R-98-53

Equivalent flow rate concept used in near field transport model COMP23

– Proposed values for SR 97

L Moreno
Department of Chemical Engineering and Technology
Royal Institute of Technology

B Gylling
Kemakta Konsult AB

November 1998

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1402-3091
SKB Rapport R-98-53

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INTRODUCTION

SKB is using NUCTRAN to calculate transport of radionuclides from a possible defective canister into the far field. NUCTRAN is included in the Performance Assessment model chain that calculates the release from the canister into the biosphere. In the chain, NUCTRAN is denoted COMP23.

In order to calculate the transport of radionuclides by diffusion into the flowing water in the rock, NUCTRAN uses the concept of equivalent flow rate, Q_{eq}. To calculate the value of Q_{eq} in the different paths, COMP23 needs information about the Darcy velocity, the geometry of the system, material properties and the flow porosity in the rock. At present, this information is supplied to COMP23 by means of three parameters. The aim of this note is to propose a method to calculate the flow equivalent within the SR 97 project.

This note is an updated version of Moreno and Gylling (1997). A more detailed description of the concept, illustrations and revisions due to new data are presented. Estimated intervals of the factors to adopt HYDRASTAR results to COMP23 are presented. Since it is difficult to give general validity to the factors, solely proposed factor intervals are presented to obtain equivalent flow rate values for COMP23. To obtain accurate equivalent flow rate values, information about the hydraulic conditions at canister locations in the groundwater model should be available for the near field model or the Q_{eq} values could be calculated directly in the groundwater flow model.

One of the main tasks in the SR 97 project is to show the barrier performance of the rock using different alternative models for flow and transport. In addition, the Alternative Model Project (AMP) aims to show how robust the assessment model description is, in terms of relevant far field performance measures (Ström and Selroos, 1997). In the AMP, three main approaches were used, namely, the Stochastic Continuum approach (HYDRASTAR-FARF31), the Channel Network model (CHAN3D) and the Discrete Feature Network model (FRACMAN/MAFIC-PAWORKS). Since HYDRASTAR solely calculates one flux at the canister location, we have estimated factors to represent the flux in the paths modelled in the near field code NUCTRAN.

The factor A and the exponents presented here are denoted QEQ_FACTOR and QEQ_EXPONENT, respectively, in Romero et al. (1997). These parameters are used as input data to COMP23.

CONCEPTUAL MODEL

NUCTRAN calculates the non-stationary nuclide transport in the near field of a repository. The system is divided in compartments, where the only restriction is that a compartment is formed of the same material. The model, which is a very coarsely discretized Integrated Finite Difference Model, embeds analytical solutions at locations where other models require a very fine discretization such as entrances and exits from small holes and fractures. In the repository, radionuclides leaking out through a small hole in the canister wall diffuse into the clay and may then migrate through various pathways into the flowing water in rock fractures. Figure 1 shows four possible pathways from a canister/deposition hole:

- Q_1: Into a fracture intersecting the deposition hole, the fracture is located adjacent to the damage on the canister wall
- Q_2: Into a fractured section around the upper part of the deposition hole, the Excavation Disturbed Zone (EDZ) around the deposition tunnel
- Q_3: Into the backfill in the tunnel and further to a large fracture (or small zone) intersecting the deposition tunnel
- Q_4: Into a nearby fracture or fracture zone located below the deposition hole with “good rock” between.

The intersection between the fracture/fractures and the deposition hole and between a fracture/fracture zone and the deposition tunnel may cover the whole circumference or only a fraction of the circumference. In this note, it is assumed that whole circumference for deposition holes and deposition tunnels are in contact with flowing water.

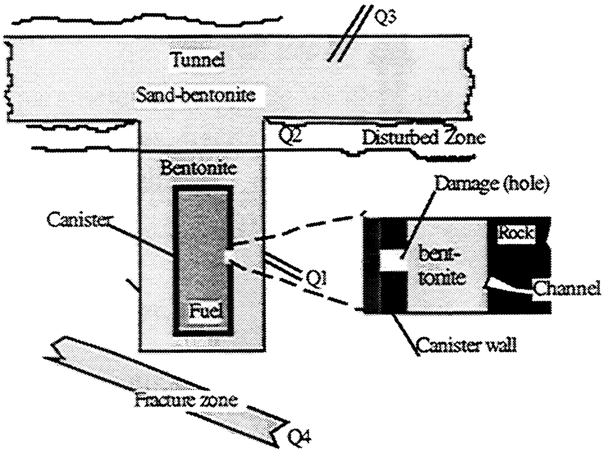

Figure 1. Schematic view of the KBS-3 repository design, showing the small hole in the canister and the location of the various possible transport path into near-field rock.

