Hydrogeology Journal _ Electronic Supplementary Material

Simplified representative models for long-term flow and advective transport in fractured crystalline bedrock

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Text A1. Statistical DFN description of the sparsely fractured rock

The DFN descriptions of the sparsely fractured rock in the complex models are defined by Fox et al. (2007) for the SNF repository site, and by SKB (2013) for the LILW repository site. Fractures are idealized as circular disks of variable radius and orientation. The sparsely fractured rock is divided into different *fracture domains* (3-D volumes within each of which the fracture population is regarded as statistically homogeneous). Within each fracture domain, multiple *fracture sets* are defined, each of which has distinct statistical properties.

In all cases, the locations of fracture centers are located by a 3-D Poisson process. This results in fracture locations that are uniformly random in three dimensions, within a given fracture domain.
The density of fractures belonging to a given fracture set is governed by the fracture intensity measure P_{32} (total fracture area per unit volume).

For each fracture set, fracture radius r has a power-law distribution of the form:

$$f(r) = \frac{k_r r_0^{k_r}}{r^{k_r+1}}, r \geq r_0 \tag{A-1}$$

where r_0 is the minimum fracture radius for which the distribution is considered to apply, and k_r is an empirical constant that describes how rapidly the number of fractures decays with increasing radius. This distribution is considered to apply for values of r ranging from some minimum value r_{min} to a maximum value r_{max}.

Orientations of fractures are described in terms of the fracture poles (i.e. the normal vectors to each disk-shaped fracture). For each fracture set, the fracture poles are treated as following a Fisher distribution (Mardia 1972). This distribution is characterized by the mean pole direction (specified in geological coordinates as a trend and plunge) and a concentration parameter κ that describes the degree of clustering about the mean.

A1.1 DFN models for the SFN repository

Three main geometrical DFN alternatives were developed in the course of SKB's site descriptive modelling of the Forsmark side, to assess uncertainty in the statistical models for fracture size in relation to fracture intensity. For simplicity in the main body of this article, these are referenced as alternatives 1, 2, and 3, which correspond to the following names used by (Fox et al. 2007):

1. r_0-fixed alternative (base case)

2. "outcrop-scale" model + "tectonic-fault" model, or OSM + TFM alternative

3. "tectonic continuum" model, or TCM alternative

Each of these alternatives is defined for both of the fracture domains defined by Fox et al. (2007) as FFM01 and FFM06. The statistical properties are summarized in Tables A-1 through A-6. The names given to the different fracture sets by Fox et al. (2007) are here replaced with numbers in order to simplify the presentation.

A1.2 DFN models for the LILW repository

The hydrogeological DFN model for the LILW repository site as specified by (SKB 2013) is defined for three depth intervals:

Shallow domain: $z > -60$ m

Repository domain: $-60 \text{ m} \geq z > -200$ m

Deep domain: $-200 \text{ m} \geq z > -1100$ m

where z is the elevation relative to the mean sea level (RHB 70 datum). For the SRM analysis, only the repository domain is considered, as being most relevant for the properties of the rock mass at repository depth. Two alternative parametrizations of this model were given by SKB (2013), referred to as the "connectivity analysis" and "tectonic continuum" variants.

The hydrogeological DFN model is statistically parametrized in terms of an orientation distribution for each fracture set, together with a power-law model for fracture radius as defined above, and a logarithmic correlation of fracture transmissivity to fracture radius of the form:

$$T = \alpha r^{\beta} \quad \text{(A-2)}$$

The values of these parameters for the five fracture sets are listed in Table A-7. Equivalent hydraulic conductivity values calculated for 50-m blocks based on stochastic realizations of the two alternative parametrizations are compared in Figure A-1.

Text A2. Length-based scaling and area-based scaling of intersection probabilities

In the SRM of the rock mass for the SNF repository, a given fracture-deposition hole intersection ***X*** is assumed to have a uniform probability p_c of connecting to the nearest discharging HCD. Two different assumptions are considered regarding this probability, length-based scaling and area-based scaling, as explained below.

