SKB TECHNICAL REPORT 91-48

A compartment model for solute transport in the near field of a repository for radioactive waste (Calculations for Pu-239)

Leonardo Romero, Luis Moreno, Ivars Neretnieks

Department of Chemical Engineering,
Royal Institute of Technology, Stockholm,
Sweden

October 1991

SVENSK KÄRNBRÄNSLEHANTERING AB
SWEDISH NUCLEAR FUEL AND WASTE MANAGEMENT CO

BOX 5864 S-102 48 STOCKHOLM

TEL 08-665 28 00 TELEX 13108 SKB S
TELEFAX 08-661 57 19

A COMPARTMENT MODEL FOR SOLUTE TRANSPORT IN THE NEAR FIELD OF A REPOSITORY FOR RADIOACTIVE WASTE
(Calculations for Pu-239)

Leonardo Romero, Luis Moreno, Ivars Neretnieks

Department of Chemical Engineering, Royal Institute of Technology, Stockholm, Sweden

October 1991

Information on SKB technical reports from 1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40) and 1990 (TR 90-46) is available through SKB.

A COMPARTMENT MODEL FOR SOLUTE TRANSPORT IN THE NEAR FIELD OF A REPOSITORY FOR RADIOACTIVE WASTE

(Calculations for Pu-239)

Leonardo Romero, Luis Moreno, and Ivars Neretnieks

Department of Chemical Engineering
Royal Institute of Technology
S-100 44 Stockholm, Sweden

1991

KAT-91/13

ABSTRACT

Radionuclides released from a damaged canister for spent fuel will leak through a damage in the canister wall and spread into the surrounding backfill. They will further migrate into water bearing fractures in the rock, through the backfill into the damaged zone around the drift and into the drift itself. Some substances may also diffuse through the rock to adjacent fracture zones. The nuclides will sorb on the materials along the transport paths. This very complex and variable transport geometry has been modelled using a compartment model which is based on simplifying a full three dimensional integrated finite difference model. The simplifications are supplemented by introducing analytical and semianalytical solutions at sensitive locations such as entrances and exits from holes and fractures and in the flowing water.

TABLE OF CONTENTS

TABLES

APPENDICES

SUMMARY

A very simple compartment model is developed to calculate the non stationary release of radionuclides for systems with a complex geometry. The model is based on dividing the complex geometry into a number of compartments. Only transport by diffusion is considered in the clay and in the rock matrix. Transport by flow is accounted for in the fractures in the rock. The interior of the canister is handled as a well mixed compartment.

The model describes the release of dissolving species of radionuclides out through a small hole through a canister wall and further out into the bentonite. The species follow different pathways to reach the various zones of flowing water.

The number of compartments can be kept low by a special technique which is based on using analytical and semi analytical solutions at the mouths of the fracture in the rock and at the mouth of hole trough the canister wall. This ensures that these very important "pinch" points are handled correctly. Because of the coarse compartmentalization the code is very flexible and can be adapted to different geometries. Different locations of fractures, damaged zones etc. can be modelled with minor changes in the specifications of the compartments. Also new pathways can be added with little effort.

The numerical code can handle radionuclide release with or without decay. To calculate the inventory of a single nuclide within the canister the code can account for solubility limitations of the dissolving nuclide. Gear's method is used to integrate the system of differential equations.

The code has been verified by comparison with a previously developed resistor network model and a three-dimensional numerical integrated finite difference code for some steady state cases.

Sample calculations using Pu-239 with a solubility limit of $2.0 \cdot 10^{-8}$ moles/l and initial inventory of 28.1 moles have been performed. Results shows a depletion time of Pu-239 in the canister about $5.4 \cdot 10^{5}$ years. After this time the concentration drops rapidly everywhere.

The results given here for Pu-239 are preliminary. The non steady state results have not yet been verified.

1 INTRODUCTION

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

Once water penetrates into the canister the nuclides dissolve and diffuse out through the damage in the canister wall and further out through the bentonite. Some species diffuse into the fracture that intersects the repository hole, some into a fracture zone below the repository hole and some up to the disturbed zone around the tunnel at the top of the repository hole. From the pathway that goes to the top of the repository hole, a part diffuses into the disturbed zone at the bottom of the tunnel. The other part diffuses up into the backfill in the tunnel, along this and into fractures that intersect the tunnel. The region adjacent to a repository hole including the tunnel and its disturbed zone, the damage in the canister wall and the different paths are illustrated in Figure 1.

To calculate the release of radionuclides for the complex geometry described above a simple compartment model is used. In this model the different regions such as the damage in the canister, the different parts of the backfill in the repository hole and the tunnel, the rock, fractures and fracture zones are modelled as a number of compartments. The process resembles that of the discretization used in finite difference or integrated finite difference models for three-dimensional problems. The main difference is that the compartment model uses much fewer cells or compartments.

Only transport by diffusion is considered in the clay and in the rock matrix because the advective transport has been shown earlier to be negligible compared to the transport by diffusion. Transport by flow is accounted for in the fractures in the rock. The interior of the canister is modelled as a well mixed compartment and therefore the concentration within the canister is the same everywhere. The damage in the canister wall, it is assumed to be a small hole which may have developed by anomalies in the fabrication process or by local corrosion. The size of this hole is assumed to be very small.

In order not to loose significant accuracy in the computations due to the coarse discretization analytical "exact" solutions are utilized to define the proper sizes and shapes of fictitious compartments at sensitive zones. These are located at the mouths of the damage in the canister wall, at the mouth of the fractures, and in the flowing water in the fractures and fracture zones.

The model has been compared to numerical solutions using a "full" three-dimensional code with fine discretization for the steady state but has not yet been compared with "fully" three-dimensional calculations for the non steady state cases.

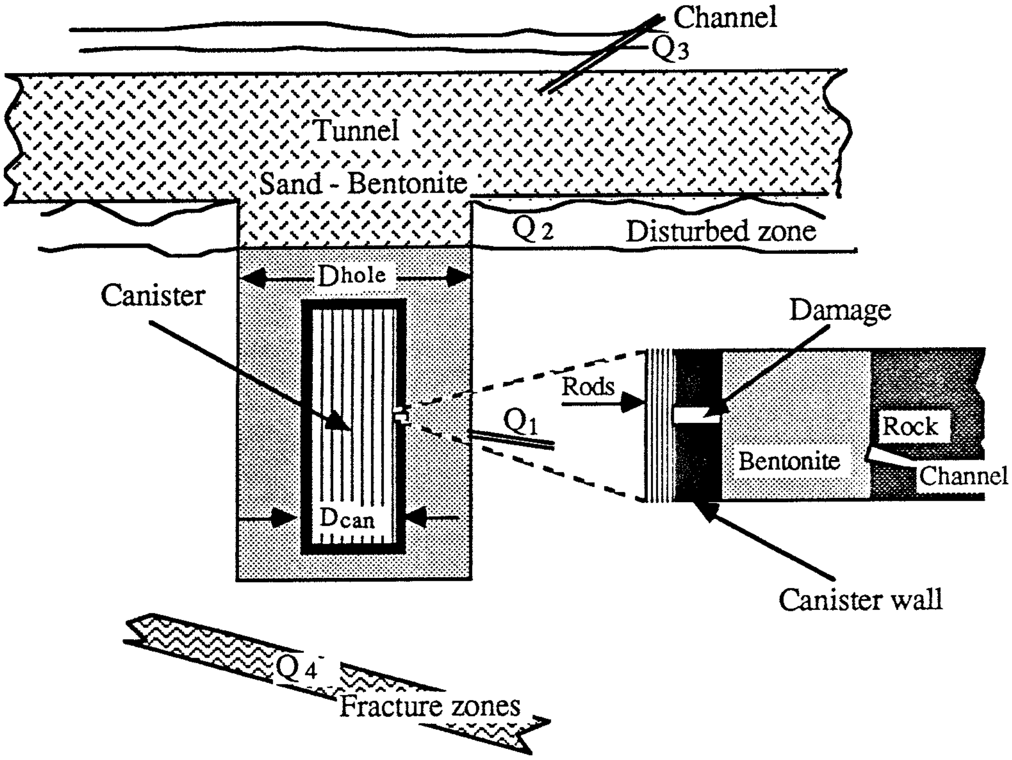


Figure 1. Schematic view of the entire system showing the geometry and the different zones where the water flows.

2 THE CONCEPTUAL MODEL

In this section we develop the conceptual basis for the model. For a system described in Figure 1 the nuclide release from a canister containing the radioactive wastes will be modelled using a compartment model. The concept of compartment is very useful when the transport is through materials with different properties and the geometry of the system is very complex. This concept is illustrated in Figure 2, for a two-dimensional case. The compartments can of course be three-dimensional.

The Figure 2 shows an arbitrary compartment "i". Every compartment "i" is surrounded by other compartments "j". The nuclides diffuse into or out of compartment "i" from the neighbouring compartments by diffusion. The direction of nuclide movement is from the higher concentration to the lower and the magnitude of the nuclide flowrate is proportional to the cross sectional area $A_{i,j}$ connecting the compartments. The nuclide flowrate is inversely proportional to the distances from the "center" points of the compartments to the contact area $A_{i,j}$. What flows into a compartment and does not flow out will accumulate. The joining line $d_{i,j}$ is perpendicular to the contact area $A_{i,j}$ between the compartments. These simple notions suffice to define the flow between and accumulation in every compartment. Radioactive decay is readily included.

