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REVIEW OF SPATIAL VARIABILITY IN PERFORMANCE ASSESSMENTS
MILESTONE (N°:M2.2.D.1)

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Foreword

The work presented in this report was developed within the Integrated Project PAMINA: **P**erformance **A**ssessment **M**ethodologies **IN** **A**pplication to Guide the Development of the Safety Case. This project is part of the Sixth Framework Programme of the European Commission. It brings together 25 organisations from ten European countries and one EC Joint Research Centre in order to improve and harmonise methodologies and tools for demonstrating the safety of deep geological disposal of long-lived radioactive waste for different waste types, repository designs and geological environments. The results will be of interest to national waste management organisations, regulators and lay stakeholders.

The work is organised in four Research and Technology Development Components (RTDCs) and one additional component dealing with knowledge management and dissemination of knowledge:

- In RTDC 1 the aim is to evaluate the state of the art of methodologies and approaches needed for assessing the safety of deep geological disposal, on the basis of comprehensive review of international practice. This work includes the identification of any deficiencies in methods and tools.
- In RTDC 2 the aim is to establish a framework and methodology for the treatment of uncertainty during PA and safety case development. Guidance on, and examples of, good practice will be provided on the communication and treatment of different types of uncertainty, spatial variability, the development of probabilistic safety assessment tools, and techniques for sensitivity and uncertainty analysis.
- In RTDC 3 the aim is to develop methodologies and tools for integrated PA for various geological disposal concepts. This work includes the development of PA scenarios, of the PA approach to gas migration processes, of the PA approach to radionuclide source term modelling, and of safety and performance indicators.
- In RTDC 4 the aim is to conduct several benchmark exercises on specific processes, in which quantitative comparisons are made between approaches that rely on simplifying assumptions and models, and those that rely on complex models that take into account a more complete process conceptualization in space and time.

The work presented in this report was performed in the scope of RTDC 2.

All PAMINA reports can be downloaded from http://www.ip-pamina.eu.

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Review of Spatial Variability in Performance Assessments

In contrast to engineered systems, the geosphere shows a strong spatial variability of facies, materials and material properties. Although this phenomenon can be interpreted as a specific type of (statistical) variability, it also results in (often considerable) uncertainties when describing and modelling a site and its hydrogeological setting. While the presence / absence of facies and their properties is often known at specific locations (outcrops, exploration drillings), the remaining larger part of the domain of interest remains unknown. Moreover, reducing uncertainties by means of drilling might result in adverse impacts on the safety functions to be performed by the geosphere and should therefore be planned with caution. Model assumptions can be made on the basis of borehole and outcrop interpretation, of geophysical measurements, but also on other (often called "soft") information, e.g., about site genesis. Such assumptions are either made "manually" based on expertise or by using mathematical models describing the evolution of a site. In both cases, however, the remaining uncertainties are not quantifiable.

Geostatistical methods provide means for uncertainty quantification but are rather weak with regard to the incorporation of "soft knowledge". Although it is recognised that the utilisation of geostatistical methods in hydrogeology might contribute to a consistent treatment of uncertainties in probabilistic safety assessments, most existing PAs are still based on manually-derived hydrogeological models. Some attempts to utilise geostatistical methods have been undertaken (e.g., (LaVenue, et al., 1992); (Zimmerman, et al., 1998); (Jaquet, et al., 1998), (Jaquet, et al., 2006); (Röhlig, et al., 2005); (Srivastava, 2007)), and these and other examples are compiled and compared.

1 General Remarks

In the frame of post-closure safety analyses for radioactive waste repositories several types of uncertainties have to be taken into account due to the complexity of the phenomena of concern and the large timeframes under consideration. During the last two decades, remarkable progress has been made in the development of deterministic and probabilistic methodologies for the treatment especially of parameter uncertainties, but also for the handling of scenario and model uncertainties. Provided that the uncertainties in question can be expressed using random variables in an adequate manner, probabilistic techniques generate estimates for the resulting uncertainties of performance indicators and give insight into the relevant processes by identifying key ("sensitive") entities. One of the advantages of such probabilistic techniques is their ability to fully explore the space of uncertain parameters and to widely cover possible parameter combinations.

