APPLICATION OF A DISCRETE-FEATURE MODEL TO ASSESS GEOLOGICAL UNCERTAINTIES IN A REGULATORY CONTEXT

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Abstract

A discrete-feature model was used to integrate deterministic and stochastic geoscientific information, to support the Swedish regulatory authorities' review of SR-Can. The discrete-feature approach was used to replicate the main geometric features of the proponents' models of the two candidate sites, including: (1) deformation zones on scales of 1 km to 10 km which are treated deterministically, (2) deterministic rock domains, (3) discrete fractures on scales of 2 m to 1 km which are treated stochastically, (4) excavation-disturbed zones around repository tunnels, where the tunnels are adapted to the deformation zones, and (5) deposition holes which are adapted to each realisation of the stochastic fractures, to avoid fractures for which mappable characteristics would indicate unacceptable seismic or hydrologic risks. Application of this approach in the SR-Can review provided independent estimates of key safety parameters including utilisation factors (the percentage of usable deposition-hole positions in a given layout), distribution of groundwater flow to canisters, and retention properties and release points for discharge paths to the biosphere. These results were provided as input to a compartment model (AMBER) which was used for both deterministic and probabilistic risk calculations. Discrete-feature model variants were used to scope uncertainties in deformation-zone properties and boundary conditions, as well as the potential for enhanced transport due to spalling of deposition holes at one of the sites which has a strongly anisotropic stress field. This application showed that a discrete-feature model with realistic complexity can provide independent evaluation of key geoscientific factors for safety, in the regulatory context.

Introduction

The SR-Can safety assessment (SKB, 2006b) was based on preliminary designs for a KBS-3 spent-fuel repository which is planned to be located at one of two candidate sites on Sweden's Baltic coast, either Forsmark to the north of Stockholm, or Laxemar to the south (Figure 1). This was the first safety assessment based on site-specific data from these two sites. The next planned safety assessment, SR-Site, will form part of the license application to start underground construction for a repository. Thus SR-Can was an important chance for the Swedish authorities to evaluate how site-specific data can be utilised and integrated in the regulatory context.

The modelling study described here was performed in support of a review of SR-Can which was conducted jointly by the Swedish Nuclear Power Inspectorate (SKI) and the Swedish Radiation Protection Institute (SSI). In this study, a discrete-feature model was used to integrate deterministic and stochastic geoscientific information to simulate the hydrogeology of the two sites, and to describe potential paths for groundwater flow and radionuclide transport through fractured crystalline bedrock. More complete results were obtained for the Forsmark site than for Laxemar (for which modelling work is ongoing), so the Forsmark model is emphasised here.

Approach

The discrete-feature conceptual model represents deformation zones, individual fractures, and other water-conducting features around a repository as discrete conductors surrounded by a rock matrix which, in the present study, is treated as impermeable. This approximation is reasonable given the very low permeability of unfractured crystalline bedrock (mainly granite to granodiorite in the area of interest at Forsmark, and granite to monzonite at Laxemar).

Figure 1. Location of the Forsmark and Laxemar candidate sites in Sweden (adapted from SKB, 2006b)



The following main types of hydrogeologic features are included in the discrete-feature model for each of the candidate sites:

- Deformation zones on scales of 1 km to 10 km (treated as deterministic with regard to geometry).
- Discrete (natural) fractures on scales of 2 m to 1 km (defined as a stochastic population within a given rock domain).
- Excavation-disturbed zone around repository tunnels (defined deterministically by the repository layout).
- Deposition holes (adapted to each realisation of the stochastic fractures).

The geometry of the deterministic features, and of the rock domains within which the stochastic fractures are generated, are taken from the site descriptive models and repository designs that form the basis of the SR-Can safety assessment (SKB, 2005; 2006abc).

Representation of deformation zones

The deformation zones on scales of 1 km to 10 km are treated as piecewise-planar transmissive features that intersect in 3-D space. Figure 2 shows the deformation zones that are included in the site-descriptive model for the Forsmark site (SKB, 2005). The treatment of these deformation zones in the discrete-feature model is essentially the same as in the discrete-feature models used in the SITE-94 performance-assessment study (SKI, 1996; Geier 1996).