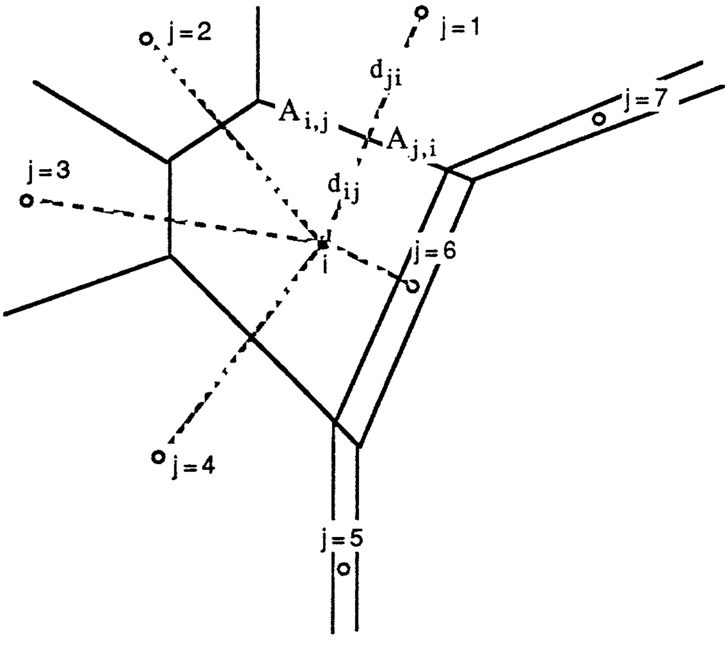
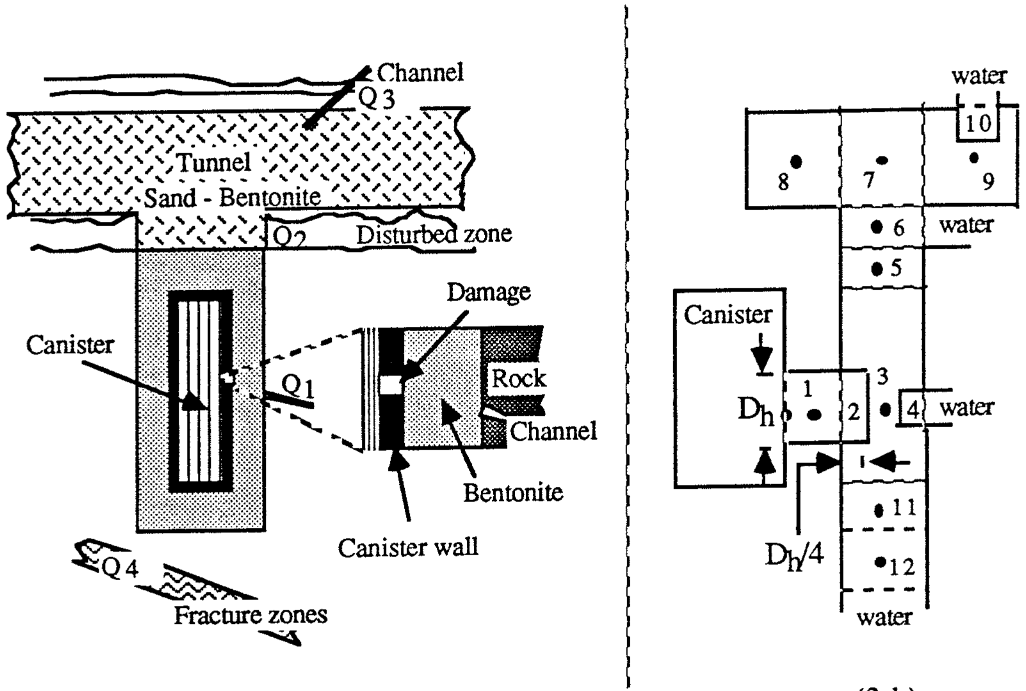


Figure 2. Schematic mesh with volume element or compartment "i" connected to other volume elements "j". There are some volumen "j" that are not in contact with the volume "i".

If we base the model on the concept defined above, the different regions of the system outlined in Figure 1 are divided into compartments each having a volume determined from the geometry. Every compartment is identified by a number and has a certain capacitance and resistivity. See Figure 3 as example of how this may be done.

Because of the low permeability of the rock matrix and backfill, the transport by flow of solute is negligible compared to that by molecular diffusion. Every compartment can thus only exchange solute with adjacent compartments by diffusion except for the flowing water in the fractures and fracture zones where transport by advective flow also takes place. These zones are denoted by Q_1 - Q_4 in Figure 1.

An important assumption is that the canister acts as a single well-mixed compartment with a volume equal the volume of water in the canister itself. This assumption means that the concentration is the same everywhere within the canister. This is probably a very conservative assumption because the diffusion path along the rods in the canister is long and narrow and will constitute a considerable resistance to transport. In addition to the nuclides in the water in the canister there may be solid phases which dissolve with known rates or which have solubility constraints.



(3-a)

(3-b)

Figure 3 (3-a) Schematic view of the entire system showing its geometry.
(3-b) Discretization in compartments of the system described in Figure 3-a. Numbers in the figure denote compartment numbers.

The discretization of the system into compartments is rather straightforward. Compartments are selected so that they include the accessible parts of the clay and rock and so that the contact areas between the compartments represent the "real" cross sections. The volumes of the compartments will define the "capacity" of the compartment to contain the nuclide either in its water volume or sorbed in/on the solid. The length(s) and cross sectional area(s) will define the resistance to transport in that direction.

Conceptually this process is straightforward but some care must be taken not to loose important processes especially when the solute moves between a large compartment and a small one with a very small connecting contact area. The small compartments cannot be neglected if they are located at some location where they form most of the transport resistance such as is the case of a small hole (damage) in the canister wall. A further difficulty which arises is that in order to make accurate calculations one needs to discretize very finely at the mouths of damages and fractures. This would counteract the purpose of this model because it would lead to many compartments and the need to rediscretize when some detail of the geometry is changed. Another approach was therefore taken, that of utilizing analytical solutions to approximate the sensitive regions.

There are several such connections in this system. One is where the hole in the canister wall (5 mm^2) connects to the clay volume around the canister. An escaping nuclide will diffuse out through the hole to its mouth and will then "see" a vast volume of clay in all directions. From the mouth of the hole the nuclide will spread out in three dimensions. The largest concentration drop will be nearest the mouth of the hole. Then a fictitious compartment is defined with a negligible volume and a resistance equivalent to the bentonite around the hole in the canister wall. The compartment in this region must be made such that the nuclide flowrate is correct at least at a final "steady state" when the concentration profiles have developed fully. This is done by analytically solving the transport equations around the mouth and using this information to define an entry resistance in the form of a plug equivalent to the total resistance of the bentonite. The equivalent thickness of this compartment was calculated to be $D_h/4$, see Appendix A.

In a similar way an analytical method developed earlier (Neretnieks, 1986) is used to define the resistance when the nuclide migrates from the clay into narrow fractures. Then, the transport resistance for the diffusion through the backfill into a fracture may be calculated assuming a fictitious compartment considering the contact area as that area calculated at the mouth of the fracture (A_f) and an equivalent thickness or diffusion length ($F \cdot \delta$) ranges from 3 to 8 times the aperture of the fracture, for the range of possible fracture apertures, spacings and locations.

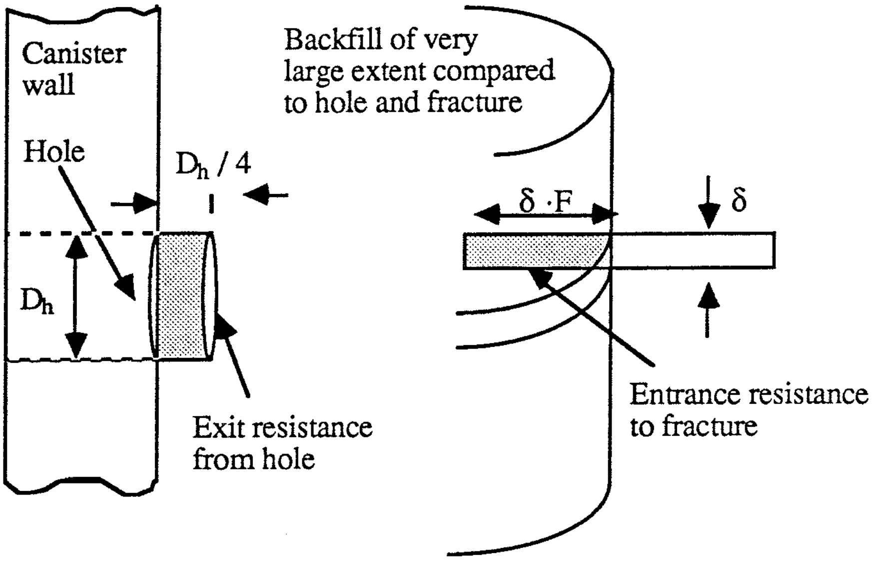


Figure 4 The sharply diverging and converging migration paths at the mouths of the hole and fracture have diffusion resistances equivalent to plugs of sizes shown in the figure.

Based on these approaches, three small compartments have been added to the system (compartment 2, 4, and 10) as shown in Figure 3. Compartment 2 is located next to the compartment representing the hole in the canister wall and at the entry of compartment 3. Compartment 4 is located at the exit of compartment 3 and next to the mouth of the fracture. In the same way, compartment 10 is positioned at the exit of compartment 9. See Figure 3. Table 3 gives a description of all compartments.

The resistance of these extra compartments is at least correct at the steady state. The resistance are in good approximation at the instationary state after the concentration in the bentonite is approximately the same everywhere. This time is rather short because the diffusion of the nuclides in the bentonite is large. During the instationary period the capacitance of these extra compartments are negligible.

3 THE MATHEMATICAL MODEL

The core of the mathematical model is the compartment with its in and outflows and accumulation of nuclides. Special compartments are introduced at the mouths of the small in and outflow locations at the damage in the canister and at fracture mouths. They are designed in such a way that they will exhibit the correct transport resistance at steady state transport but have negligible capacity for holding solute. The transport into flowing water is also formulated as a compartment but with no capacity of accumulation because the water flows away. The special compartment is that of the fuel itself. This compartment acts as a single well-mixed compartment with a volume equal to the volume of water within the canister. There are two options. Nuclides which are entirely soluble are dissolved in the small water volume in the interior of the canister. This water volume is then depleted as the nuclide escapes and decays. The other case is where the nuclide either has a solubility limit and cannot totally dissolve or when it is released with a given rate due to the dissolution of the spent fuel matrix. In the latter case the nuclide is constantly released by dissolution to a known concentration or at some known rate.

In this section we develop the basic equation for a compartment model. The equations will later be supplemented to include chain decay of nuclides and the presence of a solubility limited inventory.