It seems however conceptually difficult to address spatial variability of the geosphere and resulting uncertainties consistently in probabilistic safety assessments. Problems arise due to the wide variety of qualitatively different information sources (exploration drillings, outcrops, geophysics, knowledge of site genesis, pumping and tracer tests, etc.). Traditionally, models are derived "manually" from the available geological and hydrogeological information. This allows accounting for the variety of "soft" information and knowledge which is typical of geosciences but also causes a certain degree of subjectivity. In any case, the traditional approach usually results in one "best estimate" image of reality (or, at the most, in a very limited number of "variant" images). With the rapidly growing capacities and capabilities of electronic computing, it became manageable to derive geological and hydrogeological models of great complexity based on geomathematical algorithms. It became also feasible to generate a multitude of realisations for a model domain of concern which is an essential prerequisite for accounting for the associated uncertainties in probabilistic assessments.

In their review of methods Koltermann & Gorelick (Koltermann, et al., 1995) distinguish between

- structure-imitating methods,
- process-imitating methods, and
- descriptive methods,

the “traditional” approach belonging to the latter. Although the review is restricted to sedimentary basins, the categorisation seems to be applicable to crystalline formations as well.

According to (Koltermann, et al., 1995), structure-imitating methods comprise spatial statistical methods and sedimentation pattern methods. The former interpret reality as a realisation of a random function (of position), while the latter model the temporal evolution of sedimentation patterns, but without accounting for flow processes or transport of sediments. Statistical methods are able to produce best-estimates as well as series of realisations, both for so-called categorical (discrete) variables (indicating the presence or absence of stratigraphic, petrographic, hydrogeological, or other units) and continuous variables (for entities such as permeability or porosity). They can account for “hard” information coming, e.g., from borehole logs. In contrast, sedimentation pattern methods generate single realisations (best estimates) for categorical variables based on “soft” information.

Process-imitating methods imitate either groundwater flow processes or geologic processes. Under the former category, summarise “aquifer model calibration methods”, i.e., inverse approaches. There exists a variety of geologic process models, accounting for phenomena such as flow processes, transport of sediments, tectonics, climate changes, changes of sea level, etc. These models generate single realisations (best estimates) for continuous variables based on “soft” information.

In the opinion of the authors of this paper, the categorisation by (Koltermann, et al., 1995) is comprehensive although one might argue about details. E.g., it seems that sedimentation pattern methods are more closely related to geologic process models than to aquifer model calibration methods since both methods, sedimentation pattern methods as well as geologic process models, attempt to model site generation while aquifer model calibration models are concerned with a different kind of process (groundwater flow). Moreover, aquifer model calibration models in most cases do not work from scratch but require the existence of an initial model which has to be generated by means of one of the other methods as, e.g., in (Zimmerman, et al., 1998).

Given the specific context of our work (performance and safety assessment), we suggest a categorisation somewhat deviating from (Koltermann, et al., 1995) with regard to statistical methods. There, a distinction between Kriging, Gaussian, and non-Gaussian methods (the latter comprising indicator methods, simulated annealing, Boolean methods, and Markov chains). We propose to distinguish either

- by the type of result to be produced ([best] estimate vs. multiple realisations), or
- by the underlying models for the random functions in use.

In the latter case, models such as

- spatial co-variance / variogram (“classical” geostatistics),
- objective functions (simulated annealing),
- marked point processes (Boolean models, e.g. fracture networks), and
- transition probabilities (Markov chains)

can be identified.

In this study we have compiled a list of articles and reports dealing with geostatistical methods in the light of performance assessment. We focused on methods with the potential to account for variability and resulting uncertainty in probabilistic analyses, i.e., on the statistical methods in Koltermann & Gorelick’s categorisation. Nevertheless, not all of the reports and articles reviewed explicitly strive for feeding probabilistic analyses.