Representation of fractures

The natural fractures on scales of 2 m to 1 km are treated as a stochastic population of discshaped features, described by probability distributions for fracture size (disc radius), orientation, transmissivity, and location for a given rock domain, according to the statistical models defined in SKB site-descriptive models. The larger fractures in this population most likely represent minor deformation zones, rather than discrete, simple fractures, but the treatment of these by discrete, planar features is consistent with the treatment of larger deformation zones.

Figure 2. Deformation zones that are included in the 15 km × 11 km × 2.1 km deep site-descriptive model for the Forsmark site, viewed to the north (from SKB, 2005) Zones shown in darker shades of grey are considered to exist with high to medium confidence; pale grey zones are assessed as having a low level of confidence and are excluded from the base-case model of the site.



Representation of excavation-disturbed zone around repository tunnels

The excavation-disturbed zone (EDZ) around each tunnel in the repository layout, which results from various factors including blasting damage and stress concentrations, is idealised as four discrete features forming a tube of rectangular cross-section (Figure 3), at a distance approximately 1 m outside the tunnel wall. These features are considered to account for the permeability and porosity of the bentonite backfill within the tunnel, as well as the EDZ.

Placement of deposition holes

Deposition holes are represented explicitly as internal boundaries in the model. The locations of deposition holes are adapted to each realisation of the stochastic fractures, to avoid fractures for which

mappable characteristics would indicate unacceptable seismic or hydrologic risks. The criteria for accepting or rejecting a given deposition hole, as set forth in the SR-Can system description (SKB, 2006b), are implemented by explicit simulation of the subsurface mapping procedure was proposed in SR-Can (Figure 4), to identify potentially large fractures that are considered to pose an unacceptable seismic or hydrologic risk to a spent-fuel canister.



Figure 3. Discrete-feature representation of repository tunnels and EDZ

Figure 4. Simulation of deposition-hole placement based on full-perimeter intersection criterion used in the SR-Can safety assessment



Utilisation of deposition tunnels

Figure 5 shows an example of EDZ and deposition-hole features for one section of the repository at Forsmark, after applying these criteria with respect to one realisation of the stochastic fracture population. The degree to which repository tunnels can be utilised is measured as:

$$\varepsilon = \frac{N_{accept}l_{spacing}}{\sum_{i}L_{usable,i}}$$

where N_{accept} is the number of accepted positions, $l_{spacing}$ is the minimum distance between depositionhole centrelines (specified as a design criterion based primarily on rock thermal properties), and $L_{usable,i}$ is the "usable" length of the *i*th deposition tunnel (after subtracting the portions that are reserved for the plug at the start and for equipment clearance at the blind end of each tunnel). The utilisation factor ε is important for assessing the feasibility of a repository in a limited volume of rock, and thus this is a direct delivery to the safety-assessment review. Figure 5. Example of a repository layout for a portion (approximately 1/3) of a designed repository at the Forsmark site, with transport tunnels and deposition tunnels based on the SR-Can design layout, and canister positions (darker dots) conditioned to a realisation of the stochastic discrete-fracture model



Implicit representation of fractures as anisotropic block-scale conductivity

To reduce the computational burden for flow and transport calculations, the contributions of smaller and/or lower-transmissivity fractures to rock mass hydraulic conductivity are approximated by an orthogonal grid of block-scale features, while the larger and/or higher-transmissivity fractures are represented explicitly. The choice of which fractures to represent implicitly by block-scale features (rather than explicitly) depends on the distance from the deposition tunnels; details are given by Geier (2008).

The implicit contribution of a single fracture i to the block-scale hydraulic conductivity tensor **K** is calculated from Snow's law (Snow, 1969) which can be written in matrix form as:

$$\mathbf{K}_i = \frac{T_i}{s_i} [\mathbf{I} - n \otimes n]$$

where T_i is the fracture transmissivity, s_i is the effective fracture spacing, n is the a unit normal vector to the fracture plane, **I** is the 3x3 identity matrix, and $n \otimes n$ denotes the outer (tensor) product. The effective fracture spacing s_i is here taken as V/A_i where A_i is the area of the fracture that lies within the volume V of the rock block. After summing the contributions \mathbf{K}_i over all fractures that are represented implicitly, the resulting anisotropic tensor \mathbf{K} for a given block is represented by three orthogonal features, with transmissivity adjusted in different zones of the features to reproduce the diagonal components of \mathbf{K} .