3.1 STABLE SPECIES

The equation of conservation of mass for the species in compartment "i" accounting only for diffusion may be described by Equation (1) below

$$K_i \cdot V_i \cdot \frac{dc_i}{dt} = \sum_{j \neq i} A_{i,j} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \cdot (c_j - c_i) \qquad (1)$$

or

$$\frac{dc_i}{dt} = \sum_{j \neq i} g_{i,j} \cdot (c_j - c_i) \qquad (2)$$

Where

$$g_{i,j} = \frac{A_{i,j}}{K_i \cdot V_i} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \qquad (3)$$

The term at the left hand side in Equation (1) accounts for the accumulation of nuclide in the water and in the solid by sorption. K_i is a distribution coefficient. The term on the right hand side accounts for the transport by diffusion in and out of the compartment from all adjacent compartments.

The sub-indices "i,j" define the direction of the flowrate of radionuclides from the compartment "i" to "j". The contact area between compartment "i" and "j" is designated by $A_{i,j}$ and the volume of the compartment by V_i. The term $(D_{eff}/d)_{i,j}$ is the conductance defined by Equation (4) below obtained by adding the diffusion resistances d/D of respective compartments which are coupled in series.

$$\left(\frac{D_{eff}}{d}\right)_{i,j} = \frac{1}{(d_{i,j}/D_i + d_{j,i}/D_j)} \tag{4}$$

The distribution coefficient, K_i, in compartment "i" is defined including the nuclides dissolved in the water and sorbed in the solid.

$$K_i = \varepsilon_{p,i} + (1 - \varepsilon_{p,i}) \cdot K_{d,i} \cdot \rho_i \tag{5}$$

K_d is the sorption coefficient for the solid, ε_p is the porosity, and ρ is the density of the solid in the compartment.

By rearrangement of Equation (2), the following equation is obtained

$$\frac{dc_i}{dt} = -c_i \cdot \sum_{j \neq i} g_{i,j} + \sum_{j \neq i} g_{i,j} \cdot c_j \tag{6}$$

Equation (6) for i = 1 and j = 0 to m can be rewritten in the following form

$$\frac{dc_1}{dt} = - c_1 \cdot \sum_{j \neq i} g_{1,j} + c_0 \cdot g_{1,0} + c_2 \cdot g_{1,2} + \cdots\cdots + c_m \cdot g_{1,m} \tag{6-a}$$

where "m" is the number of compartments, including those in which the concentration of nuclides in the compartment is known or imposed as is the case of the boundary conditions. Most $g_{i,j}$:s are zero because only adjacent compartments in contact with each other will directly exchange nuclide between them.

If the terms with known concentrations are grouped in a vector of boundary conditions, Equation (6) can be rewritten and expressed in matrix form. The number of equations and independent variables is "n". Then the system of equations finally obtained is

$$\frac{d\bar{c}}{dt} = \bar{\bar{F}} \cdot \bar{c} + \bar{B} \tag{7}$$

Where:

- The term ($d\bar{c}/dt$) of the left hand side accounts for the change of concentration with time. It is a vector of dimension n.
- The first term ($\bar{\bar{F}} \cdot \bar{c}$) of the right hand side accounts for transport by diffusion. $\bar{\bar{F}}$ is a matrix of dimension nxn and $\bar{c}$ is a vector of dimension n.
- The second term ($\bar{B}$) of the right hand side accounts for the boundary conditions. It is a vector of dimension n.

The matrix $\bar{\bar{F}}$ has constant coefficients. Every compartment connection is represented in the matrix. The elements of the diagonal of the matrix are equal to the sum of all possible connections of a compartment with the neighboring compartments including those connections with the regions considered as boundary conditions.

$$F_{i,j} = \begin{pmatrix} g_{i,k} & i \neq j \\ \\ -\sum_{k=0}^{m} g_{i,k} & i = j \end{pmatrix} \tag{8}$$

Equation (7) is the basic system which will be integrated. We now proceed to introduce the modifications needed to handle for radioactive decay and to account for a finite inventory of dissolving decaying solid.

3.2 DESCRIPTION OF BOUNDARY CONDITIONS

The initial conditions are $c_i = 0$, except inside the canister where $c = c_0$. The boundary conditions at the cells adjacent to the flowing water are determined by assigning a fictitious compartment which has the same resistance as the mass transfer resistance into the flowing water. The concentration of species is zero in this compartment. The size of the compartment can be visualized by assuming a diffusion length Δx to it. See Appendix B for the calculation of this length.

These conditions may be formulated as follows (see Figure 3) :

$c = 0$ in some location of those regions in which the water flows.
These regions are: in the fracture intersecting the repository hole
in the disturbed zone
in the fracture intersecting the tunnel
in the fracture zone.

To describe the boundary condition inside the canister, two different cases are considered:

> In the first case the concentration is limited by solubility. It means that the concentration is constant and equal the solubility, $c = c_o$, as long as a solid phase exists.
>
> In the second case the concentration inside the canister is not solubility limited and the compartment behaves like a normal compartment except that it is not fed from other compartment. It is only depleted.

3.3 INTRODUCING RADIOACTIVE DECAY

The radionuclide release of a single nuclide with decay may be described in the same way as was described for a single species without decay. A decay term must be added in Equation (1) for the calculations when decay is considered. The following equation is obtained

$$K_i \cdot V_i \cdot \frac{dc_i}{dt} = \sum_{j \neq i} A_{i,j} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \cdot (c_j - c_i) - K_i \cdot V_i \cdot \lambda \cdot c_i \qquad (9)$$

The terms $F_{i,j}$ in the $\overline{\overline{F}}$ matrix become

$$F_{i,j} = \begin{pmatrix} g_{i,k} & i \neq j \\ -\lambda - \sum_{k=0}^{m} g_{i,k} & i = j \end{pmatrix} \tag{10}$$

The boundary conditions in the flowing water do not change. Theses conditions are the same independent if the calculations are made with or without decay. The boundary condition inside the canister is dependent on if the calculations are made with or without solubility limitations. If the calculations are made without solubility limitations, the concentration inside the canister is determined by decay of the inventory in addition to the depletion by migration to the next compartment.

When there is no solid present within the canister, the decrease of the inventory dissolved in the water is due to the decay of the nuclide and by transport by diffusion out of the canister. The equation becomes

$$\frac{dc_o(t)}{dt} = - c_o(t) \cdot \lambda - \frac{A \cdot D_{eff}}{V_o \cdot d} [c_o(t) - c_1(t)] \tag{11}$$

The concentrations in the canister and in the hole in the canister wall are c_o and c_1 respectively. In this case c_o is time-dependent.

If the calculations are made with solubility limitations, the concentration inside the canister remains constant and equal to the solubility, $c = c_o$, as long as a solid phase exists. A special calculation must be set up to follow the inventory of the solid which is depleted by decay and by dissolution. This is shown later.

For computation purposes it is sometimes advantageous to formulate the equations in terms of activity instead of concentration. This is done next.

To convert units of concentration in units of activity, we use

$$a = \lambda \cdot c \tag{12}$$

where "a" denotes activity concentration, λ is the decay constant, and c is the concentration.

The substitution of this conversion in Equation (9) gives the analogue formulation in activity units Equation (13)

$$K_i \cdot V_i \cdot \frac{da_i}{dt} = \sum_{j \neq i} A_{i,j} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \cdot (a_j - a_i) - K_i \cdot V_i \cdot \lambda \cdot a_i \qquad (13)$$

The boundary condition inside the canister becomes

$$a = a_o \qquad \text{for solubility limit} \qquad (14)$$

For chain decay Equation (9) is supplemented by a term which accounts for the generation of the daughter nuclide "I" by decay of the mother "I-1". The system of equations becomes larger but still can be written in the form of Equation (7). The details of these equations together with the initial and different sets of boundary conditions are presented in Appendix-D.

3.4 HANDLING THE INVENTORY FOR A SIMPLE DISSOLVING NUCLIDE

The initial inventory of a particular nuclide is defined as the amount deposited in the canister at some zero time.

The initial inventory (M^o) is the sum of the amount of solid (M_s) in the canister plus the amount of nuclide dissolved (M_{dis}) in the volume (V_o) of water in the canister.

$$M^o = M_s + M_{dis} \qquad (15)$$

At time t after canister breaching, the inventory of the nuclide within the canister will decrease with time at a rate given by the dissolution rate and the decay. For this case the dissolution rate is determined by resistances to the transport by diffusion offered by the different pathways located around the canister.

For the case when no decay is considered, the variation of the inventory of solid with time ($M_s(t)$) is

$$\frac{dM_s(t)}{dt} = -N(t) \tag{16}$$

If the concentration in the canister is solubility limited it means that the concentration within the canister remains constant and equal the solubility (c_o) of the nuclide. The rate of dissolution N is determined by the expression below

$$N = \frac{A \cdot D_{eff}}{d} (c_o - c_1(t)) \tag{17}$$

and therefore the rate of loss of the solid phase is

$$\frac{dM_s(t)}{dt} = -\frac{A \cdot D_{eff}}{d} [c_o - c_1(t)] \tag{18}$$

$M_s(t)$ is the mass of nuclide in solid form in the inventory, c_o is the solubility of the nuclide in the canister, and $c_1(t)$ is the concentration in a point located within the first compartment adjacent to the canister. In this case the water in the hole.

When decay is considered, the inventory will decrease by decay of nuclide in the solid, by decay of the dissolved nuclide and by the transport out of the canister by diffusion (N).

Considering all theses effects together and assuming that the concentration within the canister is limited by solubility, the differential equation obtained by material balance to express the loss of the nuclide inventory in the canister is

$$\frac{dM_s(t)}{dt} = -M_s(t) \cdot \lambda \ - \ V_o \cdot c_o \cdot \lambda \ - \ \frac{A \cdot D_{eff}}{d} [c_o - c_1(t)] \tag{19}$$

The term of the left hand side is the loss of mass of the solid phase present in the canister. The terms of the right hand side represent the decay of nuclide in the solid inventory, decay of dissolved nuclide, and transport by diffusion out of the canister respectively. λ is the decay constant for the nuclide. The concentrations in the canister and in the hole in the canister wall are denoted by c_o and c_1 respectively.