EQUIVALENT FLOW RATE CONCEPT

For compartments in contact with water flowing in fractures in the rock, the diffusive transport is determined by an equivalent flow rate Q_{eq}. This parameter is a fictitious flow rate of water that carries a concentration equal to that at the compartment interface. It has been derived by solving the equations for diffusional transport to the passing water by using boundary layer theory (Neretnieks, 1979). The value of Q_{eq} is dependent on the geometry of the contact area, the water flux, the flow porosity and the diffusivity. To illustrate the entities used in the definition of the equivalent flow rate, the water flow in the rock surrounding the deposition hole is shown in Figure 2. The Darcy velocity in the rock around the deposition hole is denoted U_0. The length of the water path is L. W in Equation 1 below is used to calculate the interface area for diffusion and equal to the height of the canister. In this case, since the water flows around both sides of the canister, 2W is used in the calculations.

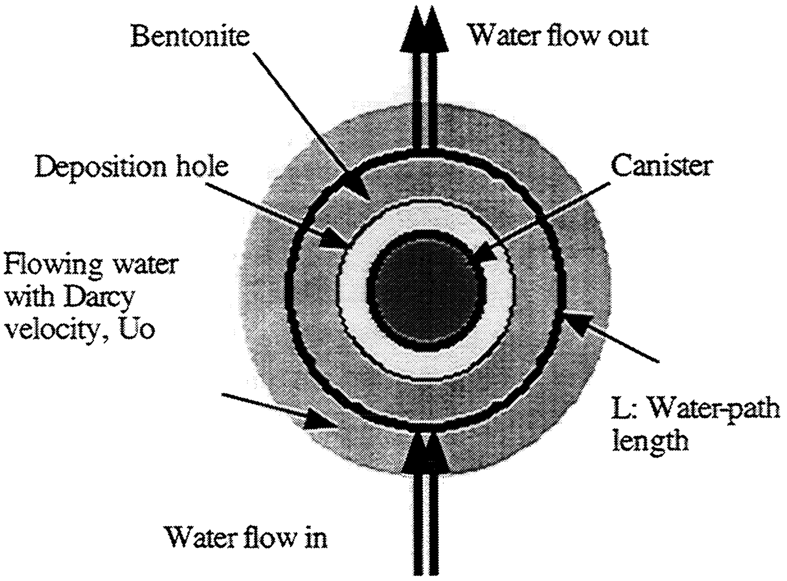

Figure 2. Schematic view of the water flow around in the rock surrounding the deposition hole.

To define the equivalent flow rate the following equation is used (Romero, 1995):

$$Q_{eq} = 2 \cdot W \cdot U_0 \cdot \bar{\eta} = 2 \cdot W \cdot U_0 \cdot \sqrt{\frac{4 \cdot D_w \cdot t_w}{\pi}} \tag{1}$$

The contact time with the flowing water is determined from the Darcy velocity U_0, the flow porosity ε_f, and the length of the pathway L in contact with the flowing water.

$$t_w = \frac{L \cdot \varepsilon_f}{U_o} \tag{2}$$

where:

U_o is the Darcy velocity (water flux) determined from HYDRASTAR, $[m^3/m^2/year]$

W is a geometric parameter used for the width of the surface area in contact with the flowing water in fractures, fracture zones, or EDZ, [m].

$\bar{\eta}$ is the mean thickness of the penetration in the fracture by diffusion from the compartment, [m]

D_w is the diffusivity in water, [m^2/year]

t_w is the time the water is in contact with the compartment, [year]

L is the length of the pathway in contact with the flowing water, [m]

ε_f is the flow porosity, [-]

IMPLEMENTATION IN COMP23

As discussed above, COMP23 requires the following input data:

- The geometry of the system
- The groundwater velocity and flow porosity in fractures intersecting the canister deposition hole, U_1 and ε_{f1}.
- The groundwater velocity and flow porosity in the disturbed zone, U_2 and ε_{f2}.
- The groundwater velocity and the flow porosity in a fracture zone intersecting the tunnel, U_3 and ε_{f3}.
- The groundwater velocity and flow porosity in a fracture zone close the deposition hole, but not intersecting it, U_4 and ε_{f4}.