Finite-element mesh assembly and flow calculations

The discrete features representing deformation zones, explicit fractures, anisotropic block-scale hydraulic conductivity (due to implicit fractures), EDZ around tunnels, and deposition holes as well as

surface topography are assembled in a triangular mesh that represents the geometry of the entire discrete-feature network (Figure 6). After imposing appropriate boundary conditions and hydraulic properties, the groundwater heads and fluxes within the discrete-feature network are computed by conventional finite-element techniques for uniform-density, steady-state fluid flow. Details of the numerical techniques are given by Geier (2005).

Figure 6. Close-up of plan view of finite-element mesh based on the assembled discrete features for Forsmark. Stochastic fractures are modelled explicitly for the immediate vicinity of the repository; the remaining fractures are represented implicitly by block-scale features (here seen as an orthogonal grid).



Calculation cases

For a given realisation of the discrete-feature model, calculations can be carried out for different boundary conditions and hydraulic properties within the discrete-features, representing different stages of climate evolution and/or uncertainty in the properties of the natural system. Variants were used to scope uncertainties in deformation-zone properties and temporally varying boundary conditions, as well as the potential for enhanced transport due to spalling of deposition holes due to the strongly anisotropic stress field at Forsmark; details are given by Geier (2008).

Flow rates to deposition holes

Groundwater flow rates to individual deposition holes are obtained as an immediate result of the finite-element computations. These flow rates are of direct relevance for safety assessment, as they can affect physical and chemical processes in the bentonite buffer (including bentonite erosion and colloid formation), canister corrosion, and transport of dissolved radionuclides away from the near-field in the event of a breached canister. Hence the computed flow rates to deposition holes are provided as input to the AMBER compartment model (Maul *et al.*, 2008) for independent consequence calculations in support of the authorities' review.

Characterisation of transport paths

Transport paths from deposition holes become important when canisters fail, either due to initial defects, or later events such as shearing during an earthquake or corrosion following buffer erosion. The potential for transport of radionuclides along these paths is characterised by advective-dispersive particle tracking in the discrete-feature network (see Geier 2005 and 2008 for details), and integration of various properties along the segments τ_i of a given particle trajectory. The most important of these properties for consequence calculations is the transport resistance:

$$F_r = \sum_{\tau_i} \frac{a_w(\tau_i) \Delta l}{v(\tau_i)} = \sum_i \frac{2\Delta t}{b_T(\tau_i)}$$

where Δl and Δt are the increments of distance and time, b_T is the transport aperture in a given feature segment, $a_w = 2/b_T$ is the local wetted surface per unit volume water, *T* is the local transmissivity, and $v = \Delta l/\Delta t$ is the magnitude of the local advective velocity. Integrals of *F* and other path properties are calculated for each class of features traversed (deformation zones, fractures, *etc.*) as well as for the entire path from the deposition hole to the surface.

The local fluid velocity and aperture at the source are also recorded, along with the exit location which can subsequently be related to the biosphere receptor (lake, sea, mire etc.) in the landscape for risk calculations. For detailed models of transport along streamlines, the properties of features traversed by each particle are also recorded. These data are provided as input for independent consequence calculations using the AMBER compartment model (Maul *et al.*, 2008).

Principal results

Utilisation factors

Mean utilisation factors calculated for Forsmark and Laxemar were 70% and 53% respectively. Both of these values are significantly lower than the corresponding values for comparable cases presented in SR-Can. The discrepancy appears to be at least partly due to non-conservative simplifying assumptions of the approach used in SR-Can, but finite-domain effects in the discretefeature model may also be a factor. Further investigation is needed to resolve this issue.

Flows to deposition holes

Distributions of flows to deposition holes for the Forsmark base-case model and the variants that were analysed for SR-Can review are shown in Figure 7. Variation between realisations of the stochastic fracture population (DFN) appears to be minor. The distribution of flow to deposition holes is robust with respect to the set of variants considered. Note however that these variants did not include alternative conceptual models for the DFN, or variants with respect to its key properties, such as a correlation of size to transmissivity.

Figure 7. Distribution of flow rates to deposition holes for the Forsmark Base Case model, late temperate climate (Variant cT), present-day temperate climate (Variant cTS), the uniform deformation-zone transmissivity variant (Variant c), and spalling variants (Variants cspT and cspxT). Results are shown for two realisations of the base case (R1 and R2) and for a single realisation (R1) of the other variants



The flow distribution to deposition holes is not very sensitive either to the hydrologic properties of the large-scale deformation zones or the time-dependent boundary conditions in a temperate setting. The main controls on this distribution appear to be the DFN submodel, the excavation-damaged zone

(EDZ) around tunnels, and spalled zones in the deposition-hole walls (if present).