To convert units of concentration in units of activity, the following conversions are used

$$a = \lambda \cdot c \qquad \text{and} \qquad M_s = \frac{V_o \cdot a}{\lambda} \tag{20}$$

The substitution of these variables in Equation (19) gives the analogue formulation in activity units. Then, the rate of change of activity of the solid phase is

$$\frac{dA_s(t)}{dt} = -A_s(t) \cdot \lambda - a_o \cdot \lambda - \frac{A_{0,1}}{V_o} \left(\frac{D_{eff}}{d}\right)_{0,1} \cdot [a_o - a_1(t)] \tag{21}$$

where A_S is the activity of the nuclide in the solid phase in the canister, a_o and a_1 are the solubility of the nuclide in activity units and the activity in compartment 1 respectively.

3.5 SOLUTION OF THE SYSTEM OF EQUATIONS

Equation (7) is the basic system of equations to solve. This is done by using standard numerical techniques. We use the Stiff solver based on Gear's method. This solve a problem of n-ordinary differential equations of the form $dY(I)/dt = F(Y(I), T)$, given the initial conditions $Y(I) = YI$ (Kahaner et al., 1988).

The solution is straightforward once the initial and boundary conditions have been defined. These are defined by the uptake in the flowing water on one hand and on the release from the fuel on the other hand. The latter consists of two different cases which are handled separately. In the first case all nuclide is dissolved initially in the water in the canister. This compartment is only depleted as it is not replenished from anywhere. In the other case this compartment is replenished from the dissolving fuel or precipitated nuclide until the source is exhausted. Thereafter the solution continues as in the first case. The system of equations is solved in a few minutes on a Macintosh SE/30 computer for about 20 compartments.

4 CALCULATIONS

Pu-239 will be used as an example and test case for the model. The case is set up as follows. A canister contains a solid matrix which is leached releasing Pu-239 to the water in the canister. The solubility of the plutonium is limited to $2.0 \cdot 10^{-8}$ moles/l and all plutonium cannot dissolve in the water.

The dissolved plutonium diffuses out through the hole in the canister wall. It moves further out to the clay and spreads out towards the other compartments. The concentration in the various compartment will change in time and depend on their volume, sorption capacity, resistance to diffusion and the decay of the nuclide.

The model needs data on geometry, physical properties and chemical properties. The basic geometry data including information of volumes, cross section areas and diffusion distances are compiled in Table 1. In this table also information on the equivalent flowrates in the different regions with flowing water are given. Table 2 contains data on physical properties such as density, porosity and sorption data for Pu-239.

The geometrical dimensions required for every compartment and the connections between them are defined in Tables 3 and 4 respectively. In these calculations a very coarse division into compartments is made at present.

Another form to represent the whole system is shown in Figure 5. The division of the system in compartment may be represented in a very convenient way by defining the capacity of each compartment by its "time constant" and the connections with adjacent compartments by the respective resistances (R). The value of the time constant, τ_i, is the time required for that the concentration in the compartment reaches approximately 2/3 rds of the concentration that the compartment could obtain at the steady state for a nuclide that does not decay.

A compartment connected to other compartments by resistances has a time constant calculated from Equation (7)

$$\tau_i = 1 / \sum_{j \neq i} g_{i,j} \tag{22}$$

The concentration that a compartment reaches at steady state directly depends on the concentration of the sorrounding compartments.

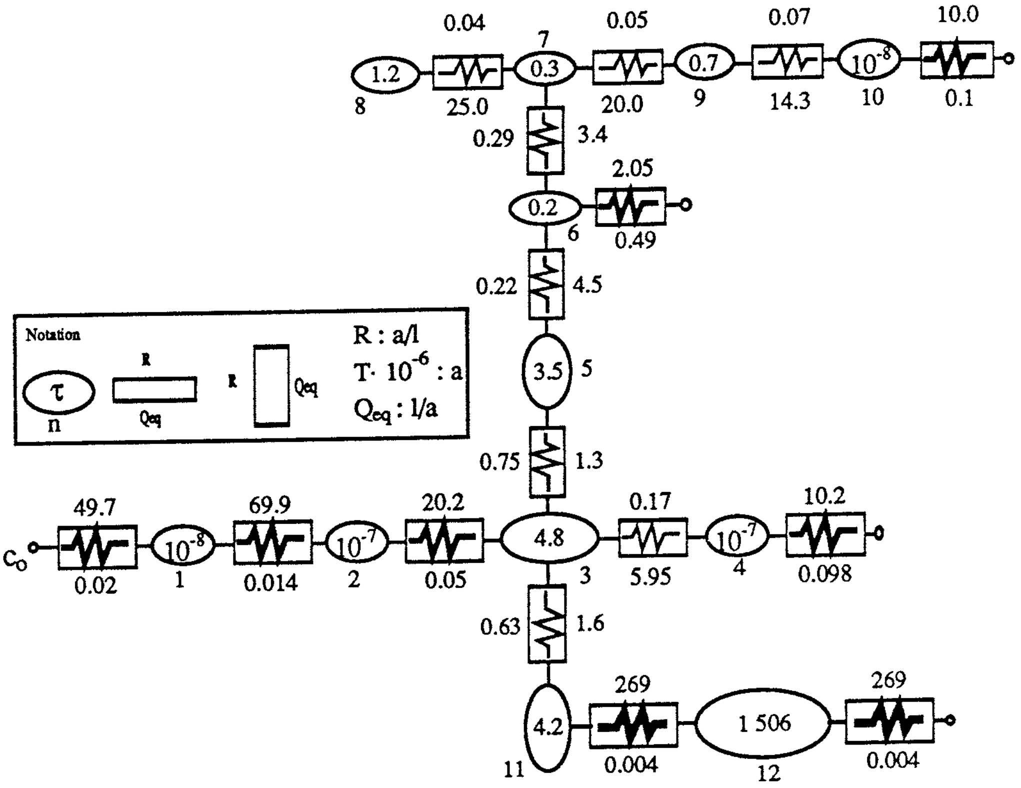


Figure 5 The whole system represented by the connection between compartments by resistances and corresponding equivalent flowrates. The center point of the compartment is expressed in the form of a "time constant". n is the number of the compartment.

The resistor may also be characterized or expressed in another form such as the local equivalent flowrate. This is a fictitious flowrate defined as the flowrate of water which carries with it the interface concentration.

At steady state the release from the canister is in practice dominated by the resistance to the transport offred by the small hole in the canister wall. For a nuclide that does not decay the fraction of nuclide flowrate transported through the different pathways is dominated by the relation of the equivalent resistance between them.

Some relationships may be obtained directly from Figure 5:

- The maximum release of nuclides into the water for each pathway is less than the minimum of any local equivalent flowrate found in each pathway.
- Approximate times may be calculated to reach concentrations approximately 2/3 rds of the maximum concentration that the compartment reaches, for a nuclide that does not decay or with a very long half-life.

On the other hand if we are interested to know the time it takes for a compartment to reach a certain very small fraction of the concentration at steady state this time may be obtained using a linear relationship

$$t \cong x_f \cdot \tau_i \tag{23}$$

Where x_f is a fraction of concentration the compartment would have at steady state if the nuclide does not decay.

5 RESULTS

Preliminary results are shown here for the Pu-239 in Figures 6 to 8. They are based on a minimum division into compartment. Later some of the present compartments will be subdivided.

Figure 6 shows how the concentration of Pu-239 changes in the different compartments. The concentration in the water in the hole in the canister is very near the solubility limit and builds up its concentration almost immediately. The compartment outside (3) takes a very long time to attain its steady state concentration ($\approx 10^5$ years). The other compartments have decreasingly lower concentrations. The inventory of solid Pu-239 in the canister is depleted in about $5.4 \cdot 10^5$ years and the concentrations then drop rapidly everywhere.

Figure 7 shows the flowrate of Pu-239 to the different mobile waters in the rock. It is seen that in this example the release from the canister "N-input" is small, ($\approx 10^{-10}$ mol/a). The release rate is limited by the presence of the very small hole in the canister wall. This is the largest transport resistance in the whole system. The release to the flowing water in the fracture ($N_{4,w}$) is more than 3 orders of magnitude smaller because the Pu-239 decays during its transport through the clay. The next largest release is to the water in the disturbed zone around the repository hole below the tunnel. The other paths are even less. The small flowrate is due to the decay of the nuclide during its transport up through the backfill. Here it is delayed due to sorption in the backfill giving the nuclide time to decay considerably. A nuclide with different sorption and/or decay properties would behave in different way.

Figure 7 shows also the total release (N-out) into the different flowing waters. The releases were calculated considering the compartment adjacent to the canister for the N-input and those adjacent to the flowing water for $N_{i,w}$. Figure 8 shows the variation of the inventory of Pu-239 with time.

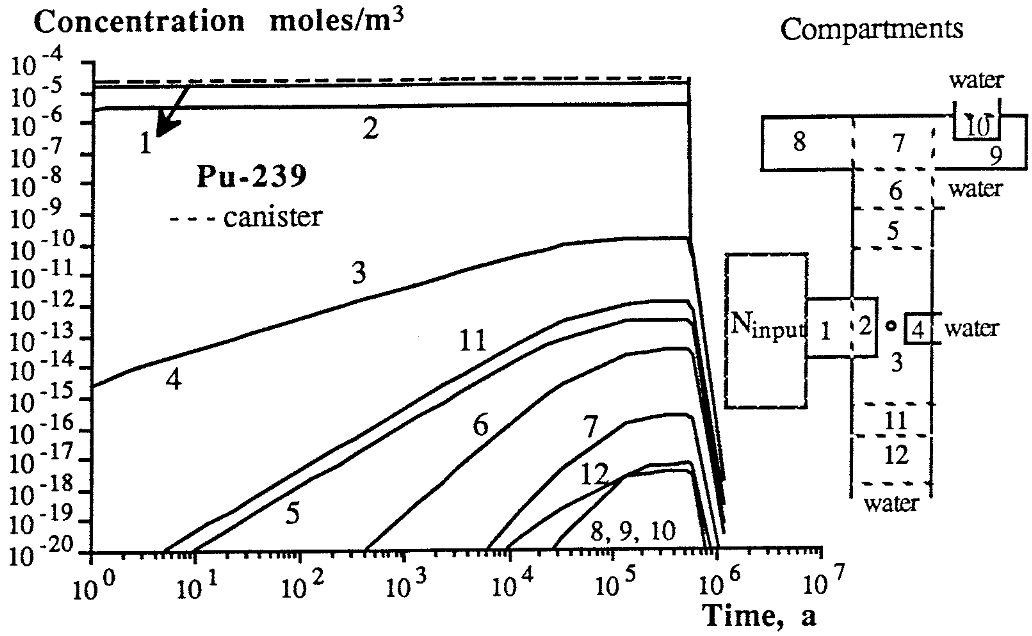


Figure 6 Concentration in the different compartments versus time. The number on the lines refers to the compartment. The numbers can be identified in the adjacent figure.