At present only one groundwater velocity is used, the Darcy velocity U_o in the zone where the canister is located. The values for the different paths are calculated in function of this Darcy velocity. The procedure used is described below.

Introducing Eq. [2] into Eq. [1], Q_{eq} is expressed as the product of the squared root of the Darcy velocity and the coefficient A, defined in Eq. [4]. The coefficient A takes into account the Darcy velocities, the flow porosity, the nuclide diffusivity in the free water, and the geometry of the interface area.

$$Q_{eq} = 2 \cdot W \cdot \sqrt{U_0} \cdot \sqrt{\frac{4 \cdot D_w \cdot L \cdot \varepsilon_f}{\pi} \left(\frac{U_i}{U_0} \right)} = A \cdot \sqrt{U_0} \tag{3}$$

from Eq. [3] , the parameters A is defined

$$A = 2 \cdot W \cdot \sqrt{\frac{4 \cdot D_w \cdot L \cdot \varepsilon_f}{\pi} \left(\frac{U_i}{U_0} \right)} = f \cdot A_0 \tag{4}$$

U_o is the Darcy velocity in the rock surrounding the canister and it is obtained directly from HYDRASTAR at present. This flux is assumed to be representative for the rock mass. The value of the parameter A for the other pathways is determined by the Darcy velocity (assumed or calculated) in the rock where the actual pathway is located, U_i, and the length and width of the interface area for that pathway. The figure 2 in the equations above is due to that the water is assumed to flow on both sides of the deposition hole and tunnel.

In COMP23, the equivalent flow rate in each pathway is defined by using three values: the Darcy velocity, U_o, the exponent of the Darcy velocity in Eq. [3], in this case 0.5, and the coefficient A. In order to determine Q_{eq}, the value of the coefficient A is calculated for the different pathways. The Darcy velocity, U_o, is the same for all the pathways.

The value of the parameter A may be obtained directly from Eq. 4. It may also be expressed in function of A_o, the value for the parameter A in the pathway Q1. The parameter A_o is defined for a situation where the Darcy velocity is U_o, the flow porosity of the rock surrounding the deposition hole is 0.0001, the width of the contact surface area is 5m, i.e. approximately equal to the canister height, and the path length is 2.75 m,

$$A_0 = 2 \cdot 5 \cdot \sqrt{\frac{4 \cdot D_w \cdot 2.75 \cdot 0.0001}{\pi}} \tag{5}$$

The proposed intervals of the factor f are shown in Table 1 for the different pathways. For the EDZ, two situations are studied. A tunnel bored by using TBM (Tunnel Boring Machine) and a tunnel excavated by using drilling and blasting (Push et al., 1991; Olsson et al., 1996). The drill and blast method for tunnel construction is denoted DB in Table 1.

Table 1. Data for the different pathways. The first row corresponds to the case where A_o is defined:

	W_i (m)	L_i (m)	Flow Porosity ε_f	Water flux U_i, (m/year)	f
Path-Q1-ref.	5	2.8	0.0001	1.0 U_o	1.0
Path-Q1	5	2.8	0.0001-0.001	1-5 U_o	1-7
Path-Q2, TBM	1	2.8	0.0001 - 0.001	2-5 U_o	0.5-1.5
Path-Q2, DB	2	2.8	0.0003-0.001	10 – 100 U_o	2-15
Path Q3	2.5	7	0.001	100-1000 U_o	25-80
Path Q4	2.5	5	0.001	100-10000 U_o	20-220

Motivations for the values in Table 1

Path Q1 – The reference case

The reference case is based on a deposition hole located in rock mass of good quality with a normal fracture frequency. It is assumed that the flow porosity is 10^{-4}. For this path W_l is 5m. The geometric parameters W_l and L are illustrated in Figure 3.

Path Ql

It is assumed that the flow porosity may vary between 0.0001 and 0.001 around the deposition hole. A higher fracture density or fractures with a larger aperture may cause the larger value. The same reasons may explain the larger water flux. It is estimated that this may vary from the reference to five times the reference flux, U_0.

