservatism in our SFL 5 model due to this simplification.

b) The conceptual models are quite different in the sense that SKB has an approach that allows to examine the near-field release in a “3D-mode” although the SKB model is not a real 3D model, but a compartment based “equivalent 3D-approach”.

c) It is very difficult to be sure on the input data used actually by SKB due to the lack of transparency of the SKB reports in respect to this aspect.

In respect to c) the SKB approach is more complete than our 2D model, because our model of a cross section needs to average in a simplistic way the spatial variability along the vault. On the other hand the SKB model is not transparent and it is difficult to follow the code implementation to extract the needed information from it. If information of the radionuclide contents along the vault had been available it would be possible to study different cross-sections and to make a weighted-average. The other way that seems to us more efficient is to develop a 3D model of the vaults allowing taking into account the migration of the radionuclides along the roof of the vault and of the lateral cages before leaving them. Considering that the SFL 3-5 repository will not be build within the next 20 or 30 years there will be time to develop more realistic and accurate models.

In respect to c) it will be necessary in the future to have a good reporting on how and where, the different packages are placed and an approximate inventory for each type of package. For instance, 200 litre drums are placed in the centre of the vault and have an approximated content of *A* Bq and cubic boxes are placed in the north part of the repository and have an average content of *B* Bq.

7 Summary and conclusions

In this work we have developed a two-dimensional model of the SFL 3 and SFL 5 deposition vaults and have applied it to calculate the near-field release rates of some representative radionuclides. To translate the models to numerical codes we have used finite elements and the toolbox FlexPDE, version 2.1.

The deposition vaults are modelled as 2D sections perpendicular to their longitudinal axis. The transport of radionuclides is accounted by advection and diffusion through the different barriers that isolate the waste and by retardation of the radionuclides in those barriers. The water flow is horizontal for the whole period, the gradients along the vertical axis are not important and therefore the model is reduced to a diffusion/dispersion controlled model.

The radionuclides of SFL 5 studied were C-14 (inorganic) and Ni-59 which are radionuclides representing cases with infinite solubility and limited solubility respectively. The release curves are in reasonable agreement with SKB results presented in their preliminary assessment. The radionuclides studied for SFL 3 were C-14, Cl-36, Cs-135, H-3, I-129 and Ni-59. The results obtained are systematically higher (exclusive H-3) than those of SKB, due to the fact that the retarding effect of concrete inside the cubic boxes have been disregarded. The reason was lack of information. However it is recommended that the development of a 3D model of the SFL 3 and 5 vaults, in conjunction with the use of input data that can represent the real distribution of the waste along the vaults.

References

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SKB, SR 97 - Deep repository for spent nuclear fuel, SR 97 - Post-closure safety, Main report - Vol. I, Vol. II and Summary, SKB TR-99-06, Swedish Nuclear Fuel and Waste Management Co, Stockholm,1999.

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Appendix I

FEM_SFL: the near-field model of the SFL 3 and SFL 5 vaults.