A2.1 Length-based scaling

Under this assumption, the frequency of transport paths per unit length of deposition hole, $P_{10,\mathrm{trans}}$, is assumed to be equal to the linear frequency of PFL anomalies that were encountered in the same fracture domain in deep boreholes:

$$P_{10,\mathrm{trans}} = P_{10,\mathrm{PFL,corr}} \tag{A-3}$$

This would be expected for a system in which the portions of PFL-anomaly fractures that carry significant flow are wide in relation to the diameters of both the boreholes and the deposition holes. In such a situation, the expected number of transport paths that intersect deposition holes is:

$$N_{\mathrm{trans}} = P_{10,\mathrm{trans}} L_{\mathrm{dh}} N_{\mathrm{dh}} = P_{10,\mathrm{PFL,corr}} L_{\mathrm{dh}} N_{\mathrm{dh}} \tag{A-4}$$

so the length-scaled probability of a given fracture/deposition-hole intersection being part of a transport path is:

$$p_{\mathrm{cL}} = \frac{N_{\mathrm{trans}}}{N_{\mathrm{X}}} = \frac{P_{10,\mathrm{PFL,corr}} L_{\mathrm{dh}} N_{\mathrm{dh}}}{N_{\mathrm{X}}} \tag{A-5}$$

where N_{X} is the total number of fracture/deposition-hole intersections in the repository section considered.

A2.2 Area-based scaling

In a strongly channelized fracture flow system where, within a given fracture, flow tends to be concentrated in channels of finite width, the length-based scaling assumption might not be conservative. If the typical flow-channel width is small relative to the deposition-hole diameter, then the probability of intersecting a given flow channel scales in proportion to the vertical cross-sectional area of the deposition holes vs. the boreholes, rather than just the length.

In the bounding situation where flow channels are effectively point flows, the frequency of transport paths that intersect deposition holes, per unit length of deposition hole, is related to the linear frequency in deep boreholes as:

$$P_{10,\mathrm{trans}} = P_{10,\mathrm{PFL,corr}} \frac{r_{\mathrm{dh}}}{r_{\mathrm{bh}}} \tag{A-6}$$

where r_{dh} is the deposition-hole radius and r_{bh} is the nominal radius of boreholes at repository depth.

In this bounding case, the area-scaled probability of a given fracture/deposition-hole intersection being part of a transport path is:

$$p_{\mathrm{cA}} = \frac{N_{\mathrm{trans}}}{N_{\mathrm{X}}} = \frac{P_{10,\mathrm{PFL,corr}} L_{\mathrm{dh}} N_{\mathrm{dh}}}{N_{\mathrm{X}}} \cdot \frac{r_{\mathrm{dh}}}{r_{\mathrm{bh}}} \qquad \text{(A-7)}$$

In practice, p_{cA} often exceeds 1, leading to the result that all fracture/deposition-hole intersections are treated as transmissive intersections.

Text A3. Transmissivity and aperture alternatives for the SNF repository

The three transmissivity variants considered are the perfectly correlated model (in which case transmissivity T is deterministically related to fracture radius r), the semi-correlated model (in which case T is logarithmically correlated to r), and the uncorrelated model (in which case T varies independently of r). These three variants are considered as separate calculation cases. All of these can be expressed in the general form of the semi-correlated model:

$$T = ar^{b} 10^{\sigma N(0,1)} \qquad \text{(A-8)}$$

where a, b, and σ are empirical parameters and $N(0,1)$ is a random value from the standard normal (Gaussian) distribution with zero mean and unit standard deviation.

For the case of the perfectly correlated model, $\sigma = 0$ so this reduces to:

$$T = ar^{b} \qquad \text{(A-9)}$$

For the case of the uncorrelated model, $b = 0$ so the general form reduces to:

$$T = a \cdot 10^{\sigma N(0,1)} \qquad \text{(A-10)}$$

or alternatively (SKB 2010):

$$T = 10^{\mu + \sigma N(0,1)} \qquad \text{(A-11)}$$

where $\mu = \log_{10}(a)$, so $a = 10^{\mu}$. The values of these parameters for the depth zone $z < -400$ m, are listed in Table A-8.

