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# COMP23 – Study of the connection between the hole in the canister wall and the surrounding bentonite

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Kemakta Konsult AB

August 1998

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# Summary

The input data in the near field compartment model concerning the connection between the hole in the canister wall and the surrounding bentonite has been studied.

The calculations show that Z_AREA and A_ZERO must be given equal values in order to achieve consistent dimensions of the hole and the equivalent plug.

The usage of an equivalent plug in the connection between the small hole and a large bentonite compartment is valid only if the hole is small compared to the area of the surrounding bentonite. It was shown that a hole with an area larger than about 0.001 $m^2$ overestimates the resistance between the hole and bentonite. An alternative is to make the model without the plug. However, in many cases with large hole the plug resistance is small compared to the total resistance and there is no need to take away the plug. In the case of an initially large hole it is better to exclude the plug from the model.

The different resistances in the system from the source to the release at Q1 were studied. It was then concluded that usage of the CANISTER_TYPE CUFE gives an internal plug with dimensions equal to the plug between the hole and bentonite and an effective diffusivity of $10^{-10}$ $m^2/s$. Usage of the CANISTER_TYPE LEAD_FILLED gives no resistance inside the canister wall and is recommended for future use.

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# Introduction

The near field compartment model COMP23 will be used in the SR97 calculations for SFL 2. The division of the near field into model blocks is shown in Figure 1. A detailed description of the dimensions used for the discretization is given in Appendix A.

In this study the connection between the hole in the canister wall and the surrounding bentonite is studied, especially the influence of the area of the hole. In the input data to COMP23 the area of the hole in the canister wall is given at two locations, Z_AREA and A_ZERO. The area of the hole is used to calculate the resistance of the hole and also to calculate the resistance in an equivalent plug. The equivalent plug is used in the code to represent the resistance in the connection between the small hole compartment and the large bentonite compartment.

Several calculation cases have been set up, where Z_AREA and A_ZERO were varied on different levels. The total release rate of U-238 and the concentration of U-238 in the source, the hole and the inner bentonite compartment are presented in figures. The resistances in the different compartments are calculated and the results are discussed.

The usage of an equivalent plug in the connection between the small hole and large bentonite compartment is valid only if the hole is small compared to the area of the surrounding bentonite. The limit for the size of the hole will be discussed.