Properties of transport paths

Particle-tracking results have been produced only for Forsmark, in the work thus far. A continuous EDZ intersecting all deposition holes and extending along all repository tunnels is included in all Forsmark variants, and turns out to be a dominant feature for flow and transport, due to the apparent sparseness of the fracture population in the repository volume. It was found that transport paths originating at one deposition hole often pass through other deposition holes along their way to the surface, because of the dominance of the EDZ.

Distributions of transport resistance F for the Forsmark base-case model and variants are shown in Figure 8. The safety-critical lower portion of the distribution of F is not strongly sensitive to most of these variants. Spalling around deposition holes produces a slight increase in F due to increased porosity and wetted surface at the start of each release path. This result is likely sensitive to the assumptions regarding hydraulic properties of the spalled zones, which have been arbitrarily specified for lack of relevant data. Further investigation of the sensitivity of the F distribution to assumptions regarding these parameters is warranted. The lower end of the F distribution is also sensitive to stochastic realisations of the DFN submodel. This suggests that further attention to major conceptual uncertainties in the DFN submodel (e.g. the possibility of clustering or hierarchical structure) is warranted.

Figure 8. Distribution of *F* for discharge paths from deposition holes to the surface, for the Forsmark Base Case model, late temperate climate (two realisations, Variant cT), uniform deformation-zone variant (Variant c), spalling variants (Variants cspT and cspxT), and mid-temperate climate (Variant cTS). Results are shown for two realisations of the base case (R1 and R2) and for a single realisation (R1) of the other variants



Cumulative fraction

Discharge locations in the surface environment

Figure 9 shows two examples of the surficial discharge locations for potential radionuclide transport paths originating from deposition holes. Stochastic variability in the DFN submodel, variability in large-scale deformation zone properties and future climate states are all found to influence which parts of the repository produce the fastest arrivals, and where these arrive in the biosphere.

Figure 9. Example of spatial distribution of release points for nonreactive solute from a repository at the Forsmark site

(advective-dispersive transport in the absence of matrix diffusion or other retention mechanisms), calculated for (a) latetemperate period base case and (b) uniform-transmissivity variant. Plan view showing source canister locations (tiny dots) and arrival locations (larger squares. Grid lines are at 1 km increments. The thick, pale grey line represents the coastline of the mainland and offshore islands at Forsmark, with the open waters of the Baltic toward the upper right-hand corner (northeast)



Figure 9. Example of spatial distribution of release points for nonreactive solute from a repository at the Forsmark site (Cont'd)



None of the model variants thus far have included large-scale heterogeneity within deformation zones. Based on previous analysis (SKI, 1996), discrete-feature models that incorporate large-scale, spatially correlated properties within deformation zones can be expected to exhibit greater large-scale heterogeneity, with more chance for extreme, low-F pathways, and thus should be considered for further analysis.

Conclusions

Application of the discrete-feature approach in the SR-Can review yielded independent estimation of key safety parameters including utilisation factors, distribution of groundwater flow to canisters, and, in the event of canister failure, the retention properties of discharge paths and release points in the biosphere.

Experience with application of the discrete-feature approach in SR-Can review showed that a model with realistic complexity can be used to provide independent evaluation of key geoscientific factors for repository safety, in the regulatory context. Some limitations of the approach with respect to computational resources were encountered, which required (1) simulation of just one-third of each repository layout at a time, (2) upscaling of discrete-fracture network properties over most of the model volume by means of an equivalent-continuum approximation, and (3) limited number of realisations. Although advances in software and computer technology may alleviate these limitations to some extent, it must also be expected that site models advanced by repository proponents in the future will also grow in complexity to take advantage of technological advances. Hence it should be expected that regulators will always need a strategic approach for applying such models in a review context.

This application showed that a discrete-feature model with realistic complexity can provide independent evaluation of key geoscientific factors for safety, in the regulatory context. However, the scope of application was limited by the computational requirements of the approach. Hence, although some improvements in efficiency are foreseen, it is expected that regulators will need a strategic approach for deploying such models in a review context – that is, using these models to focus on particular issue of concern rather than attempting to fully replicate a probabilistic safety assessment.

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