In this appendix we list the script used in the commercial 2D program FlexPDE (version 2.1) for modelling the SFL 3 and 5 vault of. This code (script) is for solubility-limited radionuclides. It differs from the code for non-solubility radionuclides by a term in the transport equation as explained in the main text.

```
TITLE 'SFL5 at SFL; Ni-59, Release rate (Bq/yr)'

! The Darcy flow is horizontal

SELECT printmerge=on
! nodelimit=20000
painted=on
COORDINATES cartesian2

VARIABLES C

DEFINITIONS

! solubilty limit Csol

Csol= 9.30858e12

! see main text -forward and backward rate constants (kf*c-kb):

r=(0.7*C-(0.7*C-Csol))
F= if (r>-0.001 and r<+0.001) then 1 else 0

Cmax=C

dC=-grad(C)

{coordinates}

x0=0.0          x1=-5.4      x2=+5.4          x3=x2            x4=4.8           x5=-4.8

x6=-5.4         x7=-x6       x8=5.4+0.371     x9=5.4+0.371     x10=x4           x11=x10

x12=x10         x13=x5       x14=x5           x15=-x9          x16=-x8          x17=-x7

x18=-7.0        x19=x18      x20=x18          x21=7.0          x22=x21          x23=x21

x24=x2          x25=x21      x26=x25-1.117    x27=x26-1.117    x28=x27-1.117    x29=x28-1.117

x30=x29-1.117   x31=0        x32=x31-1.460    x33=x32-1.117    x34=x33-1.117    x35=x34-1.117

x36=x35-1.117   x37=x20      x38=0            x39=x5           x40=x4           x41=0

x42=x0-0.8      x43=x5+0.8   x44=x43          x45=x42          x46=x0+0.8       x47=x4-0.8
```

```
x48=x47        x49=x46        x50=x49        x51=x48        x52=x51        x53=x50
x54=x0-0.8     x55=x44        x56=x55        x57=x54

y0=0.0         y1=0.275       y2=y1          y3=0.825       y4=0.825       y5=y4
y6=y5          y7=9.225       y8=y7+0.371    y9=10.975      y10=y9         y11=y10-0.55
y12=y7         y13=y11        y14=y10        y15=y10        y16=y8         y17=y7
y18=y7         y19=y6         y20=0          y21=0          y22=y3         y23=y7
y24=y7         y25=16.8       y26=y25+0.858  y27=y25+1.341  y28=y25+1.932  y29=y25+1.932
y30=y25+2.093  y31=19.0       y32=y30        y33=y29        y34=y28        y35=y27
y36=y26        y37=y25        y38=y3+4.8     y39=y38        y40=y38        y41=y11
y42=y38-0.8    y43=y42        y44=y5+0.8     y45=y44        y46=y45        y47=y46
y48=y42        y49=y48        y50=y38+0.8    y51=y50        y52=y11-0.8    y53=y52
y54=y53        y55=y54        y56=y50        y57=y56
Left= x20-5
Right=x21+5
Bottom=x20-2
Top=y31+5
z=0.1
! ------------------------------------------------------------------------------------------------------------------
! RO, KD, D, EPS are values of the rock surrounding the repository
! region seven has a negligible effect – it is not included just now, so the values for RO7, KD7, EPS7 and
! D7 are dummies

RO=2700        RO1=2.7e3      RO5= 2.7e3     RO7=0          RO8=2.7e3
KD=0.1         KD1=0.04       KD5=0.1        KD7=0          KD8=0.1
D=31557600*(2.8e-14)          D1=31557600*(1.0e-11)         D5=31557600*(6.0e-10)
D7=0                          D8=31557600*(6.0e-10)
EPS=5e-3       EPS1=0.15      EPS5=0.37      EPS7=0         EPS8=0.30
UX=0.0                        UY=0.0
```

! Water flow in the vault (backfill) is 62 m^3/yr according to Table 7-3 in (SKB, 1999a).
!
! This value was not used in (Pettersson et al. 1999), but the value given below waterflow=43.712

```
RO2=RO1        RO3=RO1        RO4=RO1        RO6=RO5

D2=D1          D3=D1          D4=D1          D6=D5

KD2=KD1        KD3=KD1        KD4=KD1        KD6=KD5

EPS2=EPS1      EPS3=EPS1      EPS4=EPS1      EPS6=EPS5


! int8 given the flux in the roof and int8a gives the area of region 8
! intou gives the flux in the outline region and intoua gives the area of that region

int8=integral(Cmax,'eight')
int8a=integral(1,'eight')

int4=integral(Cmax,'four')
int4a=integral(1,'four')

int6=integral(Cmax,'six')
int6a=integral(1,'six')


lamda=0.693/7.6e4



! total activity of Ni-59 1.4e15 Bq


C0=1.4e15/(7961.8) {activity, Bq}          {inventory, page 2-5, Table 2-1 (SKB, 1999a)}


! isotop dilution (Ni-59) => 0.01 in the next line

M=0.01*(0.25*C0*(upulse(x-x44,x-x45)*upulse(y-y44,y-y42))+0.25*C0*(upulse(x-x46,x-
    x47)*upulse(y-y46,y-y49))+0.25*C0*(upulse(x-x56,x-x57)*upulse(y-y56,y-
    y55))+0.25*C0*(upulse(x-x50,x-x51)*upulse(y-y50,y-y53)))



INITIAL VALUES C=M
EQUATIONS

(1/(1+RO*KD*(1-EPS)/EPS))*D*dxx(C)+(1/(1+RO*KD*(1-EPS)/EPS))*D*dyy(C)-(1/(1+RO*KD*(1-
    EPS)/EPS))*UX*dx(C)-(1/(1+RO*KD*(1-EPS)/EPS))*UY*dy(C)+F*(0.7*C-(0.7*C-Csol))-
    lamda*(C)=dt(C)


BOUNDARIES region 1 start (Left,Bottom) natural(C)=0 line to

               (Right,Bottom) to (Right,Top) to (Left,Top) to finish
```

```
region 'one' UX=0.0 UY=0.0 RO= RO1 KD=KD1 EPS=EPS1 D=D1
        start (x1,y1) line to
                  (x2,y2) line to
                  (x3,y3) line to
                  (x6,y6) line to finish

region 'two' UX=0.0 UY=0.0 RO= RO2 KD=KD2 EPS=EPS2 D=D2
        start (x4,y4) line to
                  (x3,y3) line to
                  (x7,y7) line to
                  (x8,y8) line to
                  (x9,y9) line to
                  (x10,y10) line to finish

region 'three' UX=0.0 UY=0.0 RO= RO3 KD=KD3 EPS=EPS3 D=D3
        start (x10,y10) line to
                  (x14,y14) line to
                  (x13,y13) line to
                  (x11,y11) line to finish

region 'four' UX=0.0 UY=0.0 RO= RO4 KD=KD4 EPS=EPS4 D=D4
        start (x14,y14) line to
                  (x15,y15) line to
                  (x16,y16) line to
                  (x17,y17) line to
                  (x6,y6) line to
                  (x5,y5) line to finish
```

```
     region 'five' UX=0.0 UY=0.0 RO= RO5 KD=KD5 EPS=EPS5 D=D5

               start (x19,y19) line to
                         (x6,y6) line to
                         (x17,y17) line to

                         (x18,y18) line to finish

     region 'six' UX=0.0 UY=0.0 RO= RO6 KD=KD6 EPS=EPS6 D=D6 {gravel and sand in region six}

               start (x3,y3) line to

                         (x22,y22) line to

                         (x23,y23) line to

                         (x7,y7) line to finish

!    region 'seven' UX=0 UY=Uroof RO= RO6 KD=KD6 EPS=EPS6 D=D6
!
!              start (x20,y20) line to
!
!                        (x21,y21) line to
!
!                        (x22,y22) line to
!
!                        (x3,y3) line to
!
!                        (x2,y2) line to
!
!                        (x1,y1) line to
!
!                        (x6,y6) line to
!
!                        (x19,y19) line to finish

region 'tanks' UX=0 UY=0 RO= 1890 KD=KD1 EPS=EPS1 D=3.15e-2
               start (x5,y5) line to

                         (x0,y5) line to

                         (x38,y38) line to

                         (x39,y39) line to finish

               start (x44,y44) line to

                         (x43,y43) line to

                         (x42,y42) line to
```