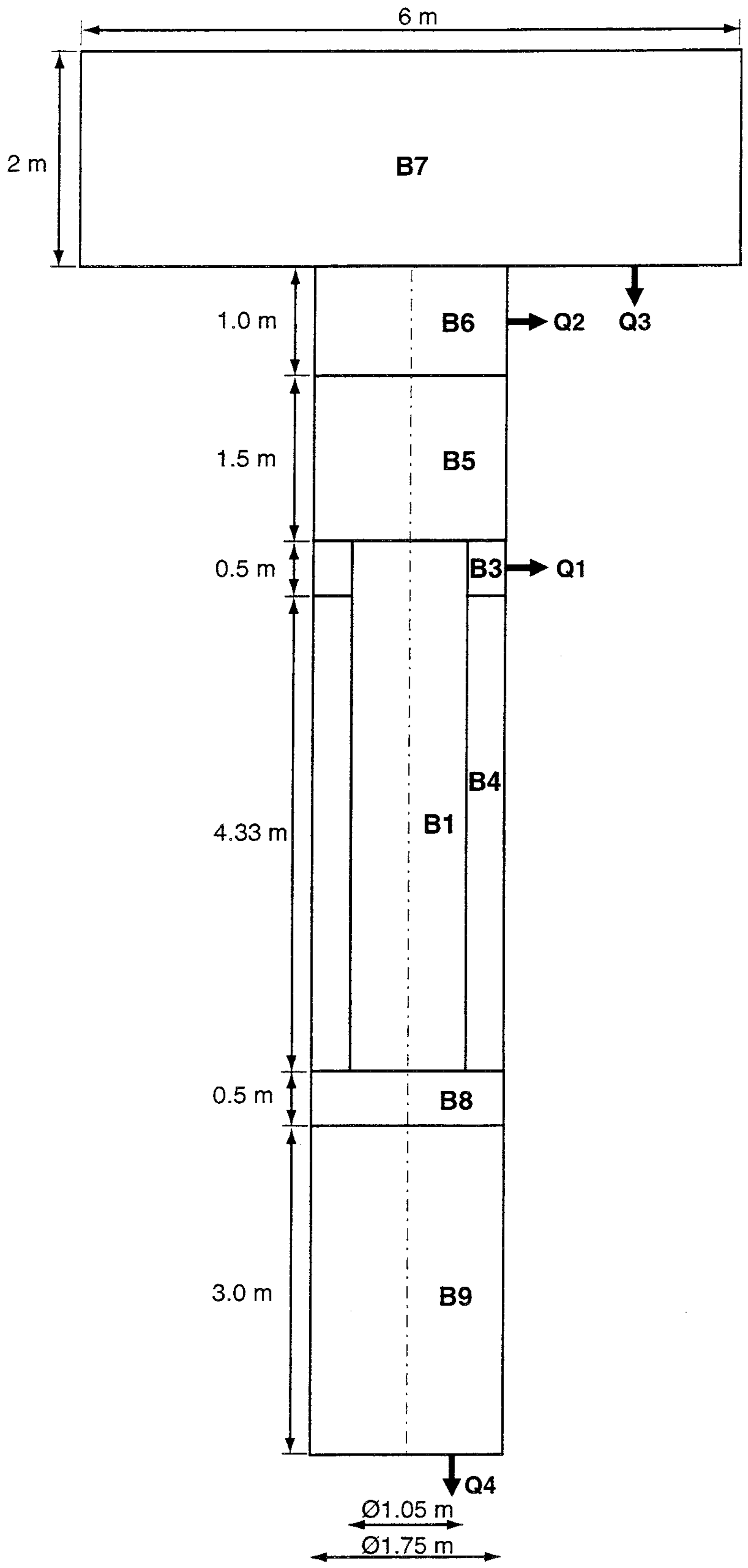


*Figure 1 Division of the near field into model blocks.*

# Calculations with different Z_AREA and A_ZERO

## Input data

The area of the hole in the canister wall may be given at two different locations. The first location is at the definition of BLOCK 2, where the hole area is given as Z_AREA and if the possibility of area change is chosen, a function for the growth of the hole is to be given at another location. In these calculations a step function was used, starting at T_ZERO with the area A_ZERO and at the time T_LIMIT the area changes to A_LIMIT. T_ZERO were in all cases set to zero years. In order to evaluate the actual influence of varying the input data concerning the size of the hole several calculation cases have been set up. The cases and the used input data are given in Table 1.

**Table 1 Calculation cases and input data.**

| Case | Input data | | | |
|---|---|---|---|---|
| | Z_AREA | A_ZERO | T_LIMIT | A_LIMIT |
| base | 5.00E-06 | 5.00E-06 | 1E8 | 0.4 |
| fa5 | 5.00E-06 | 5.00E-05 | 1E8 | 0.4 |
| fa4 | 5.00E-06 | 5.00E-04 | 1E8 | 0.4 |
| fa3 | 5.00E-06 | 5.00E-03 | 1E8 | 0.4 |
| fz5 | 5.00E-05 | 5.00E-06 | 1E8 | 0.4 |
| fz4 | 5.00E-04 | 5.00E-06 | 1E8 | 0.4 |
| fz3 | 5.00E-03 | 5.00E-06 | 1E8 | 0.4 |
| fz5a5 | 5.00E-05 | 5.00E-05 | 1E8 | 0.4 |
| fz4a4 | 5.00E-04 | 5.00E-04 | 1E8 | 0.4 |
| fz3fa3 | 5.00E-03 | 5.00E-03 | 1E8 | 0.4 |
| fz2a2 | 5.00E-02 | 5.00E-02 | 1E8 | 0.4 |
| fz1a1 | 5.00E-01 | 5.00E-01 | 1E8 | 0.4 |
| fz6al3 | 5.00E-06 | 5.00E-06 | 0.1 | 5.00E-03 |
| fz6al3t1e4 | 5.00E-06 | 5.00E-03 | 1E4 | 5.00E-03 |

## Results

The results will be presented as the release rates of U-238 as a function of time for the different cases. The calculations show that changes in only A_ZERO give small changes in the release rate, see Figure 2. Changes in Z_AREA give somewhat larger effect, see Figure 3. Changes of both A_ZERO and Z_AREA give larger effects, see Figure 4. In Figure 5 the release rates for the cases with step function at the beginning (fz6al3) and after 10 000 years (fz6al3t1e4) together with cases with equal values of Z_AREA and A_ZERO is shown. The case with a step function after 0.1 year and the case with a step function (actually without step since A_ZERO=A_LIMIT) show that Z_AREA and A_ZERO are used in the beginning and A_LIMIT after the step.

The release rates of U-238 at 16 000 year are given in Table 2. The ratio between the release rate in the actual case and the base case are also given in Table 2.

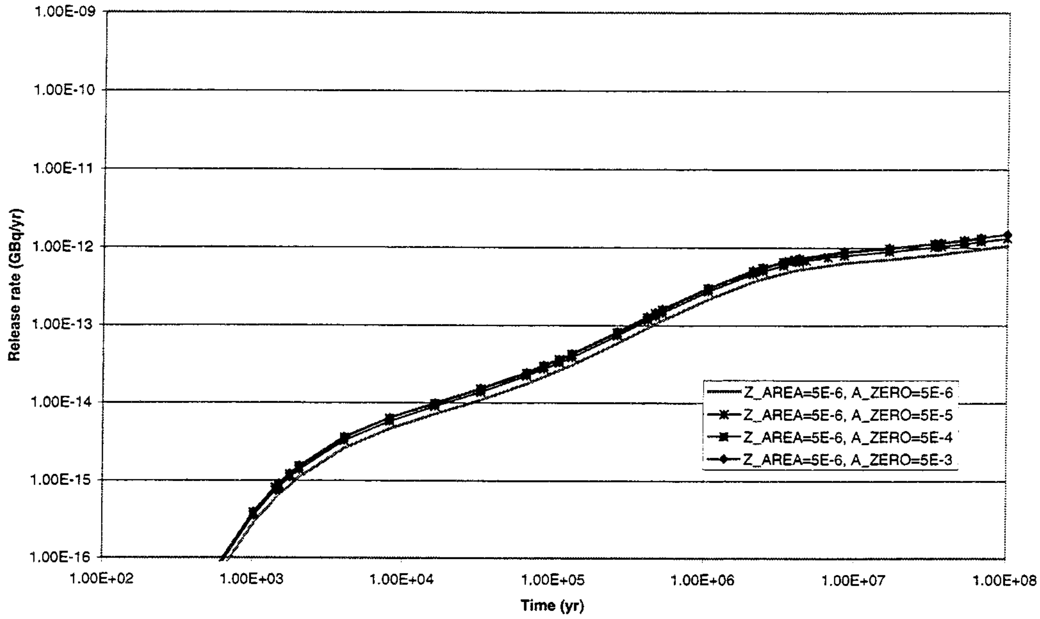


*Figure 2 Release rate of U-238 as a function of time for cases with different values of A_ZERO.*