Both estimate (kriging) and multiple realisation methods (simulation) are considered. The underlying models are either of the variogram type with the objective of estimating and/or simulating spatial distributions of facies and/or parameters or Boolean with the objective of simulating fracture networks. Upscaling methods have been comprehensively dealt with elsewhere in PAMINA's work package 2.2.D (Milestone 2.2.D.2).

We connect the considered reports with the safety functions related to the layout of the repository under consideration. All papers discuss the modelling of the groundwater flow, so that the safety function under consideration is the delay or attenuation of radionuclide migration in the host rock or the overburden. We also study if the articles deal with a normal evolution scenario or with alternative scenarios (glaciation, leakage, human intrusion by drilling through the repository). A third item of attention is whether validation / calibration techniques have been applied to strengthen the confidence in the used model.

In the reviewed papers, the following three approaches can be identified to model the spatial variability and heterogeneity:

- Direct simulation of hydraulic conductivity, sorption, etc.
- Distribution of strata (binary approach): clay / silt, sand / salt, etc.
- Simulation of fracture networks

These approaches may be mixed to form realistic models. For example, first a material type is determined per grid element, and then the material properties are varied within certain boundaries prescribed by the material type. Or, lower-dimensional fracture networks are included in an otherwise continuous porous media model.

2 Compilation of examples

With the rapid development of computing power in the last decades the usage of geostatistically generated distributions of permeabilites or transmissivities in hydrogeological models became more and more practicable (Delhomme, 1979), (Ahmed, et al., 1987), (Gelhar, 1993), (Gutjahr, et al., 1993). Although the potential of these methods for the assessment of the log-term safety of repositories was known (Bonano, et al., 1993), steps into the development of such an approach were only taken reluctantly. As a notable exception, the studies conducted within the WIPP project take up this development. Remarkably, the performance assessments conducted within the licensing process were based on probabilistic calculations of geostatistical models, see Section 2.1.

Geostatistical methods were also used in studies for locations in Sweden (Section 2.3), Switzerland and France (Section 2.4). Studies conducted in Germany at the Gorleben site are considered in Section 2.2. For literature on the simulation of fracture networks carried out for locations in Sweden, Belgium, and Canada see Section 2.5.

An overview of the studied literature can be found in the table below.

Reference	Location	Target	Remarks
(Porter, et al., 1997), (Röhlig, 1999)-(Röhlig, et al., 2005)	Gorleben (Salt): – sedimentary overburden	Modelling of heterogeneities Handling of incomplete geospatial knowledge	Geostatistics 3D, modelling 2D vertically, scale 10^4 x 10^2 m^2, stepwise integration of different information types, probabilistic for fresh water calculations, iterative approach to density flow
(LaVenue, et al., 1992), (LaVenue, et al., 1995), (Capilla, et al., 1998), (Beauheim, et al., 2007)	WIPP (Salt): overlying beds	Modelling of heterogeneities Handling of incomplete geospatial knowledge Derivation of local sensitivities regarding ground water travel times→ location of new wells	2D horizontally, scale 10^4 x 10^4 m^2, probabilistic in licensing procedure (US DOE, 1996), (US DOE, 2004), later works not for compliance, but for supporting geological understanding in the safety case, calibration with ground water heads
(Jaquet, et al., 1998)	Wellenberg: claystone	Handling of incomplete geospatial knowledge	3D, scale 10^3 x 10^3 x 10^3 m^3, "probabilistic" (12 realisations)
(Deraisme, et al., 2004), (Jaquet, et al., 2003), (Jaquet, et al., 2006)	Äspö: crystalline	Modelling of heterogeneities	3D, scale 10^5 x 10^4 x 10^3 m^3, density dependent flow, used for licensing in (Auqué, et al., 2006), (SKB, 2006)