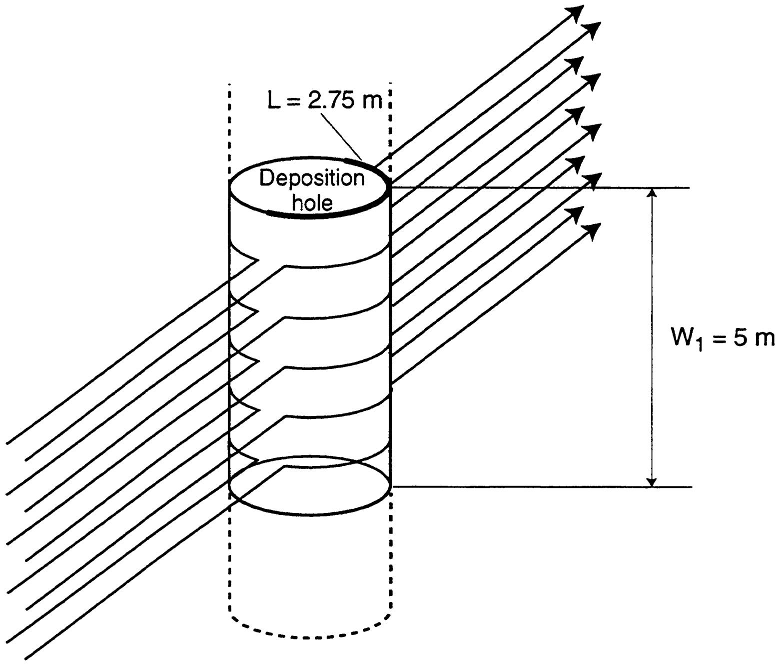

Figure 3. Schematic illustration of flow for $Q_{eq,1}$, around the deposition hole in the vicinity of the canister.

Path Q2, TBM

The values given in Table 1 have been revised according suggestions given in Rhén (1998). It is proposed that only 0.03 m around a TBM tunnel is damaged and the conductivity is increased by a factor 10-100 compared to the undisturbed rock mass. We have used a factor 100. A disturbed zone is also distinguished where the same hydraulic conductivity as for the undisturbed rock is proposed. The flux is estimated to be increased by a factor 2-5, calculated for a region of 1 m from the tunnel wall, compared to the reference flux. For this path W_2 is 1m. The geometry for path Q2 is shown in Figure 4.

Path Q2, DB (Drill and Blast)

In Rhén (1998), it is suggested that the damaged zone extends to about 2m from the tunnel wall with increased conductivity of a factor 10-100 compared to the rock mass. In addition, there is a region of disturbed rock that extends to about 4 m from the tunnel wall with the same conductivity as the rock mass. For a region of 2 m from the tunnel wall it is estimated that the flux may increase with a factor 10-100. A larger flow porosity is also assumed.

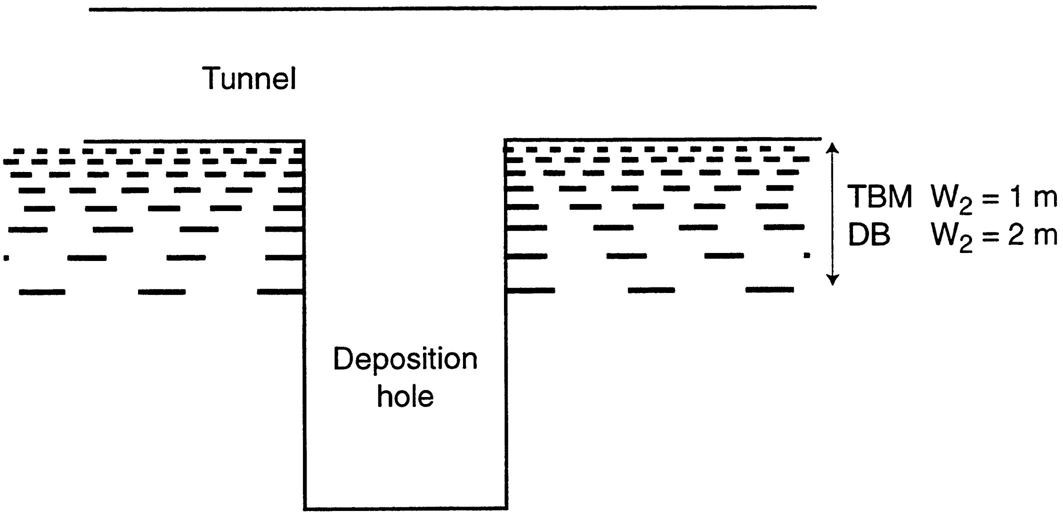

Figure 4. Schematic view of the damaged and disturbed zone for path Q2.