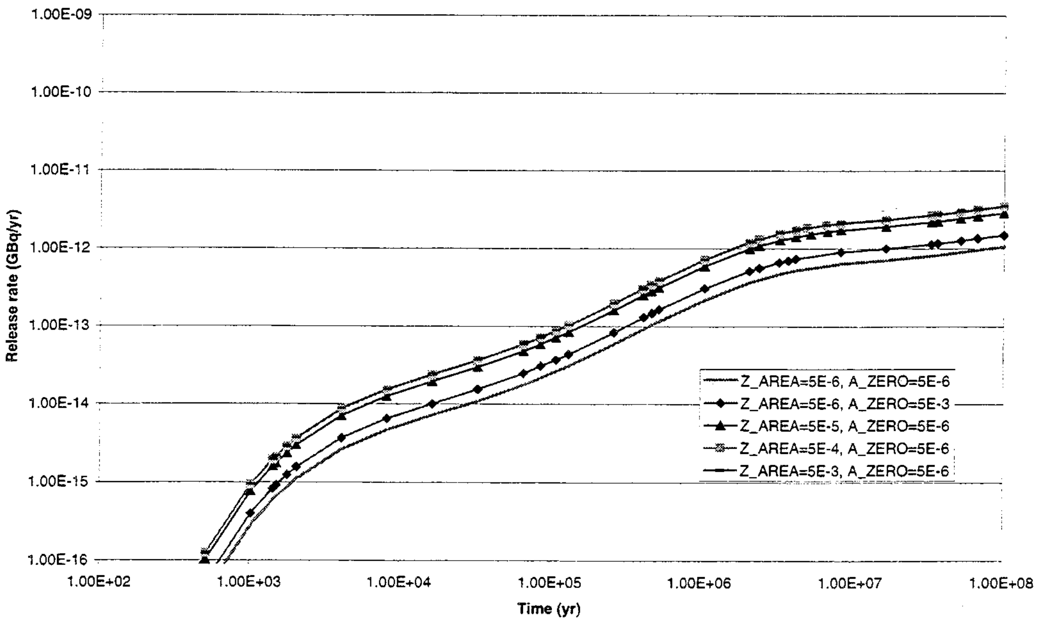


*Figure 3 Release rate of U-238 as a function of time for cases with different values of Z_AREA.*

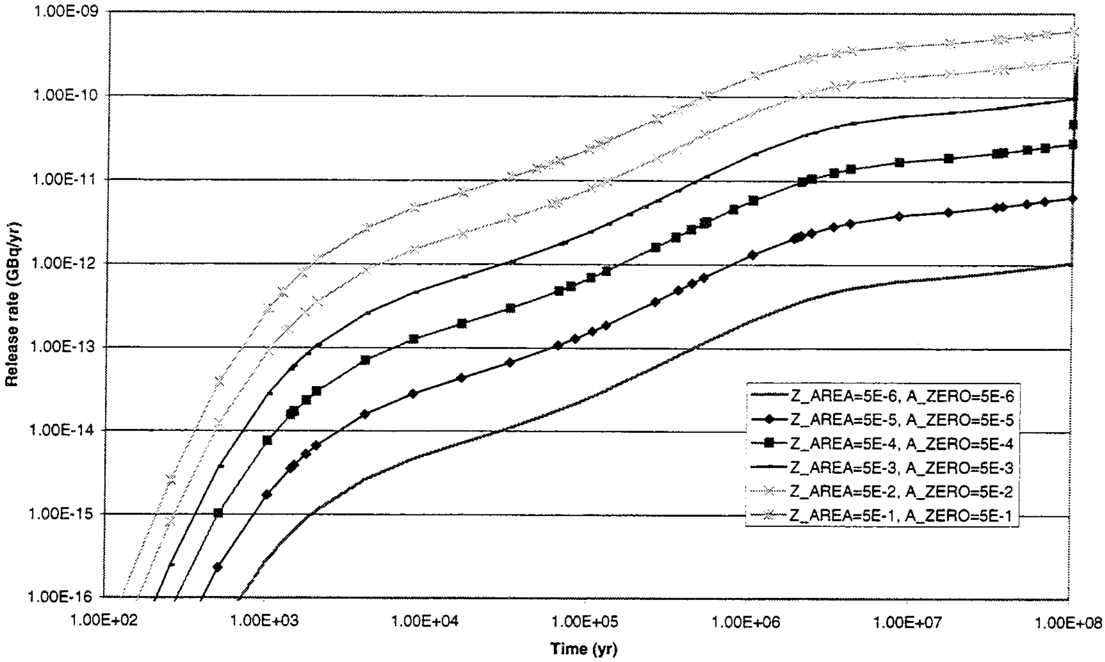


*Figure 4 Release rate of U-238 as a function of time for cases with different values of Z_AREA and A_ZERO.*