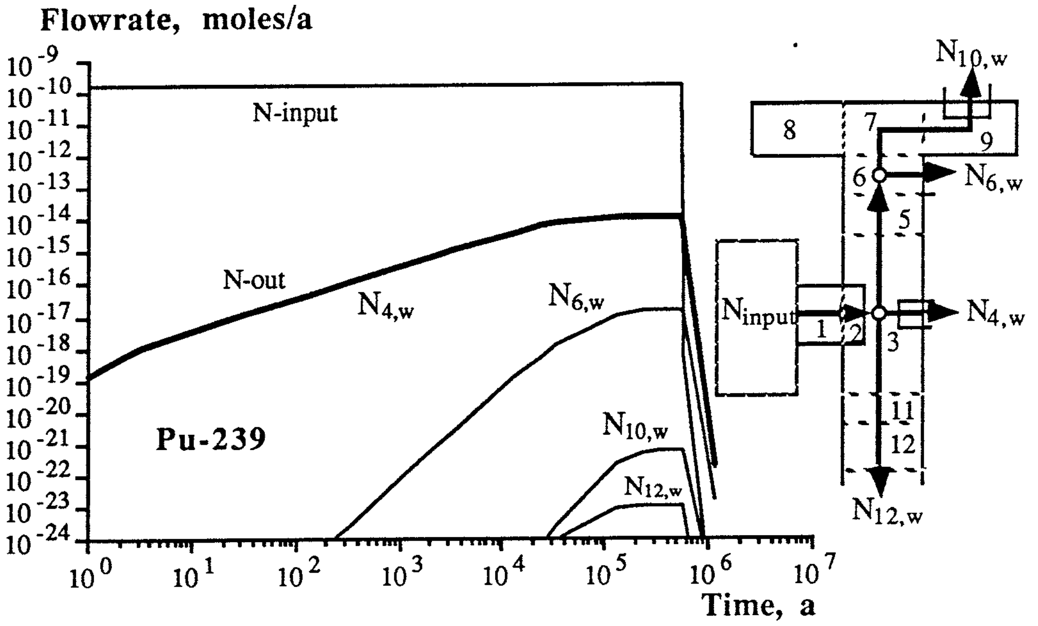


Figure 7 Flowrates of nuclide through different pathways versus time. The notation on the lines $N_{i,w}$ refers to the release of nuclide from the compartment into the water. The notation can be identified in the adjacent figure.

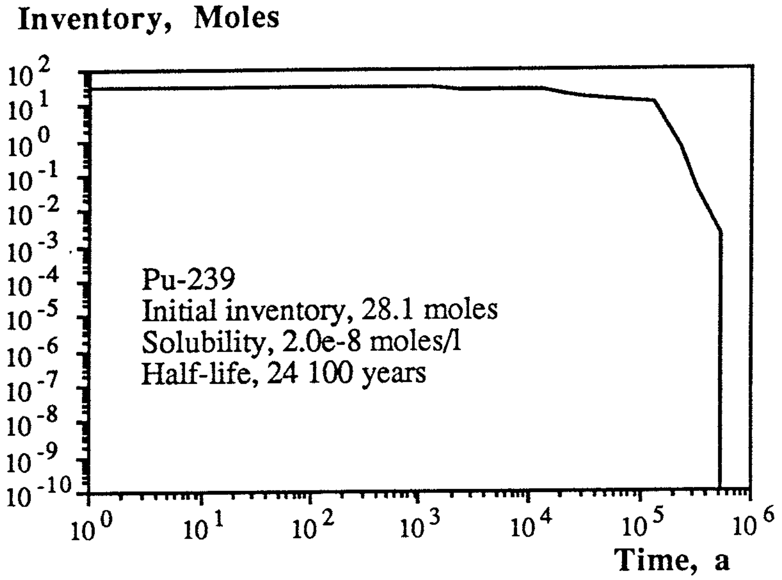


Figure 8 Variation of the nuclide inventory in the canister with time.

The total amount of moles released into the bentonite is less than 10^{-6} times the initial inventory (28.1 moles) for Pu-239. Of this release, less than a fraction 10^{-4} of the mass released reaches the flowing water. This occurs almost entirely through the fracture intersecting the repository hole, through the path formed by the compartments 3, 4, and the flowing water. The rest decays.

6 DISCUSSION AND CONCLUSIONS

There is no simple way to verify the proposed compartment model in all its aspects. The approach we have taken is the steady state comparisons with known analytical solutions.

Inherently the model has its main resistances in the hole in the canister wall, in the flowing water in the fractures and at the mouth of the hole in the canister wall and fractures. The model handles these regions by use of analytical solutions which are very robust. In the steady state thus the model behaves well and gives results which can be checked by comparison with known solutions.

The non steady state results have not been verified yet. The approach we intend to take is to increase the number of compartments in the regions with large volumes and sorption capacities until further increase in accuracy is not warranted. We also intend to compare some simple cases with "full" 3-D calculations.

The model developed is aimed to be very simple and flexible. This is of course at the expense of loss of accuracy. The accuracy during the unsteady state phase is low when few compartments are used but can be increased to get very high accuracy if more and more compartments are chosen. For scoping calculations few compartments should suffice and when accuracy need be increased compartments can be subdivided in the sensitive zones.

NOTATION

$A_{i,j}$	Contact area (compartment i and j)	m^2
A_f	Contact area at the mouth of the fracture	m^2
A_s	Activity concentration in the canister	GBq/m^3
a_o	Activity concentration (equivalent to the solubility)	GBq/m^3
a_i	Activity concentration in the i-th compartment	GBq/m^3
$\overline{B}$	Vector of boundary conditions	
c	Concentration	$moles/m^3$
c_o	Concentration in canister	$moles/m^3$
c_1	Concentration in compartment 1 (small hole)	$moles/m^3$
D_{eff}	Effective diffusivity	m2/a
D_{can}	Canister diameter	m
D_{hole}	Repository hole diameter	m
D_h	Small hole diameter	m
$d_{i,j}$	Diffusion length in compartment i to j	m
F	Diffusion length, plug at the mouth of the fracture	m
$\overline{\overline{F}}$	Matrix of coefficients	
K_i	Distribution coefficient	-
$K_{d,i}$	Sorption coefficient	m^3/kg
L_{can}	Canister length	m
L_i	Compartment length	m
m	number of independent variables (total)	-
M^o	Initial inventory	moles
M_s	Inventory of nuclide in the solid phase in the canister	moles
M_{dis}	Inventory of nuclide dissolved in the canister	moles
n	Number of independent variables	-
N	Flowrate of nuclide	moles/a
N_{input}	Flowrate of nuclide from the canister	moles/a
N_{out}	Total release of nuclide into the flowing water	moles/a
Q	Local equivalent flowrate	m^3/a
r	Radius	m
R	Resistance	a/m^3
t	Time	a
V_i	Compartment volume	m^3
V_o	Water volume in canister	m^3
δ	Aperture	m
Δx	Equivalent diffusion length	m
$\varepsilon_{p,i}$	Porosity (compartment i)	-
ρ_i	Density (compartment i)	kg/m^3
λ	Decay constant	a^{-1}
τ	Time constant	a

REFERENCES

Brandberg F., Skagius K.,"Porosity, sorption and diffusivity data compiled for the SKB 91 study", SKB Technical report, 91-16, 1991.

Bruno J., Sellin P., "Radionuclide solubilities to be used in SKB 91", SKB arbetsrapport, AR 91-02, 1991.

Kahaner D., Moler C., Nash S., "Numerical Methods and Software", Prentice hall 1988.

Neretnieks I., "Transport mechanisms and rates of transport of radionuclides in the geosphere as related to the swedish KBS concept", in Proceedings of symposium om "Underground disposal of radioactive wastes", Vol II, p 108, OTANIEMI 2-6 july 1979, IAEA, 1979.

Neretnieks I., "Stationary transport of dissolved species in the backfill surrounding a waste canister in fissured rock: some simple analytical solutions", Nuclear Technology, 72-194, 1986.

Wiborgh M.,Lindgren M., "Database for the radionuclide transport calculation for SFR", SKB Progress report, SFR 87-09, 1987.

Table 1 Parameter values required for calculations.