Transport-path apertures b_{T} are calculated based on specified correlations to transmissivity T, depending on the variant considered. Four variants have been considered in the present calculations (b_{T} expressed in units of m and T in units of $\mathrm{m^2/s}$, in all cases):

1. Empirical model based on data from Äspö, Sweden (Dershowitz et al. 2003) used here as a base case:

$$b_{\mathrm{T}} = 0.5T^{0.5} \qquad \text{(A-12)}$$

2. Stochastic model based on the Äspö model but with a half-order-magnitude standard deviation:

$$b_{\mathrm{T}} = 0.5 \cdot 10^{0.5N(0,1)} T^{0.5} \qquad \text{(A-13)}$$

3. Empirical model of Hjerne et al. (2010):

$$b_{\mathrm{T}} = 0.28T^{0.3} \qquad \text{(A-14)}$$

4. The cubic law which can be written as:

$$b_{\mathrm{T}} = \left(\frac{12\mu_{\mathrm{w}}}{\rho_{\mathrm{w}} g} \right)^{1/3} \cdot T^{1/3} \qquad \text{(A-15)}$$

where μ_{w} is the dynamic viscosity of water, ρ_{w} is the density of water, and g is gravitational acceleration.

Table A-1 Statistical parameters for DFN base case (r_0-fixed alternative), fracture domain FFM01. For all sets r_{min} = 3 m and r_{max} = 564.2 m.

Set	Mean pole trend (°)	Mean pole plunge (°)	Fisher concentration κ	r_0 (m)	k_r	P_{32} (m^{-1})
1	314.9	1.3	20.94	0.039	2.72	1.7330
2	270.1	5.3	21.34	0.039	2.75	1.2920
3	230.1	4.6	15.70	0.039	2.61	0.9480
4	0.8	87.3	17.42	0.039	2.58	0.6240
5	157.5	3.1	34.11	0.039	2.97	0.2560
6	0.4	11.9	13.89	0.039	2.93	0.1690
7	293.8	0.0	21.79	0.039	3.00	0.6580
8	164.0	52.6	35.43	0.039	2.61	0.0810
9	337.9	52.9	17.08	0.039	2.61	0.0670

Table A-2 Statistical parameters for DFN base case (r_0-fixed alternative), fracture domain FFM06. For all sets r_{min} = 3 m and r_{max} = 564.2 m.

Set	Mean pole trend (°)	Mean pole plunge (°)	Fisher concentration κ	r_0 (m)	k_r	P_{32} (m^{-1})
1	125.7	10.1	45.05	0.039	2.79	3.2990
2	91.0	4.1	19.49	0.039	2.78	2.1500
3	34.1	0.8	16.13	0.039	2.66	1.6080
4	84.3	71.3	10.78	0.039	2.58	0.6400
5	155.4	8.3	20.83	0.039	2.87	0.1940
6	0.0	47.5	12.71	0.039	2.61	0.4290

Table A-3 Statistical parameters for DFN alternative 2 (outcrop-scale model/tectonic-fault model), fracture domain FFM01.

For all OSM sets r_{min} = 3 m. For all TFM sets r_{min} = 28 m. For all sets r_{max} = 564.2 m.

Set	Mean pole trend (°)	Mean pole plunge (°)	Fisher concentration κ	r_0 (m)	k_r	Base case P_{32} (scaled) (m^{-1})
OSM-1	314.9	1.3	20.94	0.0385	2.60	0.0800
OSM-2	270.1	5.3	21.34	0.0385	2.90	0.0222
OSM-3	230.1	4.6	15.70	0.0385	2.44	0.0827
OSM-4	0.8	87.3	17.42	0.0385	2.61	0.0321
OSM-5	157.5	3.1	34.11	0.0385	2.20	0.0283
OSM-6	0.4	11.9	13.89	0.0385	3.06	0.0015
OSM-7	293.8	0.0	21.79	0.0385	3.00	0.0075
OSM-8	164.0	52.6	35.43	0.0385	2.61	0.0042
OSM-9	337.9	52.9	17.08	0.0385	2.61	0.0034
TFM-1	315.3	1.8	27.02	28	3.00	0.0285
TFM-2	92.7	1.2	30.69	28	2.20	0.0003
TFM-3	47.6	4.4	19.67	28	2.06	0.0003
TFM-4	347.4	85.6	23.25	28	2.83	0.0286
TFM-5	157.9	4.0	53.18	28	3.14	0.0871
TFM-6	186.3	4.3	34.23	28	2.85	0.0014

Table A-4 Statistical parameters for DFN alternative 2 (outcrop-scale model/tectonic-fault model), fracture domain FFM06.