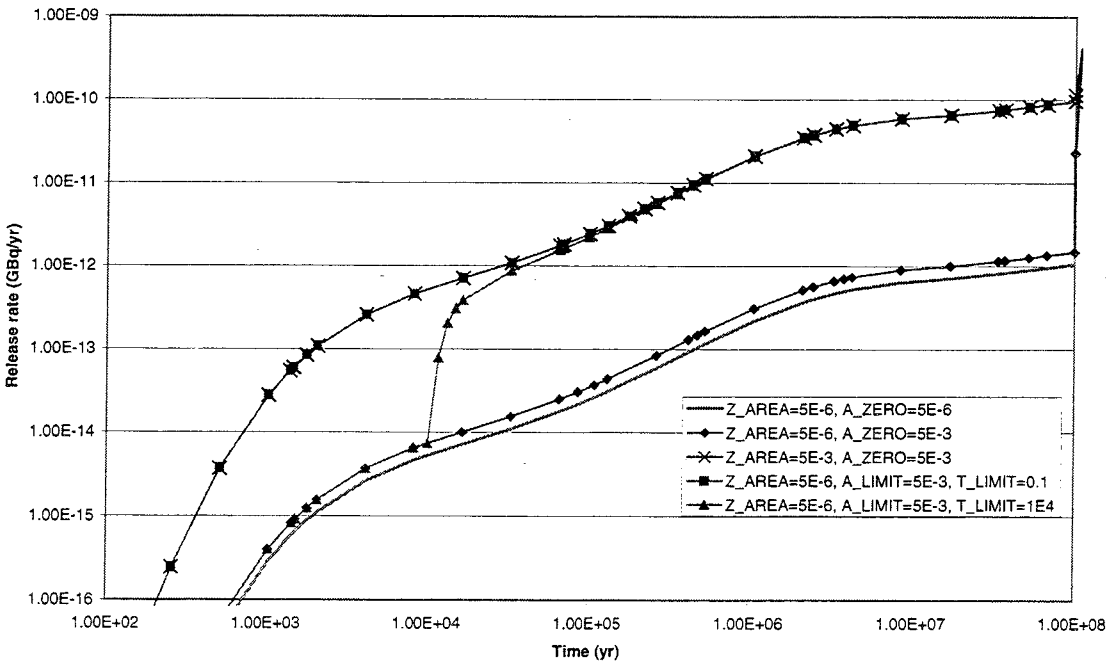


*Figure 5 Release rate of U-238 as a function of time for cases with different step functions.*

**Table 2 Release rates of U-238 at 16 000 yr and relative release rates.**

| Case | Input data | | Results | |
|---|---|---|---|---|
| | Z_AREA | A_ZERO | Release (GBq/yr) | Release Case/base |
| base | 5.00E-06 | 5.00E-06 | 1.06E-12 | 1.0 |
| fa5 | 5.00E-06 | 5.00E-05 | 1.33E-12 | 1.3 |
| fa4 | 5.00E-06 | 5.00E-04 | 1.45E-12 | 1.4 |
| fa3 | 5.00E-06 | 5.00E-03 | 1.49E-12 | 1.4 |
| fz5 | 5.00E-05 | 5.00E-06 | 2.86E-12 | 2.7 |
| fz4 | 5.00E-04 | 5.00E-06 | 3.45E-12 | 3.3 |
| fz3 | 5.00E-03 | 5.00E-06 | 3.52E-12 | 3.3 |
| fz5a5 | 5.00E-05 | 5.00E-05 | 6.39E-12 | 6.1 |
| fz4a4 | 5.00E-04 | 5.00E-04 | 2.81E-11 | 27.0 |
| fz3a3 | 5.00E-03 | 5.00E-03 | 9.69E-11 | 98.1 |
| fz2a2 | 5.00E-02 | 5.00E-02 | 2.77E-10 | 323.1 |
| fz1a1 | 5.00E-01 | 5.00E-01 | 6.20E-10 | 1008.4 |
| fz6al3 | 5.00E-06 | 5.00E-06[a)] | 1.03E-10 | 98.1 |
| fz6al3t1e4 | 5.00E-06 | 5.00E-03[b)] | 1.03E-10 | 53.5[c)] |

a) A_LIMIT=5E-3, T_LIMIT=0.1
b) A_LIMIT=5E-3, T_LIMIT=1E4
c) The release rate is at this time (16 000 yr) strongly affected by the step function

## Discussion

If a time dependent size of the hole is used both the hole and the plug dimensions should follow the function. The results show that the results are dependent both of Z_AREA and A_ZERO. In order to evaluate how these values are used two different alternative will be discussed. In the first alternative Z_AREA is used to calculate the plug and A_ZERO to calculate the hole. In the second alternative Z_AREA is used to calculate the hole and A_ZERO is used to calculate the plug. To understand the different results achieved, the resistance in the system from the canister to the release at Q1 was calculated, see Figure 7. Release through Q1 is the dominating release path for U-238 during the first about 100 000 years.

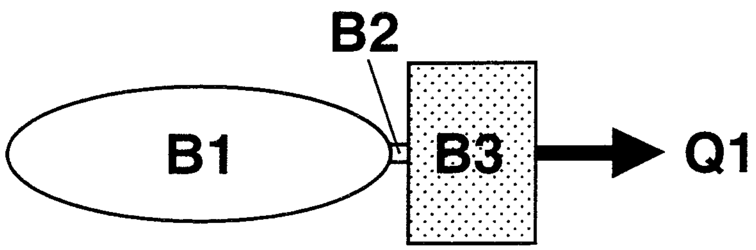


*Figure 7 Schematic illustration of the system from the canister to the release at Q1.*

The resistance in a block is given by:

$$R = \frac{x}{A \cdot D_e}$$

where x is the diffusion length of the block, A is the cross-sectional area of the block perpendicular to the direction of the transport and $D_e$ is the effective diffusion coefficient.