Symbol	Description	Units	Range	central-value	Ref.
D_{can}	Diameter of canister	m	-	0.8	-
D_{hole}	Diameter of repository hole	m	-	1.5	-
D_h	Hole diameter in canister wall	m	10^{-3} - 10^{-1}	0.0025 (5 mm^2)	-
YL_{tun}	Height of tunnel	m	-	4.5	-
ZL_{tun}	Width of tunnel	m	-	3	-
L_1	Thickness of canister	m	-	0.06	-
L_{can}	Length of canister	m	-	4.5	-
L_5	Length (see Fig.3)	m	-	1.5	-
L_6	Length (see Fig.3)	m	-	1.0	-
L_8	Length (see Fig.3)	m	0 - 3	2.5	-
L_9	Length (see Fig.3)	m	0 - 3	2.5	-
L_{11}	Length (see Fig.3)	m	-	0.5	-
L_{12}	Length (see Fig.3)	m	0-10	3	-
δ_1	Aperture (channel)	m	10^{-5} - 10^{-3}	10^{-4}	-
δ_2	Thickness (disturbed zone)	m		1	
δ_3	Aperture (channel)	m	10^{-5} - 10^{-3}	10^{-4}	-
δ_4	Thickness (fracture zone)	m	0.2 - 2		
Local equivalent flowrate					
Q_1	channel (repository hole)	l/a	0.03 - 3	0.1	...
Q_2	disturbed zone	l/a	0.03 - 3	0.5	...
Q_3	channel (tunnel)	l/a	0.03 - 3	0.1	...
Q_4	fracture zones	l/a	0.03 - 100	100	...
Equivalent diffusion length for compartment at the mouth of fracture					
F_4	in repository hole	m	$(3 - 8)\cdot\delta$	$5*\delta$	-
F_{10}	in tunnel	m	$(3 - 8)\cdot\delta$	$5*\delta$	-
V_o	Water volume in canister	m^3	-	0.02	-

Table 2Data used in the calculations. Pu-239

Symbol		Units	Range	central-value	Ref.
M^o	Initial inventory	moles		28.1	-
c_o	solubility	moles/l		$2.0 \cdot 10^{-8}$	AR 91-02
τ	Half-life	a	.....	24 100	
Diffusivity (Deff)					
D_{water}	in water	m^2/s	.....	$3.9 \cdot 10^{-9}$	SKB 89-38
D_{bent}	bentonite	m^2/s	.....	$1.0 \cdot 10^{-10}$	SKB 91-16
$D_{s\text{-}b}$	in sand-bent. (90/10)	m^2/s	.....	$1.0 \cdot 10^{-10}$	SFR 87-09
D_{rock}	in rock	m^2/s	.....	$1.0 \cdot 10^{-13}$	SKB 91-16
D_{hole}	hole in canister wall	m^2/s	.....	$3.9 \cdot 10^{-9}$	SKB 89-38
Sorption					
$K_{d\text{-}bent}$	in bentonite	m^3/kg	0.6 - 11.0	5.0	SKB 91-16
$K_{d\text{-}(s\text{-}b)}$	in sand-bent. (90/10)	m^3/kg	.....	0.5	-
$K_{d\text{-}rock}$	in rock	m^3/kg	.....	3.0	SKB 91-16
$k_{d\text{-}hole}$	in hole in canister wall	m^3/kg	.....	0.0	
Porosity					
$\varepsilon_{p\text{-}bent}$	in bentonite	-	.....	0.25	SKB 91-16
$\varepsilon_{p\text{-}(s\text{-}b)}$	in sand-bent. (90/10)	-	.....	0.25	SFR 87-09
$\varepsilon_{p\text{-}rock}$	in rock	-	.....	0.005	SKB 91-16
$\varepsilon_{p\text{-}hole}$	in hole in canister wall	-	.....	1.0	-
$\varepsilon_{p\text{-}dist}$	in disturbed zone	-	.....	0.01	-
Density					
ρ_{bent}	wet bentonite	kg/m^3	.....	2000	SKB 91-16
$\rho_{s\text{-}b}$	sand-bent. (90/10)	kg/m^3	.....	2000	SFR 87-09
ρ_{rock}	rock	kg/m^3	.....	2700	"
ρ_{hole}	hole in canister wall	kg/m^3	.....	1000	-

Table 3 Defining the geometry of the system

Compartment (i)	Diffusion length (d_i)	Volume (V_i)
1	L_1	$L_1 \cdot A_h$
2	$D_h/4$	$(D_h/4)\ A_h$
3	L_{can}	$L_{can} \cdot (A_{hole} - A_{can})$
4	$F{*}\delta$	$F \cdot \delta^2 \cdot P_{hole}$
5	L_5	$L_5 \cdot A_{hole}$
6	$dy_6 = L_6\ ,\ dx_6 = D_{hole}$	$L_6 \cdot A_{hole}$
7	$dy_7 = YL_{tun},\ dx_7 = D_{hole}$	$D_{hole} \cdot A_{tunnel}$
8	L_8	$L_8 \cdot A_{tunnel}$
9	L_9	$L_9 \cdot A_{tunnel}$
10	$F{*}\delta$	$F \cdot \delta^2 \cdot P_{tunnel}$
11	L_{11}	$L_{11} \cdot A_{hole}$
12	L_{12}	$L_{12} \cdot A_{hole}$

* $A_{hole} = \frac{\pi \cdot D_{hole}^2}{4}$ $A_{can} = \frac{\pi \cdot D_{can}^2}{4}$

* $A_{tunnel} = YL_{tunnel} \cdot ZL_{tunnel}$ $A_h = \frac{\pi \cdot D_h^2}{4}$

* $P_{tunnel} = (\ 2YL_{tun} + ZL_{tun}\ )$ $P_{hole} = \pi \cdot D_{hole}$

Table 4 Defining the connections of compartments in the whole system

Connection i,j	Length d_i	Contact area $A_{i,j}$	Volume V_i
1 0	$d_1/2$	A_h	V_1
1 2	$d_1/2$	A_h	V_1
2 1	$d_2/2$	A_h	V_2
2 3	$d_2/2$	A_h	V_2
3 2	0	A_h	V_3
3 4	0	$\delta_1 \cdot P_{hole}$	V_3
3 5	$d_3/2$	$(A_{hole} - A_{can})$	V_3
3 11	$d_3/2$	$(A_{hole} - A_{can})$	V_3
4 3	$d_4/2$	$\delta_1 \cdot P_{hole}$	V_4
4 w_1	$d_4/2$	$\delta_1 \cdot P_{hole}$	V_4
5 3	$dy_5/2$	$(A_{hole} - A_{can})$	V_5
5 6	$dy_5/2$	A_{hole}	V_5
6 5	$dy_6/2$	A_{hole}	V_6
6 w_2	$dy_6/2$	$\delta_2 \cdot P_{hole}$	V_6
6 7	$dy_6/2$	A_{hole}	V_6
7 6	$dy_7/2$	A_{hole}	V_7
7 8	$dy_7/2$	A_{tunnel}	V_7
7 9	$dy_7/2$	A_{tunnel}	V_7
8 7	$d_8/2$	A_{tunnel}	V_8
9 7	$dx_9/2$	A_{tunnel}	V_9
9 10	-	$\delta_3 \cdot P_{tunnel}$	V_9
10 9	$d_{10}/2$	$\delta_3 \cdot P_{tunnel}$	V_{10}
10 w_3	$d_{10}/2$	$\delta_3 \cdot P_{tunnel}$	V_{10}
11 3	$d_{11}/2$	$(A_{hole} - A_{can})$	V_{11}
11 12	$d_{11}/2$	A_{hole}	V_{11}
12 11	$d_{12}/2$	A_{hole}	V_{12}
12 w_4	$d_{12}/2$	A_{hole}	V_{12}

APPENDIX A: Calculation of the equivalent diffusion length for mass transport from a small hole into a large body.

In this appendix an equivalent plug length, Δx_a, will be calculated. The transport by diffusion takes place from a small area into a large body.

When a species diffuses out of a small hole into a very large volume of clay it will spread out in a spherical way. Very near the hole, the cross section for diffusion is still on the order of the size of the hole. Further away the cross section for diffusion has increased considerably as the "sphere" grows. The cross section area increases proportionally to the distance squared whereas the diffusion distance increases only proportionally to the distance. It can be intuitively conceived that most of the resistance to diffusion will be concentrated very near the mouth of the hole. In the following we show how all the resistance can be contained in a short plug with the diameter of the hole and a length equal to 1/4 of the hole diameter. Figure A1 illustrates the "real"case, the model approach and the equivalent plug.

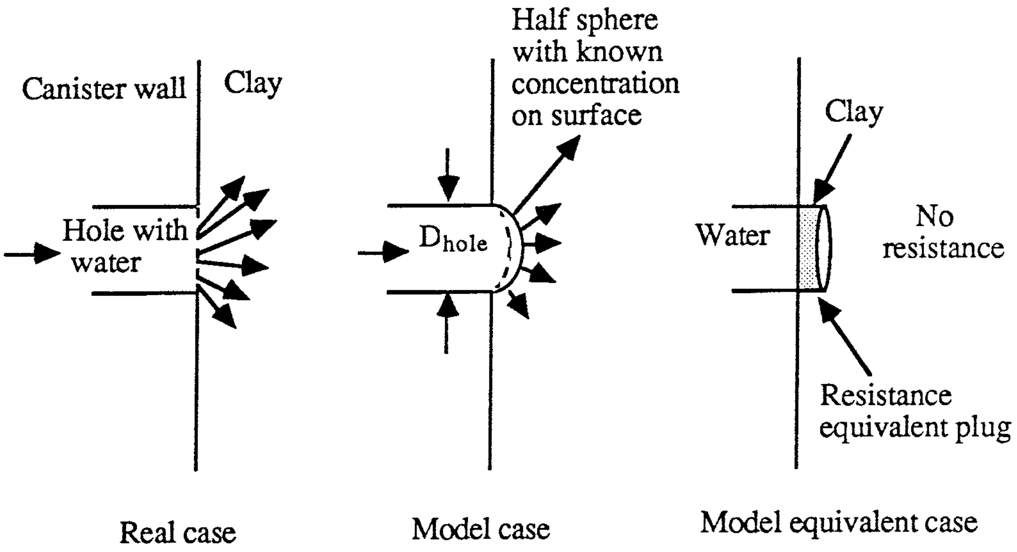


Figure A1 Schematic view of the real case and the model case to get the resistance equivalent plug.