For all OSM sets r_{min} = 3 m. For all TFM sets r_{min} = 28 m. For all sets r_{max} = 564.2 m.

Set	Mean pole trend (°)	Mean pole plunge (°)	Fisher concentration K	r_0 (m)	k_r	Base case P_{32} (scaled) (m^{-1})
OSM-1	125.7	10.1	45.05	0.0385	2.64	0.26800
OSM-2	91.0	4.1	19.49	0.0385	2.90	0.07390
OSM-3	34.1	0.8	16.13	0.0385	2.44	0.23280
OSM-4	84.3	71.3	10.78	0.0385	2.61	0.05720
OSM-5	155.4	8.3	20.83	0.0385	2.20	0.04130
OSM-6	0.0	47.5	12.71	0.0385	2.61	0.03840
TFM-1	315.3	1.8	27.02	28	3.00	0.02851
TFM-2	92.7	1.2	30.69	28	2.20	0.00034
TFM-3	47.6	4.4	19.67	28	2.06	0.00026
TFM-4	347.4	85.6	23.25	28	2.83	0.02861
TFM-5	157.9	4.0	53.18	28	3.14	0.08707
TFM-6	186.3	4.3	34.23	28	2.85	0.00138

Table A-5 Statistical parameters for DFN alternative 3 (tectonic continuum model), fracture domain FFM01. For all sets r_{min} = 3 m and r_{max} = 564.2 m.

Set	Mean pole trend (°)	Mean pole plunge (°)	Fisher concentration K	r_0 (m)	k_r	Base case P_{32} (unscaled) (m^{-1})
1	314.9	1.3	20.94	0.6592	3.02	1.7332
2	270.1	5.3	21.34	0.0593	2.78	1.2921
3	230.1	4.6	15.70	0.5937	2.85	0.9478
4	0.8	87.3	17.42	0.8163	2.85	0.6239
5	157.5	3.1	34.11	0.3249	3.25	0.2563
6	0.4	11.9	13.89	0.1700	3.10	0.1686
7	293.8	0.0	21.79	0.0385	3.00	0.6582
8	164.0	52.6	35.43	0.0385	2.61	0.0812
9	337.9	52.9	17.08	0.0385	2.61	0.0669

Table A-6 Statistical parameters for DFN alternative 3 (tectonic continuum model), fracture domain FFM01. For all sets r_{min} = 3 m and r_{max} = 564.2 m.

Set	Mean pole trend (°)	Mean pole plunge (°)	Fisher concentration K	r_0 (m)	k_r	Base case P_{32} (unscaled) (m^{-1})
1	125.7	10.1	45.05	0.3509	3.02	3.2987
2	91.0	4.1	19.49	0.0385	2.78	2.1504
3	34.1	0.8	16.13	0.3193	2.85	1.6078
4	84.3	71.3	10.78	0.7929	2.85	0.6396
5	155.4	8.3	20.83	0.7400	3.25	0.1940
6	0.0	47.5	12.71	0.0385	2.61	0.4294

Table A-7 Intensity, size and transmissivity distribution parameters of DFN model for the LILW repository domain ($-60 \geq z > -200$ m RHB 70) as specified by (SKB 2013).

Set	P_{32} (m^2/m^3)	Connectivity analysis			Tectonic continuum		
		k_r	α	β	k_r	A	β
1	1.44	3.1	$2.1\cdot10^{-9}$	1.1	2.63	$7.9\cdot10^{-11}$	1.4
2	0.81	3.0	$1.1\cdot10^{-8}$	1.1	2.596	$1.3\cdot10^{-9}$	1.1
3	1.00	3.3	$2.2\cdot10^{-9}$	1.3	2.752	$8.6\cdot10^{-11}$	1.35
4	1.21	2.72	$4.0\cdot10^{-9}$	0.80	2.72	$4.0\cdot10^{-9}$	0.80
5	0.95	2.55	$8.5\cdot10^{-10}$	1.35	2.55	$8.5\cdot10^{-10}$	1.35

Table A-8 Parameters of transmissivity models for the main fracture domain for depth $z < -400$ m, based on (SKB 2010).