Transport into a large compartment is treated by usage of an equivalent plug. For this plug of a cross-sectional area equal to the hole area in the canister wall and thickness $\Delta x$ given by $\Delta x = r_{hole}/\sqrt{2}$. The plug is managed by the model COMP23 as a resistance added to the coupling resistance between the two compartments (the hole in the canister wall and the bentonite compartment adjacent to this hole). This equivalent plug resistance $R_p$ as a function of the hole radius in the canister wall is:

$$R_p = \frac{x}{A \cdot D_e} = \frac{1}{\pi \cdot r_{hole} \cdot D_e \cdot \sqrt{2}}$$

The size of the block of small capacity may vary with time. If this is the case, the plug resistance will vary also.

Transport into a narrow slit is also treated by usage of an extra plug. The plug area is equal to the cross-sectional area of the fracture and the length is equal to a factor times the fracture aperture, see "Compartment model "NUCTRAN" (User´s manual), June1997 p.6.

The resistance in the plug is given by:

$$R_f = \left[ \left( F_{x,0} / \delta \right) / \delta / \left( D_e A_f \right) \right] = \begin{Bmatrix} D_e \, for \\ Nb, Ra, Sr, Tc, U \end{Bmatrix} =$$

$$= \frac{5.0E - 4\,m}{0.016\,m^2 / yr \cdot 5.5E - 4\,m^2} = 57\ yr / m^3$$

The resistance for Qeq is calculated as:

$$R_{Qeq} = \frac{1}{Qeq} = \frac{1}{QEQ\_FACTOR \cdot u^{QEQ\_EXPONENT}} = \frac{1}{0.025 \cdot 0.01^{0.5}} = 400\ yr / m^3 .$$

In Table 3 and 4 the resistances in the different components in the system are given calculated with the two alternative approaches.

**Table 3** **Resistances in the different components in the system. Alternative 1, Z_AREA is used to calculate the plug and A_ZERO to calculate the hole.**

| Case | Block 1 (plug) | Block 2 | Plug A | Block 3 | Plug B | Qeq | Total resistance | base/case |
|---|---|---|---|---|---|---|---|---|
| base | 56635 | 158730 | 11151 | 10 | 57 | 400 | 226983 | 1.00 |
| fa5 | 56635 | 15873 | 11151 | 10 | 57 | 400 | 84126 | 2.70 |
| fa4 | 56635 | 1587 | 11151 | 10 | 57 | 400 | 69840 | 3.25 |
| fa3 | 56635 | 159 | 11151 | 10 | 57 | 400 | 68412 | 3.32 |
| fz5 | 17911 | 158730 | 3526 | 10 | 57 | 400 | 180634 | 1.26 |
| fz4 | 5664 | 158730 | 1115 | 10 | 57 | 400 | 165976 | 1.37 |
| fz3 | 1791 | 158730 | 353 | 10 | 57 | 400 | 161341 | 1.41 |
| fz5a5 | 17911 | 15873 | 3526 | 10 | 57 | 400 | 37777 | 6.01 |
| fz4a4 | 5664 | 1587 | 1115 | 10 | 57 | 400 | 8833 | 25.70 |
| fz3a3 | 1791 | 159 | 353 | 10 | 57 | 400 | 2769 | 81.96 |
| fz2a2 | 566 | 16 | 112 | 10 | 57 | 400 | 1161 | 195.53 |
| fz1a1 | 179 | 2 | 35 | 10 | 57 | 400 | 683 | 332.31 |

**Table 4** **Resistances in the different components in the system. Alternative 2, Z_AREA is used to calculate the plug and A_ZERO is used to calculate the hole.**

| Case | Block 1 (plug) | Block 2 | Plug A | Block 3 | Plug B | Qeq | Total resistance | base/case |
|---|---|---|---|---|---|---|---|---|
| base | 56635 | 158730 | 11151 | 10 | 57 | 400 | 226983 | 1.0 |
| fa5 | 17911 | 158730 | 3526 | 10 | 57 | 400 | 180634 | 1.3 |
| fa4 | 5664 | 158730 | 1115 | 10 | 57 | 400 | 165976 | 1.4 |
| fa3 | 1791 | 158730 | 353 | 10 | 57 | 400 | 161341 | 1.4 |
| fz5 | 56635 | 15873 | 11151 | 10 | 57 | 400 | 84126 | 2.7 |
| fz4 | 56635 | 1587 | 11151 | 10 | 57 | 400 | 69840 | 3.3 |
| fz3 | 56635 | 159 | 11151 | 10 | 57 | 400 | 68412 | 3.3 |
| fz5a5 | 17911 | 15873 | 3526 | 10 | 57 | 400 | 37777 | 6.0 |
| fz4a4 | 5664 | 1587 | 1115 | 10 | 57 | 400 | 8833 | 25.7 |
| fz3a3 | 1791 | 159 | 353 | 10 | 57 | 400 | 2769 | 82.0 |
| fz2a2 | 566 | 16 | 112 | 10 | 57 | 400 | 1161 | 195.5 |
| fz1a1 | 179 | 2 | 35 | 10 | 57 | 400 | 683 | 332.3 |

Comparison between the differences between the release rates, Table 2 and the calculated total resistances in the system from the source to Q1 given in Table 3 and 4. It can be seen that the second alternative gives a better correspondence. The conclusion is hence that in the beginning is the dimension for the hole given in Z_AREA and the dimension for the plug is given in A_ZERO. After the step in the function the dimensions for the hole and (probably) the plug are both given in A_LIMIT. The base for the code is that the area for the hole and the plug are equal and hence the user of the code must put in equal values for Z_AREA and A_ZERO.