Reference	Location	Target	Remarks
(Jaquet, et al., 1999)	Site du Gard: clay and overlying cretaceous deposits	Modelling of heterogeneities	3D, scale 10^4 x 10^4 x 10^3 m^3
(Xu, et al., 2000), (Wörmann, et al., 2003)	Äspö: crystalline	Modelling of heterogeneities	1D calculation of migration, scale $10^{-3}…10^{-2}$ m
(Huysmans, et al., 2005)	Mol: Boom Clay (ductile)	Modelling of heterogeneities in the host rock including fracturing of the EDZ	Simplified 3D-model (symmetry assumption) for calculation of migration, scale 10^1 x 10^1 x 10^2 m^3
(Srivastava, 2007)	Hypothetical Canadian crystalline site	Modelling of large scale fractures (based on statistics of the Canadian Shield, uncertainty considerations planned for several realisations)	3D, scale 84 km^2 x 1,5 km
(Park, et al., 2004), (Park, et al., 2005)	Whiteshell / Lac du Bonnet: crystalline	Derivation of spatially varying effective properties for fractured material Prediction of tracer test results	Scale 50 m x 50 m x 50 m, calibration of conductivities, porosity, dilution by categorical Markov-realisations
(McKenna, 2001)	MIU, Japan: crystalline	Modelling of heterogeneities	3D, scale 10^3 x 10^3 x 10^3 m^3
(Iooss, 2008)	Moscow: sands and clays	Modelling of heterogeneities Sensitivity analysis	Scale 250 m × 350 m, 3 vertical layers

2.1 WIPP (overburden of a repository in bedded salt)

A series of articles spanning more than a decade deals with the Waste Isolation Pilot Plant (WIPP). The earlier works (LaVenue, et al., 1992), (Jackson, 1995), (Larsson, et al., 1997), (Capilla, et al., 1998), (LaVenue, et al., 1995) model the porosity of the Culebra dolomite layer with the help of several geostatistical methods which are derived in the associated theoretical parts (Gómez-Hernández, et al., 1997), (Capilla, et al., 1997), (RamaRao, et al., 1995). The dolomite layer is the assumed main pathway for contaminated brines in a human intrusion scenario. This scenario postulates drilling through the repository that is located below the dolomite layer in a halite layer of the Salado formation. Hence all reports of this section are concerned with a human intrusion scenario in which contaminated brine enters a highly fractured dolomite layer.

The Sandia report (LaVenue, et al., 1992) studies conditionally simulated (CS) transmissivity fields. The grid consists of 50×57×1 (x/y/z) grid blocks and has a finer grid in the central portion of the model. Grid-block dimensions range from 50m near the center of the site to approximately 2800m at the model boundary spanning an overall region of 25km×30km. Particle tracking for 70 different realisations of the transmissivity field was used to determine the most likely travel path out of the WIPP repository.

In (LaVenue, et al., 1995), this approach is extended by using the Pilot Point method of (RamaRao, et al., 1995). Conditionally simulated (CS) transmissivity fields are simulated for the previously described grid. The CS fields are calibrated with measured heads data. For each of these 70 CS fields the groundwater travel path and travel time were calculated for a point located within the WIPP boundary. To reduce the uncertainty of the model suggestions for the location of further boreholes are made.

The article (Capilla, et al., 1998) uses the self-calibrated method developed in (Gómez-Hernández, et al., 1997), (Capilla, et al., 1997) to create equally likely realisations of transmissivity fields conditional to transmissivity measurements and to steady-state head data. The simulation grid corresponds to the same area considered in the above-mentioned study. Confined groundwater flow has been simulated using finite-differences over a 61×43 mesh of square blocks of 500m×500m. Particle-tracking was used to determine travel times of 300 realisations for different scenarios.

The available data from the WIPP was also used in (Jackson, 1995) where studies of five different teams from the INTRAVAL project are considered. These results are also presented in section 4.5 of (Larsson, et al., 1997). In different stochastic approaches the transmissivity of the Culebra layer was modelled. The measured heads were in most cases not included in the model, but compared with the computed values. The AEA project team considered four different stochastic models, the model with an exponential covariance structure was studied in detail. Bi-quadratic finite elements were used on a 40×60 grid. The UPV project team generated realisations using sequential simulation, a predecessor of the self-calibrated method of (Gómez-Hernández, et al., 1997). Both transmissivity data and heads data are used for modelling. Pathlines for 300 realisations are tracked for particles starting near the center of the WIPP site. The AECB project team chose a model in which the transmissivity distribution was calibrated against the transient head data as a base model. They considered model variants with increased salinity or with freshwater everywhere. The finite-difference code works on a 2D grid with 1344 blocks. The BGR project team considered a vertical cross-section through the model area. The SNL project team explored the use of a 3D model to study the importance of vertical flow between the Culebra Dolomite and the overlying units. This model has 15 layers to model 10 stratigraphic units.