Case	a (m^2/s)	$\log_{10} a$	b (-)	σ (-)
semi-correlated	5.3×10^{-11}	-10.3	0.5	1.0
correlated	1.8×10^{-10}	-9.7	0.5	0
uncorrelated	1.58×10^{-9}	-8.8	0	1.0

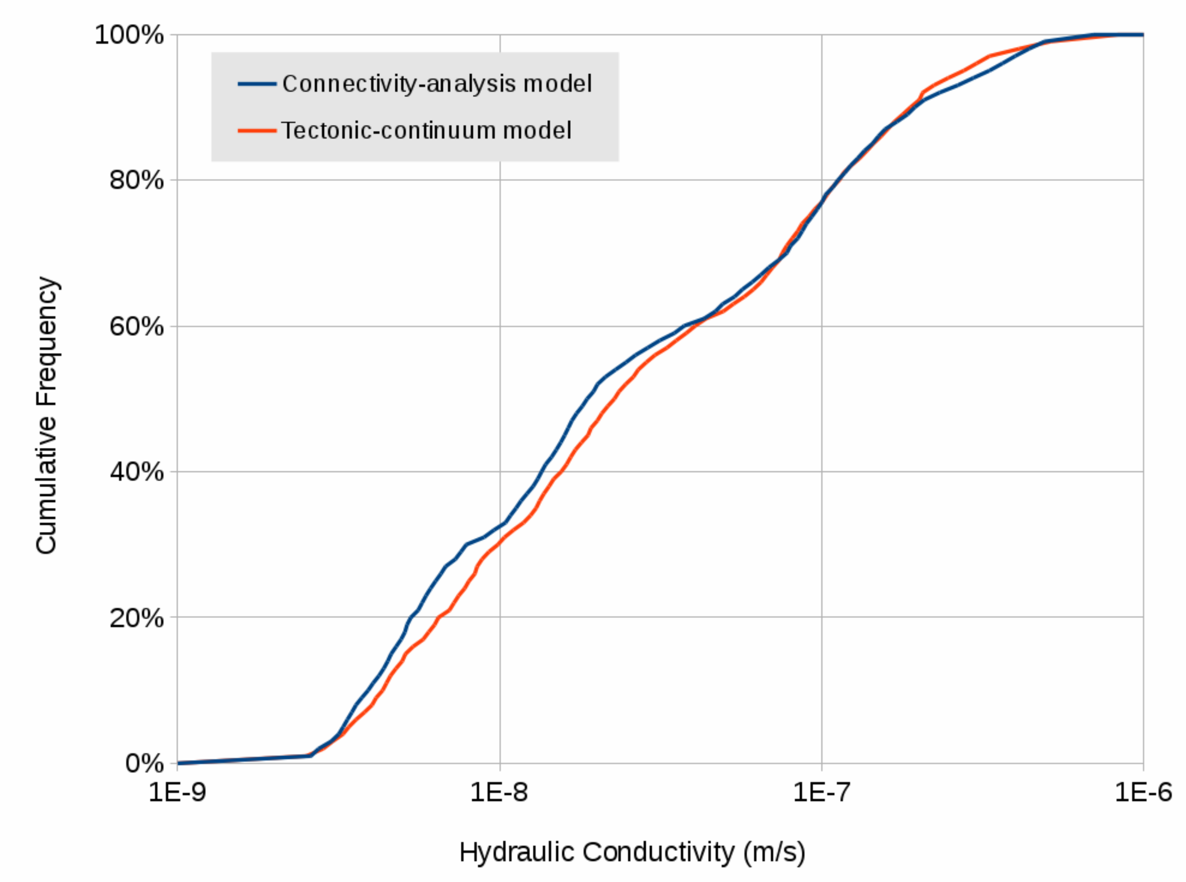

Figure A-1: Cumulative distributions of hydraulic conductivity at repository depths, calculated by geometric upscaling for 50-m scale blocks, for the two DFN parameterizations for the LILW repository site (connectivity-analysis and tectonic-continuum models). Hydraulic conductivity values for this plot are calculated as the geometric mean of the directional conductivities for each block, $K_g = (K_x\ K_y\ K_z)^{1/3.}$

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