(x45,y45) line to finish

start (x0,y5) line to

(x4,y4) line to

(x40,y40) line to

(x38,y38) line to finish

start (x46,y46) line to

(x49,y49) line to

(x48,y48) line to

(x47,y47) line to finish

start (x38,y38) line to

(x40,y40) line to

(x11,y11) line to

(x41,y41) line to finish

start (x50,y50) line to

(x53,y53) line to

(x52,y52) line to

(x51,y51) line to finish

start (x39,y39) line to

(x38,y38) line to

(x41,y41) line to

(x13,y13) line to finish

start (x56,y56) line to

(x55,y55) line to

(x54,y54) line to

(x57,y57) line to finish

```
region 'eight' UX=0.0 UY=0.0 RO= RO5 KD=KD5 EPS=EPS5 D=D5
        start (x7,y7) line to
              (x23,y23) line to
              (x25,y25) line to
              (x26,y26) line to
              (x27,y27) line to
              (x28,y28) line to
              (x29,y29) line to
              (x30,y30) line to
              (x31,y31) line to
              (x32,y32) line to
              (x33,y33) line to
              (x34,y34) line to
              (x35,y35) line to
              (x36,y36) line to
              (x37,y37) line to
              (x18,y18) line to
              (x17,y17) line to
              (x16,y16) line to
              (x15,y15) line to
              (x9,y9) line to
              (x8,y8) line to finish

time 1 to 1000000

MONITORS

PLOTS for
  t=1,2,3,4,5,6,7,8,9,10,100,200,300,400,500,600,700,800,900,1000,2000,5000,10000,20000,50000,100
  000,200000,500000,1000000

table((int8/int8a+int4/int4a+int6/int6a)*waterflow) on 'eight' export

! grid(x,y)
```

```
! vector(dC) norm

surface(C) on 'eight' as 'eight'

contour(C) on 'eight' as eight

contour(C) on 'tanks' as tanks

HISTORIES

history ((int8/int8a+int4/int4a+int6/int6a)*waterflow)

END
```

Appendix II

Data selected for the calculation cases

Table 1 *Data selected for density [ρ] from Lindgren and Pers (1991), prosity [ε] from Skagius et al. (1999), effective diffusivity [D_e] from Skagius et al. (1999) and sorption coefficients [K_d] from Skagius et al. (1999) for the reference case of SFL 5.*