Another collection of different methods is presented in the article (Zimmerman, et al., 1998) which discusses many of the used geostatistical algorithms presented in earlier WIPP articles. These algorithms have been tested on synthetic data (producing a “WIPP-like” scenario). The results have been compared with each other. This article comes to the conclusion that good results depend to a lesser extent on the type of used geostatistical method and much more on a good model (i.e., choice of variogram).

The article (Beauheim, et al., 2007) deals with the absence/presence of a halite layer above the dolomite layer, which indicates if the dolomite is washed-out and therefore fractured or if the layer is intact and therefore has a low permeability. Without this halite indicator, some of the data obtained from the wells would contradict a stationary variance assumption which has already been reported in (Capilla, et al., 1998) and in the UVP study of (Jackson, 1995).

The WIPP Compliance Certification Application and the Compliance Recertification Application (US DOE, 1996), (US DOE, 2004) both use geostatistical methods to predict the ground water flow and radionuclide migration through the repository via particle tracking.

2.2 Sedimentary overburden of the Gorleben site (salt dome)

The INTRAVAL report (Porter, et al., 1997), the Federal Ministry of Environment's (BMU) reports (Röhlig, 1999), (Röhlig, et al., 2000), (Röhlig, et al., 2001), and the article (Röhlig, et al., 2005) consider the overburden of the Gorleben salt dome which is a proposed site for a repository of heat-generating high level waste in Germany.

The considered domain in (Porter, et al., 1997) is a 2D model of a vertical cut along the so-called Gorleben erosion channel. A nonlinear transformation takes the stratigraphic data into account that is available in form of borehole logs. The clay distribution in the sedimentary overburden is modelled via indicator kriging. The cross-section is 4km long and 200m deep. A 20×50 grid is used. Note that the vertical resolution into 50 intervals is relatively dense in order to respect the stratigraphy derived from the borehole data.

In the subsequent GRS articles instationary indicator simulation is used to generate realisations for facies distributions and superimposed parameter distributions. Three dimensional studies involving the spatial variability of the thickness of clay-layers accompany the 2D model of the erosion channel overburden. Density-driven flow and radionuclide migration is calculated for the realisations and the results of the former are compared to salinity profiles measured on-site.

These approaches are not relevant for a normal evolution scenario, they are only of interest if geological and geotechnical barriers in the salinary host rock fail and particles are released into the overburden.

2.3 SKB glaciation studies (crystalline)

The reports (Svensson, 1999), (Jaquet, et al., 2003), (Jaquet, et al., 2006) consider the influence of an ice sheet located over the proposed repository on the groundwater flow and on the salinity of the water. Major fracture zones are included in the computer models. In (Svensson, 1999), the computational domain of the area around the Äspö Hardrock Laboratory has a size of 250km×10km×4km (length/width/depth) which gives 250×50×47 cells with non-uniform spacing. The hydraulic conductivity is generated on a per-cell-basis with no correlation between the cells. Cell wall conductivities are calculated as geometric means of adjacent cells and then modified to take the effects of fracture zones into account. Particles released directly below the ice sheet are tracked for at most 600 years.

The report (Jaquet, et al., 2003) extends the results of (Svensson, 1999). Some parameters and boundary conditions differ from the previous study as newly available information has been integrated, but the domain geometry (location of the ice channels and the glacier) and processes remain identical. A different software package using finite element methods replaces the finite volume code. Hydraulic properties are estimated using variograms which are based on regional experiments. The maximum time scale for tracked particles is lowered to 122 years. The porosity has proven most influential in reducing the time scale by factor 10 at which salt transfer occurs when compared with the previous study.