The mass transfer from a half sphere into a surrounding medium, the backfill clay, is

$$N = -2 \cdot \pi \cdot r^2 \cdot D_{eff} \cdot \frac{dc}{dr} \tag{A-1}$$

Integrating between the limits r_{sph}, radius of the sphere, and r

$$N = \frac{2 \cdot \pi \cdot D_{eff} \cdot \Delta c}{\frac{1}{r_{sph}} - \frac{1}{r}} \qquad \text{(A-2)}$$

If the concentration difference is spread over a large distance, $r >> r_{sph}$, we obtain

$$\frac{r_{sph} \cdot N}{2 \cdot \pi \cdot r_{sph}^{2} \cdot D_{eff} \cdot \Delta c} = 1 \qquad \text{(A-3)}$$

The nuclide flowrate N is

$$N = 2\pi \cdot r_{sph} \cdot D_{eff} \cdot \Delta c \qquad \text{(A-4)}$$

As the diameter of the sphere is equal to that of the hole, an equivalent flowrate would be obtained by a plug of thickness Δx and radius r_{sph}

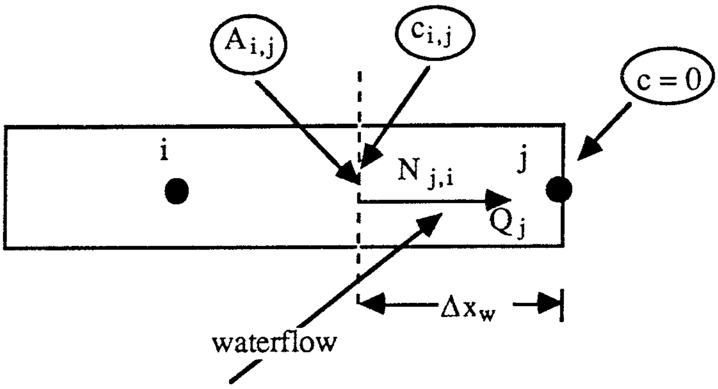
$$N = \frac{D_{eff} \cdot \pi \cdot r_{sph}^{2}}{\Delta x} \Delta c \qquad \text{(A-5)}$$

Equating Equations (A-4) and (A-5) gives

$$\Delta x = \frac{r_{sph}}{2} = \frac{r_{hole}}{2} = \frac{D_{hole}}{4} \qquad \text{(A-6)}$$

APPENDIX B: Equivalent compartment length, Δx_w, in the flowing water in the fractures

In this appendix we show how the local equivalent flowrate Q_{eq} can be transformed to be used as a boundary compartment in the model. The equivalent flowrate Q_{eq} is a fictitious flowrate of water which carries with it a concentration equal to that at the compartment interface. Q_{eq} has been derived by solving the equations for diffusional transport to the passing water (Neretnieks, 1979). The figure below shows the transport to the boundary compartment (flowing water). The water flowrate Q_{eq} approaches with concentration 0 and leaves with the interface concentration $c_{i,j}$.



The flowrate of nuclides, $N_{j,i}$, transported into the water (j-th region) is

$$N_{j,i} = Q_j \cdot c_{i,j} \tag{B-1}$$

Where Q_j is the local equivalent flowrate and $c_{i,j}$ is the interfacial concentration at the surface of contact solid-water, $A_{i,j}$.

Introducing an imaginary compartment with stagnant water with interface concentration $c_{i,j}$ on one side and concentration 0 at the other side, the nuclide flowrate through this compartment may be obtained from Fick's law

$$N_{j,i} = -\frac{D_w}{\Delta x_w} A_{j,i} \cdot \Delta c \tag{B-2}$$

where Δc is the difference of concentration between the interfacial concentration $c_{i,j}$ and a concentration zero at a fictitious position in the region in which the water flows.

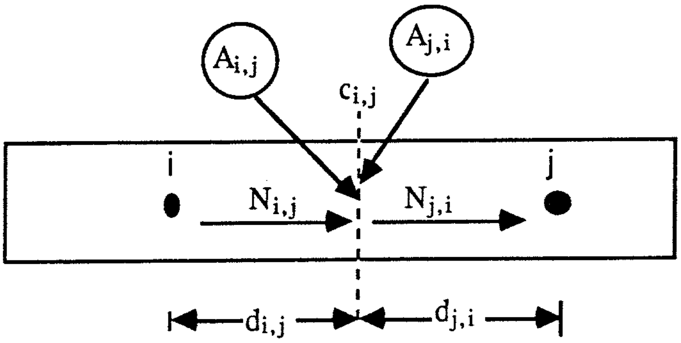
Combining the above equations we obtain the diffusion length at which the concentration of radionuclides is zero

$$d_{j,i} = \Delta x_w = \frac{D_w}{Q_i} A_{j,i} \qquad \text{(B-3)}$$

If we take as an example, the diffusion of radionuclides into the fracture intersecting the canister from the 4-th compartment (see Figure 3) for an equivalent flowrate of 0.1 l/a and for an area ($A = \delta_1 \cdot \pi \cdot D_{hole}$) of $4.7 \cdot 10^{-4}$, the equivalent length Δx_w is 0.58 m.

APPENDIX C: Conductivity between compartments, $(D/d)_{i,j}$

In this appendix the combined conductivity from a point in one compartment to a point in another compartment is derived



Knowing that the nuclide flowrates into and from the same interfacial area ($A_{i,j} = A_{j,i}$) are equal we obtain

$$N_{i,j} = N_{j,i} \tag{C-1}$$

If we express both nuclide flowrates by Fick's law, the equation obtained for the transport into the interfacial area ($A_{i,j}$) is

$$N_{i,j} = -\frac{D_i}{d_{i,j}} A_{i,j} \cdot (c_{i,j} - c_i) \tag{C-2}$$

and the nuclide flowrate out from the interfacial area ($A_{j,i}$) is

$$N_{j,i} = -\frac{D_j}{d_{j,i}} A_{j,i} \cdot (c_j - c_{i,j}) \tag{C-3}$$

Combining the above equations by eliminating the interface concentration $c_{i,j}$ gives

$$N_{i,j} = -\frac{A_{i,j}}{\left(\frac{d_{i,j}}{D_i} + \frac{d_{j,i}}{D_j}\right)} \cdot (c_j - c_i) \tag{C-4}$$

Then the conductivity between the compartments "i" and "j" is defined as

$$\left(\frac{D}{d}\right)_{i,j} = \frac{1}{\left(\frac{d_{i,j}}{D_i} + \frac{d_{j,i}}{D_j}\right)} \tag{C-5}$$

APPENDIX D: Migration of a radionuclide chain

The radionuclide release of the I-th member of a radionuclide chain may be described by a set of linear differential equations which describe the material balances of the I-th chain member and all preceding chain members over a compartment as was done to describe a single nuclide.

The calculations for the members in the chain are done in succession beginning with the first member of the chain called the mother nuclide. The mother nuclide is independent of the other nuclides in the chain. The decay term for a parent is a source term for a daughter nuclide and is included as such in the calculations for the daughter.

The following equations are obtained for a decay chain of 3 nuclides

$$K_i^I \cdot V_i \cdot \frac{dc_i^I}{dt} = \sum_{j \neq i} A_{i,j} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \cdot \left(c_j^I - c_i^I\right) - K_i^I \cdot V_i \cdot \lambda^I \cdot c_i^I \qquad \text{(D-1)}$$

$$K_i^{II} \cdot V_i \cdot \frac{dc_i^{II}}{dt} = \sum_{j \neq i} A_{i,j} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \cdot \left(c_j^{II} - c_i^{II}\right) - K_i^{II} \cdot V_i \cdot \lambda^{II} \cdot c_i^{II} + K_i^I \cdot V_i \cdot \lambda^I \cdot c_i^I \qquad \text{(D-2)}$$

$$K_i^{III} \cdot V_i \cdot \frac{dc_i^{III}}{dt} = \sum_{j \neq i} A_{i,j} \cdot \left(\frac{D_{eff}}{d}\right)_{i,j} \cdot \left(c_j^{III} - c_i^{III}\right) - K_i^{III} \cdot V_i \cdot \lambda^{III} \cdot c_i^{III} + K_i^{II} \cdot V_i \cdot \lambda^{II} \cdot c_i^{II} \qquad \text{(D-3)}$$

Assuming that only the mother nuclide is present at the initial time, the boundary conditions become

$$c_o^I(t) = c_o^I \cdot e^{-\lambda^I \cdot t} \qquad \text{(D-4)}$$

$$c_o^{II}(t) = c_o^I \cdot \frac{\lambda^I}{\lambda^{II} - \lambda^I} \left(e^{-\lambda^I \cdot t} - e^{-\lambda^{II} \cdot t}\right) \qquad \text{(D-5)}$$

$$c_o^{III}(t) = c_o^I \cdot \left(\lambda^I \cdot \lambda^{II}\right) \cdot \left(\frac{e^{-\lambda^I \cdot t}}{\left(\lambda^{II} - \lambda^I\right)\left(\lambda^{III} - \lambda^I\right)} + \frac{e^{-\lambda^{II} \cdot t}}{\left(\lambda^I - \lambda^{II}\right)\left(\lambda^{III} - \lambda^{II}\right)} + \frac{e^{-\lambda^{III} \cdot t}}{\left(\lambda^I - \lambda^{III}\right)\left(\lambda^{II} - \lambda^{III}\right)}\right) \qquad \text{(D-6)}$$

List of SKB reports

Annual Reports

1977-78
TR 121
KBS Technical Reports 1 – 120
Summaries
Stockholm, May 1979

1979
TR 79-28
The KBS Annual Report 1979
KBS Technical Reports 79-01 – 79-27
Summaries
Stockholm, March 1980

1980
TR 80-26
The KBS Annual Report 1980
KBS Technical Reports 80-01 – 80-25
Summaries
Stockholm, March 1981

1981
TR 81-17
The KBS Annual Report 1981
KBS Technical Reports 81-01 – 81-16
Summaries
Stockholm, April 1982

1982
TR 82-28
The KBS Annual Report 1982
KBS Technical Reports 82-01 – 82-27
Summaries
Stockholm, July 1983

1983
TR 83-77
The KBS Annual Report 1983
KBS Technical Reports 83-01 – 83-76
Summaries
Stockholm, June 1984

1984
TR 85-01
Annual Research and Development Report 1984
Including Summaries of Technical Reports Issued during 1984. (Technical Reports 84-01 – 84-19)
Stockholm, June 1985

1985
TR 85-20
Annual Research and Development Report 1985
Including Summaries of Technical Reports Issued during 1985. (Technical Reports 85-01 – 85-19)
Stockholm, May 1986

1986
TR 86-31
SKB Annual Report 1986
Including Summaries of Technical Reports Issued during 1986
Stockholm, May 1987

1987
TR 87-33
SKB Annual Report 1987
Including Summaries of Technical Reports Issued during 1987
Stockholm, May 1988

1988
TR 88-32
SKB Annual Report 1988
Including Summaries of Technical Reports Issued during 1988
Stockholm, May 1989

1989
TR 89-40
SKB Annual Report 1989
Including Summaries of Technical Reports Issued during 1989
Stockholm, May 1990

1990
TR 90-46
SKB Annual Report 1990
Including Summaries of Technical Reports Issued during 1990
Stockholm, May 1991

Technical Reports

List of SKB Technical Reports 1991

TR 91-01
Description of geological data in SKB's database GEOTAB Version 2
Stefan Sehlstedt, Tomas Stark
SGAB, Luleå
January 1991