Path Q3

In the case of a possible fracture zone that intersect the deposition tunnel 3 m from the centre of the canister, it is estimated that the conductivity may increase with a factor 100-1000. If the situation would be worse (larger flow rate in the fracture zone), it is assumed that the particular location of the deposition hole is rejected. Due to the resistance to diffusion in bentonite and tunnel backfill, this path is normally of less importance. The geometry for path Q3, where W_3 is 2.5m, is shown in Figure 5.

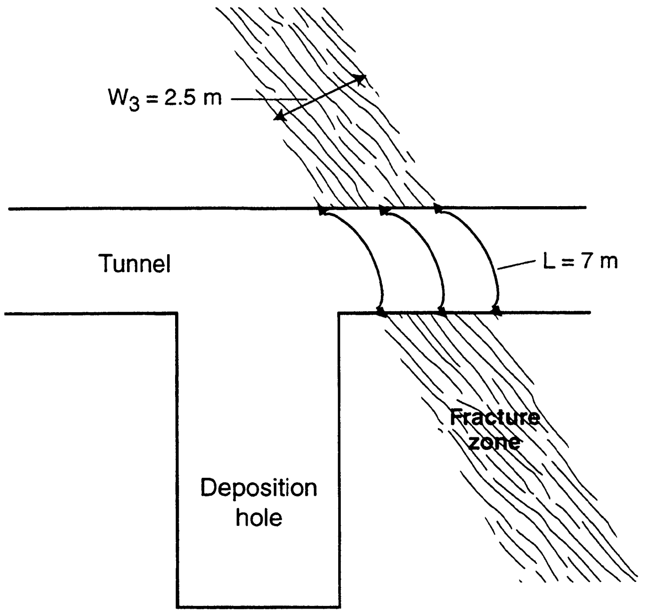

Figure 5. Illustration of the geometry for path Q3.

Path Q4

In the case of a fracture zone in the vicinity of the deposition hole (closest distance 5m), it is assumed that the flux may be increased with a factor of 100-10000. Due to the resistance to diffusion in the rock, this path is of less importance. Path Q4 is shown schematically in Figure 6. For this path is $W = 0.5W_4$ due to another geometry than the other paths. W_4 is assumed to be 5m.

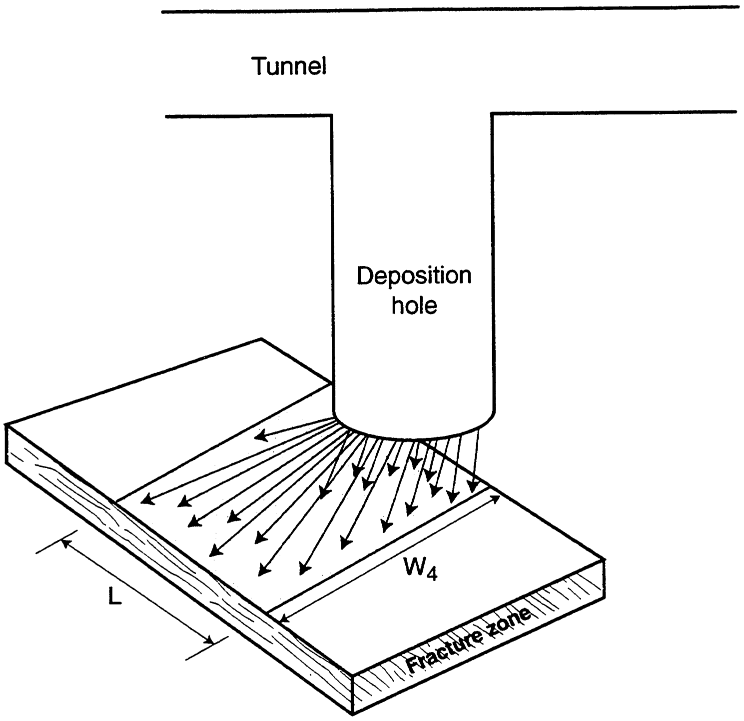

Figure 6. Simplified illustration of path Q4.