In the third report (Jaquet, et al., 2006) the set of governing equations modelling the physical processes are slightly modified, the salt transport now includes the effects of rock-matrix diffusion. The model domain contains now the Simpevarp region for which a detailed map of deformation zones is available. This regional model has a width of 21.6km and height of 13km. This height is extended for the glaciation model about 300km upstream and 100km downstream. The depth of the glaciation model is 2.3km. The 3D mesh has a horizontal resolution of 100m/300m (inside/outside the Simpevarp model area) and the vertical resolution corresponds to a global discretisation of 100m giving 3.3 million cuboid finite elements. The hydraulic conductivity and porosity outside the Simpevarp model area were estimated using a turning-bands method based on the parameters from the model area. Moreover, fractures and moulins through the glacier are modelled so that the sub-glacial groundwater flow is fed not only by basal melt water but also by glacial surface melt water. This contrasts to earlier studies where the ice channels are prescribed. Furthermore, the built-up and melt-down of the ice-sheet have been simulated. A tracking of particles starting in a depth of 500m results in average travel times of 2200 years until the surface is reached. This travel time is drastically reduced during phases of glacial build-up and retreat.

A glaciation period is considered part of the normal evolution and hence results derived from these computational experiments have direct impact on the performance assessment for this scenario.

2.4 Studies in argillaceous rock formations

The report (Jaquet, et al., 1998) studies the groundwater flow through the (in the meantime rejected) repository in Wellenberg marlstone. The questions under consideration are in which way the groundwater flow is modified by setting up a deep-underground repository and in which time-scales the undisturbed flow is re-established. To answer these questions a 3D model of the Wellenberg Mountain is considered in which hydraulic conductivity is split into a linear drift term and a kriged residual. As a result of the simulations the resaturation of the repository structure after closure takes between 400 and 29000 years. The model covers a $40km^2$ area and uses volume elements of 100m side length which results in a model of 425000 nodes. Representative tectonic faults are modelled by 2D elements. Six deep boreholes were used for hydraulic tests. These results are used for calibrating a linear drift model.

A study of the Gard site in France which had been investigated in the course of the French disposal program was conducted in (Jaquet, et al., 1999). The used model follows the above mentioned design of linear drift plus a random perturbation. Data from three boreholes were available for the study. The Gard site was given up by the French government in late 1998.

In Mol, the Belgian nuclear repository program is characterizing the host rock capacities of the Boom Clay. Some of the results are reported in (Huysmans, et al., 2005). The models under consideration include simulations of hydraulic conductivity via kriging and of fractures using Monte-Carlo methods. The local hydrogeological model has a size of 20m×15m×102m (x/y/z) with a grid spacing of 1m×0.17m×(0.2m to 1m). The results of the simulation differ only slightly from the results obtained by a simple homogeneous model.

The German Federal Office for Radiation Protection Agency (Bundesamt für Strahlenschutz) is conducting a study on the effectivity of barrier systems. In this context, the report (Colenco, 2007) applies geomathematical methods to examples in claystone (Callovo-Oxfordian and Opalinus). 2D permeability on a 1m×1m scale is simulated using a variogram model based on experimental data. In 3D, three mineral fractions are estimated for volumes of 1m×1m×1m and of 100m×200m×100m to study model upscaling. Different mineral fraction have been overlaid which different permeabilities.

2.5 Fracture Networks

In the glaciation reports considered above, the fracture topology of the region under consideration has been included in the model. There are other studies which are devoted to the study of simulating fracture networks. Examples which also consider the Äspö area are found in the article (Xu, et al., 2000) and the SKI report (Wörmann, et al., 2003). In the article (Xu, et al., 2000), a 1D solute transport model is derived based upon exponentially determined auto-covariance functions for fracture aperture and advective velocity along a trajectory. A 2D model is presented and trajectory paths for this model are simulated on a 1m×1m domain. The report (Wörmann, et al., 2003) analyses the radionuclide transport in rock fractures. It considers a 3D discrete fracture model in which a Monte-Carlo technique accounts for the randomness of the fracture network. The solute transport is computed by a 1D-code which allows for uncertainties in the parameters of the underlying partial differential equations. Moreover, the spatial variability of the host rock is honored by semi-variograms taken from data collected on-site. A demonstration case for the 3D model is based on a 5km×5km area with depth of 1km. Results for the 3D model are compared with results from the 1D model for which suitable parameters were extracted from the 3D model.