In the study it has been noticed that there is a resistance inside the canister. It was then concluded that usage of the CANISTER_TYPE CUFE gives an internal plug with dimensions equal to the plug between the hole and bentonite and an effective diffusivity of $10^{-10}$ $m^2/s$. This canister type refers to an old copper/iron canister with granulated backfill material. The plug represents the transport through the granulated material. Usage of the CANISTER_TYPE LEAD_FILLED gives no resistance inside the canister wall and is recommended for future use.

## Concentration in the inner compartments

The concentrations of U-238 in the three inner compartments, i.e. the source, the hole and the bentonite compartment adjacent to the hole are discussed below. The concentration in the source is equal to the solubility limit during the whole studied time period. The concentration in the hole is given in Figure 8 and the concentration in the inner bentonite compartment is given in Figure 9.

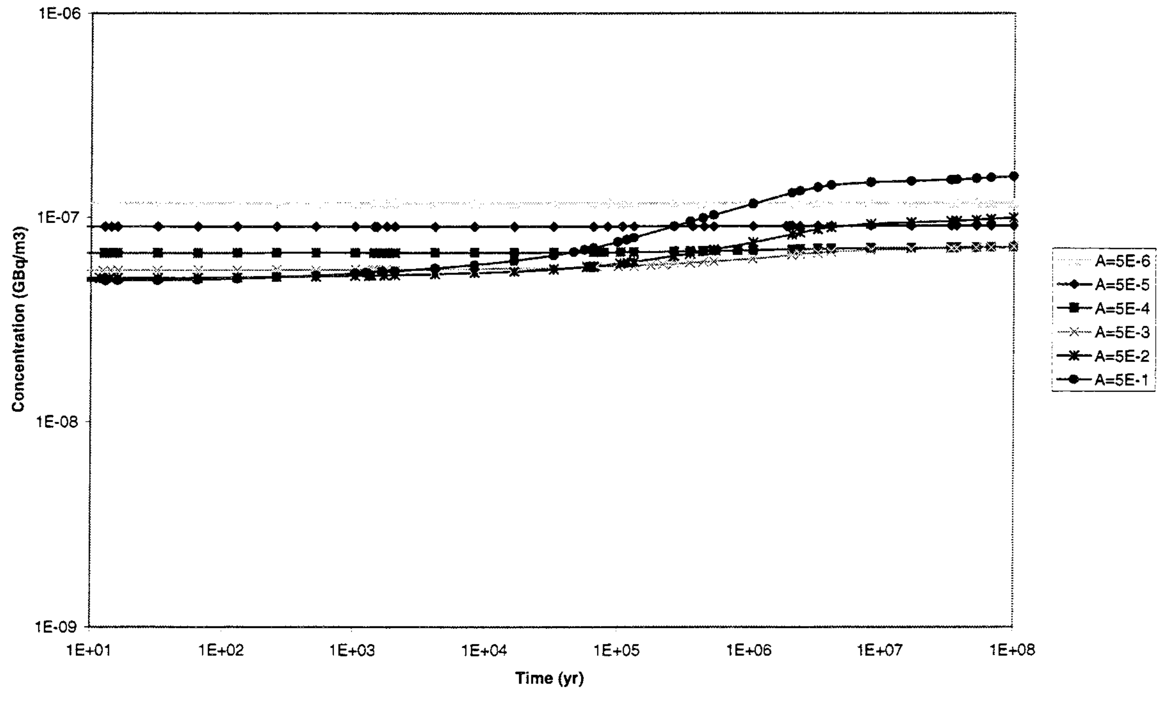


*Figure 8 Concentration of U-238 in the compartment representing the hole in the canister wall.*