Example for a specific radionuclide: Uranium

A_0 is dependent on the diffusivity of the nuclide in water. For most of the radionuclides the water diffusivity is roughly between $1\text{-}3\cdot 10^{-9}$ m^2/s. For a specific radionuclide, e.g. uranium, the value of the water diffusivity is estimated to $1\cdot 10^{-9}$ m^2/s (Ohlsson and Neretnieks, 1997). The value of A_0 is then 0.034 m$^{2.5}$/year$^{0.5}$. This means that the factor A will also be radionuclide specific.

Table 2. Proposed intervals for the values of the factor $A = fA_0$ and the exponent used in the calculations of the Equivalent Flow rate. The same exponent of U_0 applies to all pathways.

	Proposed interval of A, $m^{2.5}/year^{0.5}$	Exponent
Path-Q1-ref.	0.03	0.5
Path-Q1	0.03 - 0.25	0.5
Path-Q2, TBM	0.01-0.05	0.5
Path-Q2, DB	0.1-0.5	0.5
Path Q3	1.0-5.0	0.5
Path Q4	1.0-10.0	0.5

The estimated intervals of the factor A for the different paths shown in Table 1 are given in Table 2 for Uranium, together with the exponent of the Darcy velocity. It is proposed to choose values within the intervals in Table 2 for use in SR 97.

The factor A and the Exponent of U_0 in Table 2 are denoted QEQ_FACTOR and QEQ_EXPONENT, respectively, in Romero et al. (1997) which are used input data to COMP23.

Simplifications for use in SR 97

Ohlsson and Neretnieks (1997) reports values of diffusion in water for radionuclides in the range from $0.15\text{-}2.0 \cdot 10^{-9}$ m^2/s. For radionuclides where data is lacking it is assumed that $D_w = 1 \cdot 10^{-9}$ m^2/s. Due to the many uncertainties in the data and in the adoption of HYDRASTAR data to the equivalent flow rate concept, it is proposed to use $D_w = 1 \cdot 10^{-9}$ m^2/s for all radionuclides within SR 97. This means, that the ranges of the factor A presented in Table 2 could be used for all radionuclides in the near field calculations, but ideally nuclides specific data should be used. The increase in the A-factors is about 40% for a case with $D_w = 2 \cdot 10^{-9}$ m^2/s.

Using a concept of best estimate and pessimistic values the Tables 3 and 4 are suggested for use in SR 97. The values are in addition discussed with Andersson (personal communication, 1998). It is also assumed that the construction technique is traditional drill and blasting for the deposition tunnels (Bäckblom, 1996). Suggested values for TBM tunnels are included.

Table 3. **Best estimate** values for the different pathways based on A_o = 0.034 $m^{2.5}/year^{0.5}$.

	Flow Porosity ε_f	Water flux U_i, (m/year)	f	A, $m^{2.5}/year^{0.5}$
Path-Q1	0.0001	1 U_o	1	0.03
Path-Q2, TBM	0.0001	2 U_o	0.5	0.01
Path-Q2, DB	0.0003	10 U_o	2	0.1
Path Q3	0.001	100 U_o	25	1.0
Path Q4	0.001	100 U_o	20	1.0

Table 4. **Pessimistic** values for the different pathways based on A_o = 0.034 $m^{2.5}/year^{0.5}$.

	Flow Porosity ε_f	Water flux U_i, (m/year)	f	A, $m^{2.5}/year^{0.5}$
Path-Q1	0.001	5 U_o	7	0.25
Path-Q2, TBM	0.001	5 U_o	1.5	0.05
Path-Q2, DB	0.001	100 U_o	15	0.5
Path Q3	0.001	1000 U_o	80	5.0
Path Q4	0.001	10000 U_o	220	10.0

DISCUSSION

In the present conceptualisation the different groundwater velocities are all derived as different multiples of the Darcy velocity of the deposition hole obtained from the groundwater flow solution. When using input from HYDRASTAR (Norman, 1992) the calculated Darcy velocity represents an average over the cell size, which typically is around 30 m. From sensitivity calculations by Romero et al. (1996), it is found that the Q_1 and Q_2 pathways dominate for almost any choice of Q_3 and Q_4. This means that the proper selection of U_3 and U_4 values is not very important and conservatively high values could be selected without jeopardising the barrier function of the near field. However, it would indeed be desirable to include realistic estimates of these flows.