The following three studies consider the Whiteshell research area located in crystalline rock formations in the Canadian Shield. In (Park, et al., 2004) and (Park, et al., 2005) a porous media approximation model was calibrated with data from experiments conducted in AECL's Underground Research Laboratory. Transition probabilities between different material types (sparsely/moderately/highly fractured rocks) have been used for Monte-Carlo simulation. Realisations from this model were used to predict results from other experiments. The experimental area has a size of 58m×58m×50m (x/y/z). In (Srivastava, 2007), Sequential Gaussian Simulation (SGS) is applied to geometric attributes on an irregular grid to create a fractured zone. First, strike directions and length (using information from observed fractures) are determined via SGS on a 2D grid to create the surface traces of the network. After this simulation has completed, the propagation to depth into a 3D model is performed, again using SGS. With this procedure, fracture networks for regions with ground cover and lakes have been simulated on the basis of data from the Surface Lineament Database for the AECL's Whiteshell Research. An area of 50km×40km was studied with a depth of over 850m. The probability of intersecting a fracture at different depths has been computed with a set of 100 fracture network models.

2.6 Other studies

The SANDIA report (McKenna, 2001) considers the host rock of the Mizunami Underground Research Laboratory (MIU) (crystalline rock) in Japan. A volume of 464m×664m×962m (x/y/z) is discretised into blocks of 8m×8m×6.5m. This size matches the interval length of the conducted packer tests to measure the hydraulic conductivity. 14 borehole data were used in the study. Five additional datasets were used to perform model validation. The hydraulic conductivity is estimated via variograms.

The report (Iooss, 2008) studies the contamination and spread of Strontium-90 on the disposal site of the Russian Research Center "Kurchatov Institute" where waste packages have been flooded by leaking sewage waters. The study uses geostatistical simulations for the distribution of a coarse sand layer which influences the radionuclide transport. The model domain is 250m×350m, with a discretisation of 5m×m. Three vertical layers have been chosen in accordance with filtration and migration characteristics of the sands in the upper aquifer. A sensitivity analysis is carried out for the results of the simulation. To ease the computational burden of this analysis, meta-models are used instead of full model runs.

3 Discussion

Geospatial methods are used to increase the levels of confidence in the used modelling process, either by showing that a model can cope with variations in the geospatial layout or by verifying that already a simpler model (i.e. a model based on the "conventional/manual" descriptive approach) reflects all the important factors from a complex model. See Section 3.1 for more details.

Many of the cited articles are only indirectly connected to performance assessments; they support the local geological understanding for use in a safety case. Reports with direct impact on a safety case are mentioned in Section 3.2.

In recent years, more emphasis is put on the role of safety functions in the performance assessments. Safety functions are used to classify FEPs and to derive alternative scenarios. The connection of safety functions to geospatial variability is investigated in Section 3.3.

The role of the methods investigated in relation to probabilistic safety assessments and their potential of contributing to a safety case is briefly discussed in Section 3.4.

3.1 Reliability of models

In any scientific discussion, results including unresolved issues and newly occurring questions are fed back into the scientific community. The same holds for the stepwise evolution of a repository programme and the associated safety case. The use of methods which involve geospatial variability has the benefit of verifying or questioning possible spatial parameter distributions, proving or disproving assumptions made upon nominal models, etc., especially when combined with experimental data. For the WIPP, the locations of new boreholes were suggested via geostatistical studies so that the largest local uncertainty would be reduced. In the SKB glaciation studies questionable results are replaced by new model approaches in later reports.