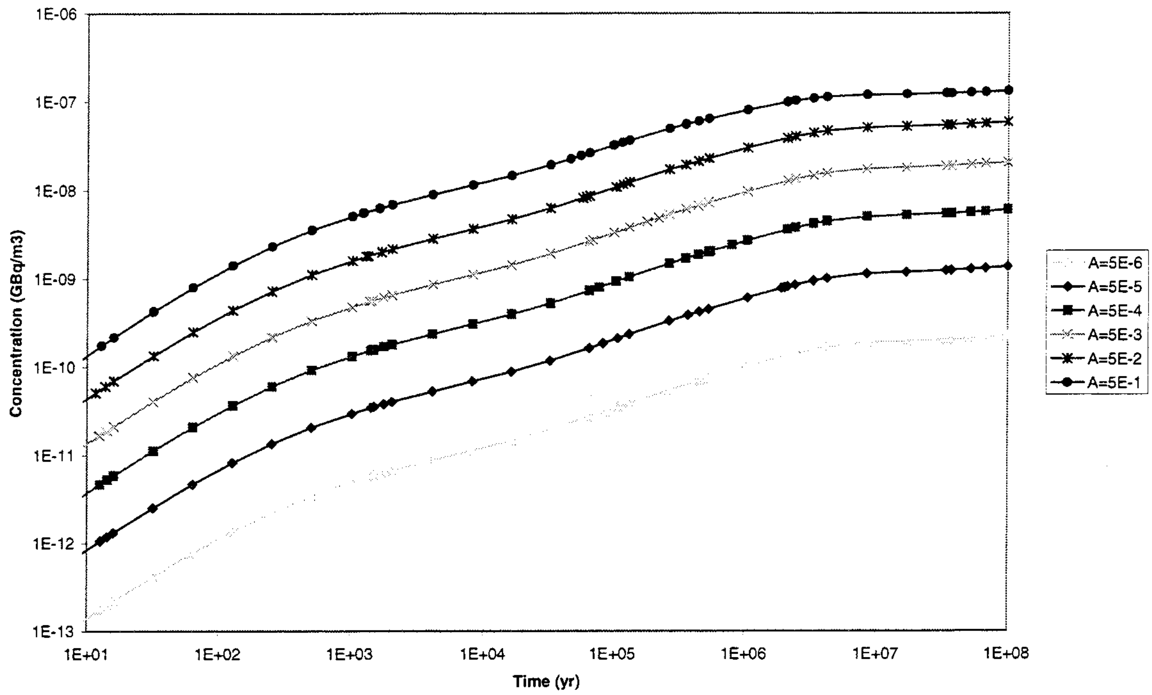


*Figure 9    Concentration of U-238 in the bentonite compartment adjacent to the hole.*

The concentration of U-238 in the hole varies only to a little extent depending on the different size of the area. The concentration in the beginning is dependent on the size of the hole, so that smaller holes result in higher concentration. This is due to the increased resistance in the connection to the bentonite for a smaller hole. If the hole is larger the concentration increases with time, this is due to the fact that the concentration in the bentonite in these cases are of the same size and hence the transport is slower and the concentration is built up.

The concentration of U-238 in the bentonite compartment adjacent to the hole show that the concentration is higher if the hole is larger. This is due to the smaller resistance in the system before this compartment if the hole is larger.

## Possible size of the hole

The theory for the connection between the hole and surrounding bentonite is based on Romero, 1995. Species diffusing out of a small hole into a very large volume of material spread out spherically. Very near the hole, the cross-section is still of the order of the size of the hole. Further away, the cross section increases considerably as the "sphere" grows. Thus, most of the resistance to diffusion is concentrated very near the mouth of the hole. This resistance is calculated by integrating the transport rate equation,

$$N = -2 \cdot \pi \cdot r^2 \cdot D_e \frac{dc}{dr},$$

from a small hemisphere into a very large volume, between the limits of the sphere radius $r_{sph}$ and an outer radius r. This result in:

$$N \cdot \left[ \frac{1}{r} - \frac{1}{r_{sph}} \right] = 2 \cdot \pi \cdot D_e \cdot \Delta c.$$

If $r >> r_{sph}$ the term 1/r is negligible in comparison to the term $1/r_{sph}$ and the transport rate is simplified to

$$N = 2 \cdot \pi \cdot r_{sph} \cdot D_e \cdot \Delta c.$$

In the model the real situation is approximated by using an equivalent plug. The transport equation for this plug is equal to the simplified transport equation for the case were $r >> r_{sph}$.

The usage of an equivalent plug in the connection between the small hole and large bentonite compartment is hence valid only if the hole is small compared to the surrounding bentonite. The thickness of the surrounding bentonite is 0.35 m. Assume a hole in the canister wall with an area of 0.001 $m^2$, corresponding to a radius of 0.02 m. This result in the fact that 1/r constitute 5 % of the term $(1/r - 1/r_{sph})$ and this value, 0.001 $m^2$ seems to be a reasonable limit for the size of the hole if the treatment with an equivalent plug should be valid. A larger hole overestimates the resistance between the hole and bentonite.

If a hole with an area larger than about 0.001 $m^2$ is to be modelled the surrounding bentonite should be divided into smaller compartments and the connection between the hole and the bentonite should not include a plug. However, in many cases with large hole the plug resistance is small compared to the total resistance and there is no need to take away the plug or change the discretization.

## References

Romero L. (1995): The Near-Field Transport in A Repository For High-Level Nuclear Waste, Ph. D. Thesis, Department of Chemical Engineering and Technology, Royal Institute of Technology, Stockholm, Sweden.

Romero L., Moreno L., Neretnieks I., Widén H., Boghammar A. (1997): Compartment model "NUCTRAN" (User´s manual), (in progress)

# APPENDIX A

## Description of the dimensions used for the discretization in COMP23

Block 1 is the internal of the canister, no transport resistance is assumed and hence both Z_LENGTH and R_LENGTH are equal to zero and Z_AREA and Z_LENGTH are equal to 1.

Block 2 is the hole in the canister wall. It is assumed to be a lying cylinder. No transport resistance is assumed in the radial direction and hence R_LENGTH is equal to zero and R_AREA is equal to 1. Z_LENGTH is the length of the hole, i.e. corresponding to the thickness of the canister wall, 0.05 m. Z_AREA is the diffusion area in the z-direction, $5\cdot 10^{-6}$ $m^2$.