TR 91-02
Description of geophysical data in SKB database GEOTAB Version 2
Stefan Sehlstedt
SGAB, Luleå
January 1991

TR 91-03
1. The application of PIE techniques to the study of the corrosion of spent oxide fuel in deep-rock ground waters
2. Spent fuel degradation
R S Forsyth
Studsvik Nuclear
January 1991

TR 91-04
Plutonium solubilities
I Puigdomènech[1], J Bruno[2]
[1]Enviromental Services, Studsvik Nuclear, Nyköping, Sweden
[2]MBT Tecnologia Ambiental, CENT, Cerdanyola, Spain
February 1991

TR 91-05
Description of tracer data in the SKB database GEOTAB
SGAB, Luleå
April, 1991

TR 91-06
Description of background data in the SKB database GEOTAB
Version 2
Ebbe Eriksson, Stefan Sehlstedt
SGAB, Luleå
March 1991

TR 91-07
Description of hydrogeological data in the SKB's database GEOTAB
Version 2
Margareta Gerlach (ed.)
Mark Radon Miljö MRM Konsult AB, Luleå
December 1991

TR 91-08
Overview of geologic and geohydrologic conditions at the Finnsjön site and its surroundings
Kaj Ahlbom[1], Sven Tirén[2]
[1]Conterra AB
[2]Sveriges Geologiska AB
January 1991

TR 91-09
Long term sampling and measuring program. Joint report for 1987, 1988 and 1989. Within the project: Fallout studies in the Gideå and Finnsjö areas after the Chernobyl accident in 1986
Thomas Ittner
SGAB, Uppsala
December 1990

TR 91-10
Sealing of rock joints by induced calcite precipitation. A case study from Bergeforsen hydro power plant
Eva Hakami[1], Anders Ekstav[2], Ulf Qvarfort[2]
[1]Vattenfall HydroPower AB
[2]Golder Geosystem AB
January 1991

TR 91-11
Impact from the disturbed zone on nuclide migration – a radioactive waste repository study
Akke Bengtsson[1], Bertil Grundfelt[1],
Anders Markström[1], Anders Rasmuson[2]
[1]KEMAKTA Konsult AB
[2]Chalmers Institute of Technology
January 1991

TR 91-12
Numerical groundwater flow calculations at the Finnsjön site
Björn Lindbom, Anders Boghammar,
Hans Lindberg, Jan Bjelkås
KEMAKTA Consultants Co, Stockholm
February 1991

TR 91-13
Discrete fracture modelling of the Finnsjön rock mass
Phase 1 feasibility study
J E Geier, C-L Axelsson
Golder Geosystem AB, Uppsala
March 1991

TR 91-14
Channel widths
Kai Palmqvist, Marianne Lindström
BERGAB-Berggeologiska Undersökningar AB
February 1991

TR 91-15
Uraninite alteration in an oxidizing environment and its relevance to the disposal of spent nuclear fuel
Robert Finch, Rodney Ewing
Department of Geology, University of New Mexico
December 1990

TR 91-16
Porosity, sorption and diffusivity data compiled for the SKB 91 study
Fredrik Brandberg, Kristina Skagius
Kemakta Consultants Co, Stockholm
April 1991

TR 91-17
Seismically deformed sediments in the Lansjärv area, Northern Sweden
Robert Lagerbäck
May 1991

TR 91-18
Numerical inversion of Laplace transforms using integration and convergence acceleration
Sven-Åke Gustafson
Rogaland University, Stavanger, Norway
May 1991

TR 91-19
NEAR21 - A near field radionuclide migration code for use with the PROPER package
Sven Norman[1], Nils Kjellbert[2]
[1]Starprog AB
[2]SKB AB
April 1991

TR 91-20
Äspö Hard Rock Laboratory.
Overview of the investigations 1986-1990
R Stanfors, M Erlström, I Markström
June 1991

TR 91-21
Äspö Hard Rock Laboratory.
Field investigation methodology and instruments used in the pre-investigation phase, 1986-1990
K-E Almén, O Zellman
June 1991

TR 91-22
Äspö Hard Rock Laboratory.
Evaluation and conceptual modelling based on the pre-investigations 1986-1990
P Wikberg, G Gustafson, I Rhén, R Stanfors
June 1991

TR 91-23
Äspö Hard Rock Laboratory.
Predictions prior to excavation and the process of their validation
Gunnar Gustafson, Magnus Liedholm, Ingvar Rhén, Roy Stanfors, Peter Wikberg
June 1991

TR 91-24
Hydrogeological conditions in the Finnsjön area.
Compilation of data and conceptual model
Jan-Erik Andersson, Rune Nordqvist, Göran Nyberg, John Smellie, Sven Tirén
February 1991

TR 91-25
The role of the disturbed rock zone in radioactive waste repository safety and performance assessment.
A topical discussion and international overview.
Anders Winberg
June 1991

TR 91-26
Testing of parameter averaging techniques for far-field migration calculations using FARF31 with varying velocity.
Akke Bengtsson[1], Anders Boghammar[1], Bertil Grundfelt[1], Anders Rasmuson[2]
[1]KEMAKTA Consultants Co
[2]Chalmers Institute of Technology

TR 91-27
Verification of HYDRASTAR. A code for stochastic continuum simulation of groundwater flow
Sven Norman
Starprog AB
July 1991

TR 91-28
Radionuclide content in surface and groundwater transformed into breakthrough curves. A Chernobyl fallout study in an forested area in Northern Sweden
Thomas Ittner, Erik Gustafsson, Rune Nordqvist
SGAB, Uppsala
June 1991

TR 91-29
Soil map, area and volume calculations in Orrmyrberget catchment basin at Gideå, Northern Sweden
Thomas Ittner, P-T Tammela, Erik Gustafsson
SGAB, Uppsala
June 1991

TR 91-30
A resistance network model for radionuclide transport into the near field surrounding a repository for nuclear waste (SKB, Near Field Model 91)
Lennart Nilsson, Luis Moreno, Ivars Neretnieks, Leonardo Romero
Department of Chemical Engineering, Royal Institute of Technology, Stockholm
June 1991

TR 91-31
Near field studies within the SKB 91 project
Hans Widén, Akke Bengtsson, Bertil Grundfelt
Kemakta Consultants AB, Stockholm
June 1991

TR 91-32
SKB/TVO Ice age scenario
Kaj Ahlbom[1], Timo Äikäs[2], Lars O. Ericsson[3]
[1] Conterra AB
[2] Teollisuuden Voima Oy (TVO)
[3] Svensk Kärnbränslehantering AB (SKB)
June 1991

TR 91-33
Transient nuclide release through the bentonite barrier - SKB 91
Akke Bengtsson, Hans Widén
Kemakta Konsult AB
May 1991

TR 91-34
SIMFUEL dissolution studies in granitic groundwater
I Casas[1], A Sandino[2], M S Caceci[1], J Bruno[1], K Ollila[3]
[1] MBT Tecnologia Ambiental, CENT, Cerdanyola, Spain
[2] KTH, Dpt. of Inorganic Chemistry, Stockholm, Sweden
[3] VTT, Tech. Res. Center of Finland, Espoo, Finland
September 1991

TR 91-35
Storage of nuclear waste in long boreholes
Håkan Sandstedt[1], Curt Wichmann[1], Roland Pusch[2], Lennart Börgesson[2], Bengt Lönnerberg[3]
[1] Tyréns
[2] Clay Technology AB
[3] ABB Atom
August 1991

TR 91-36
Tentative outline and siting of a repository for spent nuclear fuel at the Finnsjön site. SKB 91 reference concept
Lars Ageskog, Kjell Sjödin
VBB VIAK
September 1991

TR 91-37
Creep of OFHC and silver copper at simulated final repository canister-service conditions
Pertti Auerkari, Heikki Leinonen, Stefan Sandlin
VTT, Metals Laboratory, Finland
September 1991

TR 91-38
Production methods and costs of oxygen free copper canisters for nuclear waste disposal
Hannu Rajainmäki, Mikko Nieminen, Lenni Laakso
Outokumpu Poricopper Oy, Finland
June 1991

TR 91-39
The reducibility of sulphuric acid and sulphate in aqueous solution (translated from German)
Rolf Grauer
Paul Scherrer Institute, Switzerland
July 1990

TR 91-40
Interaction between geosphere and biosphere in lake sediments
Björn Sundblad, Ignasi Puigdomenech, Lena Mathiasson
December 1990

TR 91-41
Individual doses from radionuclides released to the Baltic coast
Ulla Bergström, Sture Nordlinder
Studsvik AB
May 1991

TR 91-42
Sensitivity analysis of the groundwater flow at the Finnsjön study site
Yung-Bing Bao, Roger Thunvik
Dept. Land and Water Resources, Royal Institute of Technology, Stockholm, Sweden
September 1991

TR 91-43
SKB - PNC
Development of tunnel radar antennas
Lars Falk
ABEM, Uppsala, Sweden
July 1991

TR 91-44
Fluid and solute transport in a network of channels
Luis Moreno, Ivars Neretnieks
Department of Chemical Engineering,
Royal Institute of Technology, Stockholm, Sweden
September 1991

TR 91-45
The implications of soil acidification on a future HLNW repository.
Part I: The effects of increased weathering, erosion and deforestation
Josefa Nebot, Jordi Bruno
MBT Tecnologìa Ambiental, Cerdanyola, Spain
July 1991

TR 91-46
Some mechanisms which may reduce radiolysis
Ivar Neretnieks, Mostapha Faghihi
Department of Chemical Engineering, Royal
Institute of Technology, Stockholm, Sweden
August 1991

TR 91-47
On the interaction of granite with Tc(IV) and Tc(VII) in aqueous solution
Trygve E Eriksen, Daquing Cui
Royal Institute of Technology, Department of
Nuclear Chemistry, Stockholm, Sweden
October 1991