An integration of these results into a research and development cycle is important for the scientific and public acceptance of the used modelling process. The usage of all available measurement data also improves the quality of computational models.

As another field of application, geospatial methods are used to test whether the output from a complex model is more meaningful than the output from a simple model. In the Boom Clay study (Huysmans, et al., 2005), it was shown that a simple transport model faithfully reproduces the output from the more complex model which also includes fracture network simulations. In the study (Wörmann, et al., 2003), parameters for a 1D transport model were derived from a complex 3D model.

3.2 Connection to recent safety cases

In the WIPP Compliance Recertification Application (US DOE, 2004), the article (LaVenue, et al., 1990) is referred to as source for the Culebra flow and transport model. This article is also the basis for the subsequent reports (LaVenue, et al., 1992), (LaVenue, et al., 1995).

The study (Jaquet, et al., 2006) is cited in the SR-Can climate reports (Auqué, et al., 2006) and (SKB, 2006). Here the glaciation scenario is part of the standard scenario.

The Belgian SAFIR-2 report (ONDRAF/NIRAS, 2001) predates the article (Huysmans, et al., 2005), however the investigation of fracture networks is formulated in SAFIR-2 as an active area of research. In the same way, the study of fracture network models as in (Srivastava, 2007) is part of Ontario Power's nuclear waste management research and development program, see the Annual Report 2006 (Ontaria Power Generation, 2007).

The Swiss Entsorgungsnachweis (nagra, 2002) mentions no geostatistical methods, only probabilistic parameter studies. The international review team states in (NEA, 2004) that other national projects place more emphasis on probabilistic analysis. For the Swiss legislator, see (BFE, 2008) , one criteria group for the site evaluation regarding safety and technical feasibility is the reliability of geological statements, which might be backed up by geostatistical studies in a forthcoming safety report.

3.3 The role of safety functions

With respect to performance assessment, the articles considered in this report only deal with issues related to the safety function of "delay or attenuation of radionuclide migration in the host rock or the overburden" while other safety functions like "containment" or "(mechanical/ chemical / thermodynamical /hydraulical / geological) stability" are not connected to issues of spatial variability. Maybe the study of glacial built-up and retreat can be subsumed under the study of the safety function "hydraulical stability".

The use of spatially varying parameters may, however, also be of interest when addressing the safety function "mechanical stability" by conducting geomechanical computations. This approach is not used in the reviewed literature. Presently, stress-strain calculations are usually based on the assumption of a limited number of homogeneous domains (e.g. vault, excavation disturbed zone EDZ, undisturbed host rock). The introduction of heterogeneities in these domains might have a significant impact on the mechanical performance and should therefore be investigated.

3.4 Probabilistic safety assessments: Addressing spatial variability in a safety case

Simulation (both variogram-based and Boolean) has the potential of representing uncertainties caused by spatial variability in an integrated probabilistic safety assessment model which might be either requested by regulation and/or be used to explore the space of conceivable parameter configurations as comprehensively as possible in order to gain better system understanding. Although it is recognised that the utilisation of geostatistical methods in hydrogeology might contribute to a consistent treatment of uncertainties in probabilistic safety assessments (Bonano, et al., 1993), most existing safety assessments are still based on the "manual" approach even though some attempts to utilise geostatistical methods have been undertaken. The only case of directly using such methods in the integrated modelling for probabilistic safety assessments the authors are aware of is the WIPP project where the regulation was a strong driver for doing so.

Over the last years, safety assessments and safety cases became increasingly focussed on safety functions. Hydrogeological modelling as a means for consequence calculations got decreasing weight in those concepts where host rock performance (containment or migration delay and attenuation) was paramount. The authors are nevertheless of the opinion that safety cases

- should discuss spatial variability with regard to its potential of influencing or jeopardizing the safety functions claimed,
- investigate, where necessary, its impact as discussed in Section 3.1, and
- either justify its omission in assessments or explicitly account for it.

The review presented here demonstrates that the means of doing so are available. These remarks are not restricted to the traditional application area of hydrogeological and migration modelling, but might, dependent on the safety concept, well be valid for other areas.

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