Block 3 is the bentonite outside the hole. It has a shape of a standing cylindrical shell. The compartments are made with equal thickness of the cylindrical shells. The diffusion lengths in the radial direction R_LENGTH, i.e. from the hole to the fracture, Q1, are equal for all compartments, 0.35/6=0.058 m. The diffusion areas for the transport in the radial direction R_AREA are calculated as the envelope surface of the cylindrical shells, i.e. $2\pi(ry+ri)/2\cdot h$, where h is equal to Z_LENGTH. The transport in the z-direction is described by the diffusion length Z_LENGTH, which is assumed to be 0.5 m and by the diffusion area Z_AREA, i.e. the end surface of the cylindrical shells, $\pi(ry^2-ri^2)$. The parameters for the compartments in Block 3 together with the outer and inner radius are given in Table A-1.

**Table A-1 Dimensions used for the compartments in Block 3**

| Compartment number | Z_LENGTH | Z_AREA | R_LENGTH | R_AREA | Inner radie, ri | Outer radie, ry |
|---|---|---|---|---|---|---|
| 1 | 0.500 | 0.203 | 0.058 | 1.741 | 0.525 | 0.583 |
| 2 | 0.500 | 0.224 | 0.058 | 1.924 | 0.583 | 0.642 |
| 3 | 0.500 | 0.246 | 0.058 | 2.107 | 0.642 | 0.700 |
| 4 | 0.500 | 0.267 | 0.058 | 2.291 | 0.700 | 0.758 |
| 5 | 0.500 | 0.289 | 0.058 | 2.474 | 0.758 | 0.817 |
| 6 | 0.500 | 0.310 | 0.058 | 2.657 | 0.817 | 0.875 |

Block 4 is the bentonite outside the canister below the hole. It has the shape of a standing cylindrical shell. No transport resistance is assumed in the radial direction and hence R_LENGTH is equal to zero and R_AREA is equal to 1. The diffusion length in the z-direction, Z_LENGTH, is the height of the cylindrical shells. Two compartments were made, the upper with a height of 1 m and the lower with a height of 3.33 m. The diffusion area, Z_AREA, corresponds to the end surface of the cylindrical shell, $\pi\ (ry^2-ri^2) = \pi\ (0.875^2-0.525^2) = 1.539\ m^2$.

Block 5 is the bentonite above the canister. It has the shape of a standing cylinder and has been divided into three compartments, with equal heights. No transport resistance is assumed in the radial direction and hence R_LENGTH is equal to zero and R_AREA is equal to 1. The diffusion length in the z-direction, Z_LENGTH, is equal to the height, i.e. 0.5 m for each compartment. The diffusion area Z_AREA is the end surface of the cylinder, $\pi r^2 = \pi 0.875^2 = 2.405$ m$^2$.

Block 6 is the sand bentonite above the pure bentonite above the canister. It has the shape of a cylinder. Transport is assumed in both directions. In the radial direction the transport is described by the diffusion length R_LENGTH, that corresponds to the diameter of the cylinder, 1.75 m, and by the diffusion area R_AREA, that corresponds to the envelope surface of the cylinder $2\pi rh = 2\pi 0.875 \cdot 1 = 5.5$ m. The transport in the z-direction is described by the diffusion length Z_LENGTH that corresponds to the height of the cylinder, 1 m, and by the diffusion area Z_AREA corresponding to the end surface of the cylinder, $\pi r^2 = \pi 0.875^2 = 2.405$ m$^2$.

Block 7 is the sand bentonite in the tunnel. It has the shape of a lying cylinder. Transport is assumed in both directions. The diffusion length in the radial direction, R_LENGTH, has been assigned the value 2 m, this is a smaller value than the geometrical form of the tunnel gives, but the actual distance from the upper part of the deposition hole to the locations where the diffusing radionuclide can leave the tunnel is unknown. We have assumed 2 m, which is not overly conservative and about half of the maximum diffusion length to the top of the deposition tunnel. The diffusion area, R_AREA, has been calculated as the envelope surface for the outer diameter $2\pi rh = 2\pi 1 \cdot 2.125 = 26.7$ m$^2$, $2\pi 1 \cdot 1.75 = 22.0$ m$^2$ and $2\pi 1 \cdot 2.125 = 26.7$ m$^2$ for the three compartments respectively (**however some old figures were used and they may be corrected**). The total diffusion length in the z-direction, Z_LENGTH, corresponds to the distance between two canister holes and it has been divided into three compartments one above the canister hole with the length equal to the diameter of the canister hole, 1.75 m. The two other compartments have equal length 2.125 m i.e. (6 m - 1.75 m)/2. The diffusion area, Z_AREA, is calculated as the end surface area, i.e $\pi r^2 = \pi 2^2 = 12.566$ m$^2$ (**some old figures were used and they may be corrected**).

Block 8 is the bentonite below the canister. It has the shape of a short standing cylinder. The transport in the radial direction is neglected. The transport in the z-direction is described by the diffusion length Z_LENGTH, i.e. the height of the cylinder, 0.5 m, and the diffusion area Z_AREA i.e. the end surface of the cylinder, $\pi r^2 = \pi 0.875^2 = 2.405$ m$^2$.

Block 9 is the sand bentonite in the bottom of the canister hole. It has the shape of a standing cylinder. No transport is assumed in the radial direction. The transport in the z-direction is described by the diffusion length Z_LENGTH corresponding to the height of the cylinder, 3 m, and by the diffusion area Z_AREA corresponding to the end surface of the cylinder, $\pi r^2 = \pi 0.875^2 = 2.405$ m$^2$.