SFL 5 - Reference case (Aberg)				
	Zone 1, 2, 3, 4, 10 Concrete	**Zone 5, 6, 8** Gravel backfill	**Zone 7** [(a)] Basement gravel	**Zone 9** Waste
C-14 (inorganic)				
ρ (kg/m^3)	2.77×10^3	2.77×10^3	2.77×10^3	2.60×10^3
ε (-)	0.15	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0×10^{-11}	6.0×10^{-10}	6.0×10^{-10}	2.0×10^{-9} [(b)]
K_d (kg/m^3)	0.2	0.001	0.001	0 [(b)]
Ni-59				
ρ (kg/m^3)	2.77×10^3	2.77×10^3	2.77×10^3	2.60×10^3
ε (-)	0.15	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0×10^{-11}	6.0×10^{-10}	6.0×10^{-10}	2.0×10^{-9} [(b)]
K_d (kg/m^3)	0.04	0.02	0.02	0 [(b)]

[(a)] Not used in the final calculations. [(b)] Assumed value.

Table 2 *Data selected for density [ρ] from Lindgren and Pers (1991), prosity [ε] from Skagius et al. (1999), effective diffusivity [D_e] from Skagius et al. (1999) and sorption coefficients [K_d] from Skagius et al (1999) for the reference case of SFL 3.*

SFL 3 - Reference case (Aberg)

	Zone 1, 2, 3, 4 Structural concrete	**Zone 10** Boxes, porous concrete	**Zone 5, 6, 8** Gravel backfill	**Zone 7** [(a)] Basement gravel	**Zone 9** Waste
H-3					
ρ (kg/ m^3)	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.60 x10^3
ε (-)	0.15	0.30	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0 x10^{-11}	1.0 x10^{-9} [(c)]	6.0 x10^{-10}	6.0 x10^{-10}	2.0 x10^{-9} [(b)]
K_d (kg/ m^3)	0	0	0	0	0 [(b)]
C-14 (inorganic)					
ρ (kg/ m^3)	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.60 x10^3
ε (-)	0.15	0.30	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0 x10^{-11}	1.0 x10^{-9} [(c)]	6.0 x10^{-10}	6.0 x10^{-10}	2.0 x10^{-9} [(b)]
K_d (kg/ m^3)	0.2	0.2	0.001	0.001	0 [(b)]
Cl-36					
ρ (kg/ m^3)	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.60 x10^3
ε (-)	0.15	0.30	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0 x10^{-11}	1.0 x10^{-10}	6.0 x10^{-10}	6.0 x10^{-10}	2.0 x10^{-9} [(b)]
K_d (kg/ m^3)	0.006	0.006	0	0	0 [(b)]
Ni-59					
ρ (kg/ m^3)	2.77 x10^3	2.77 x10^3	2.7 x10^3	2.77 x10^3	2.60 x10^3
ε (-)	0.15	0.30	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0 x10^{-11}	1.0 x10^{-10}	6.0 x10^{-10}	6.0 x10^{-10}	2.0 x10^{-9} [(b)]
K_d (kg/ m^3)	0.04	0.04	0.02	0.02	0 [(b)]
I-129					
ρ (kg/ m^3)	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.60 x10^3
ε (-)	0.15	0.30	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0 x10^{-11}	1.0 x10^{-10}	6.0 x10^{-10}	6.0 x10^{-10}	2.0 x10^{-9} [(b)]
K_d (kg/ m^3)	0.003	0.003	0	0	0 [(b)]
Cs-135					
ρ (kg/ m^3)	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.77 x10^3	2.60 x10^3
ε (-)	0.15	0.30	0.30	0.30	0.7 [(b)]
D_e (m^2/s)	1.0 x10^{-11}	1.0 x10^{-10}	6.0 x10^{-10}	6.0 x10^{-10}	2.0 x10^{-9} [(b)]
K_d (kg/ m^3)	0.001	0.001	0.05	0.05	0 [(b)]

[(a)] Not used in the final calculations. [(b)] Assumed value.

[(c)] This value is used to avoid numerical instability.

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STATENS KÄRNKRAFTINSPEKTION
Swedish Nuclear Power Inspectorate

POST/POSTAL ADDRESS SE-106 58 Stockholm
BESÖK/OFFICE Klarabergsviadukten 90
TELEFON/TELEPHONE +46 (0)8 698 84 00
TELEFAX +46 (0)8 661 90 86
E-POST/E-MAIL ski@ski.se
WEBBPLATS/WEB SITE www.ski.se