For SR 97, the only possible alternative is to proceed along the previous practice. However, it would be indicated that more realistic flows should be used in future performance assessments. Evidently, at least the discrete network approaches should be able to provide more realistic values of the flows in these paths and this could be evaluated in future research studies. The discrete network approaches or theoretical studies could provide estimates of the number of deposition holes, which are not intersected by fractures, i.e. the path Q_1 is not present. In this case, only the path Q_2 is important. This information may potentially be used in for setting up calculation cases to COMP23.

In the present conceptualisation of COMP23, it is assumed that migration in the backfill is driven by diffusion and not advection. The water flow in the bentonite is expected to be very small, but can not be ruled out that water flow exists in some part of the backfill. Further research into this matter could be warranted. Another issue worth commenting on is the potential correlation between near field flow and retention properties of the far-field migration paths. It seems to make sense that high U_{nf} should be correlated to low F-ratios. Exploring such a correlation would potentially be important for the total consequences and for the potential gains of an active canister emplacement policy.

In the short run, i.e. for SR 97, the following action is recommended to:

- Produce conservative values of $U_1 - U_4$ based on U_{nf} and ε_f, but point out that more realistic estimates would be desirable, For future performance assessments it is recommended to:

- Provide estimates of U_{nf} and ε_f from all conceptual variants,
- Within e.g. the Alternative Models project evaluate the correlation between U_{nf} and F-ratio.
- Exploration of the possibilities of providing more realistic input to the COMP23 pathways from the detailed scale hydrogeological models should be contemplated as a future research option.

In a stochastic simulation the conductivity may vary in a wide range, depending on the used variance in the model. For the typical variances found in granite rock, the results from the HYDRASTAR simulations show, for some canister positions, very large water flux, U_0. This means that the upper limits proposed for the Darcy velocity, U_i, may be unrealistic. On the other hand if the Darcy velocity from the simulations, U_0, is too small the intervals proposed for U_i could be non-conservative.

A better measure of the equivalent flow rate would be to use the actual conductivity and hydraulic gradient at canister locations from the particular realisation used in the groundwater model or to calculate Qeq,i directly in the groundwater model by using discrete network model as for e.g. in CHAN3D.

A discussion has been held to obtain recommended values for use in SR 97. In this note, solely estimated ranges are proposed for the factors based on that suitable rock is used at the deposition holes.

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APPENDIX A

Derivation of the f-value used to relate $Q_{eq,i}$ to the reference

$$Q_{eq} = AU_0^{0.5}$$

A is rewritten as $A = fA_0$ where f is used to relate the specific case to a reference case and A_0 is obtained for the reference case.

$$A = 2 \cdot W \cdot \sqrt{\frac{4 \cdot D_w \cdot L \cdot \varepsilon_f}{\pi} \left(\frac{U_i}{U_0} \right)}$$

$$A_0 = 2 \cdot W_0 \cdot \sqrt{\frac{4 \cdot D_{w0} \cdot L_0 \cdot \varepsilon_{f0}}{\pi}}$$

Hence, the intermediate factor, f becomes:

$$f = \frac{W}{W_0} \sqrt{\frac{D_w L \varepsilon_f U_i}{D_{w0} L_0 \varepsilon_{f0} U_0}}$$

Data, reference values and assumptions

Table A1. Base for Table 1.

Parameter	Value	Unit
Canister height	4.833	m
Hole diameter	1.75	m
Half perimeter, L	2.75	m
Ref. flow porosity	0.0001	-

In the design, the height of the canister is 4.833m, which is approximated to 5m in these considerations. The geometric parameter 2W is 10m since it is assumed that the flow for path Q1 is surrounding the deposition hole. W in this case is used together with the half perimeter to determine the contact area between the deposition hole and the flowing water.