Application of Geostatistical Methods to Long-Term Safety Analyses for Radioactive Waste Repositories

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Abstract: Long-term safety analyses are an important part of the design and optimisation process as well as of the licensing procedure for final repositories for radioactive waste in deep geological formations. For selected scenarios describing possible evolutions of the repository system in the post-closure phase, quantitative consequence analyses are performed. Due to the complexity of the phenomena of concern and the large timeframes under consideration, several types of uncertainties have to be taken into account. The modelling work for the far-field (geosphere) surrounding or overlaying the repository is based on model calculations concerning the groundwater movement and the resulting migration of radionuclides which possibly will be released from the repository. In contrast to engineered systems, the geosphere shows a strong spatial variability of facies, materials and material properties. The paper presented here describes the first steps towards a quantitative approach for an uncertainty assessment taking into account this variability. Due to the availability of a large amount of data and information of several types, the Gorleben site (Germany) has been used for a case study in order to demonstrate the method.

1. INTRODUCTION

Long-term safety analyses are an important part of the design and optimisation process as well as of the licensing procedure for final repositories for radioactive waste in deep geological formations. For selected scenarios describing possible evolutions of the repository system in the post-closure phase, quantitative consequence analyses are performed. Being an essential part of the barrier system, the geosphere (far-field) surrounding or overlaying the repository is one of the subsystems under consideration. The performance assessment for the far-field is based on model calculations concerning the groundwater movement and the resulting migration of radionuclides which possibly will be released from the repository.

Due to the complexity of the phenomena of concern and the large timeframes under consideration, several types of uncertainties have to be taken into account in the long-term safety analyses. During the last decade, 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. Within the CEC projects EVEREST and SPA, it has been demonstrated that probabilistic uncertainty and sensitivity analyses are powerful tools in this context. Provided 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 in the relevant processes by identifying key ("sensitive") entities [1-5].

However, there is still a need to develop and improve methods to deal with uncertainties which are typical of geological modelling. In contrast to anthropogenic (engineered) systems, the geosphere shows a strong spatial variability of facies, materials and material properties. The knowledge about the hydrogeologically significant features of a site comes from very different sources (e.g. expertise concerning site genesis, exploration drillings, hydrogeological and geophysical tests) but will never be complete.

The paper presented here describes the first steps towards an approach for the integration of several types of knowledge and information into an quantitative uncertainty and sensitivity assessment for groundwater flow and nuclide migration models. Due to the availability of a large amount of data and information of several types, the Gorleben site (Germany) has been used for a case study in order to demonstrate the method.

2. SPATIAL STATISTICAL METHODS

Traditionally, hydrogeological models are derived "manually" from the geological and hydrogeological information available. This allows to account for the variety of "soft" information and knowledge which is typical for geosciences but causes also 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). In contrast, probabilistic safety assessment methods are based on stochastic models describing the variety of conceivable possibilities for the phenomena, systems, parameters, and evolutions in question.

In the last decades, several different mathematical methods have been developed for what the oil industry knows as "reservoir characterisation" and what in hydrogeology can be called "aquifer characterisation". Due to the different nature of the several information types to be integrated into hydrogeological models, an approach as mentioned in the introduction will probably integrate several of these methods. In their review of methods for the description of heterogeneous sedimentary structures, Koltermann and Gorelick [6] identify spatial statistical methods as a possibility

- to generate images of such structures which can be conditioned using "hard data" (which means the image will honour e.g. data coming from borehole logs)

and

- to generate either best estimates for such images or series of realisations which are equally probable under given assumptions.

The latter would allow fitting such methods into a framework of probabilistic uncertainty analyses. Therefore it has been decided to use spatial statistical methods as a starting point for the method to be developed.

The entities of interest might be the presence or absence of certain geological or hydrogeological units or the values of specific parameters (for hydrogeological models e.g. conductivity, for other applications e.g. ore content). Both types of entities can be expressed using functions of position – the former by discrete ("categorical", "indicator"), the latter by continuous variables. Spatial statistical methods see each of these "regionalised variables" as one single realisation of a random function of position. Because a single realisation does not allow performing statistics, additional prerequisites are needed. Usually an assumption of invariance of certain characteristics of the random function will be made. This assumption, called stationarity, very often concerns the moments of the random function. E.g. the so-called "weak stationarity" implies a constant expected value for each position

$$\mathrm{E}\{Z(\boldsymbol{x})\} = \mathrm{E}\{Z\} = \mathrm{const}$$

E............... expected value
$\boldsymbol{x}$, $\boldsymbol{y}$........... position vectors
Z............... random variable

and a covariance between values at pairs of positions which is only dependent on the distance vector ("lag") but not on the positions themselves

$$\mathrm{Cov}(\boldsymbol{x},\boldsymbol{y}) = \mathrm{E}\{(Z(\boldsymbol{x}) - \mathrm{E}\{Z\})\bullet(Z(\boldsymbol{y}) - \mathrm{E}\{Z\})\} = \mathrm{Cov}(\boldsymbol{x} - \boldsymbol{y}) = \mathrm{Cov}(\boldsymbol{h})$$

Cov........... covariance
$\boldsymbol{h} = \boldsymbol{x} - \boldsymbol{y}$.... distance vector, lag

[7]. This allows one to perform statistics for the covariance for a given series of lags (provided that enough data pairs are available for each lag) and thus to characterise the degree of spatial connectivity of a variable. Instead of the covariance, the semivariogram

$$\gamma(\boldsymbol{h}) = \mathrm{Cov}(\boldsymbol{0}) - \mathrm{Cov}(\boldsymbol{h})$$

γ................ semivariogram

is often used. Usually, the semivariogram will increase with increasing distance. The functional dependency of the semivariogram on the lag estimated from the existing data is one important basis to interpolate the entity in question between the position where it is known ("kriging") or to generate equally probable pictures of the data distribution, each honouring a given distribution function and semivariogram ("geostatistical simulation"). For the latter it is possible to honour given data ("conditional simulation").

3. THE GORLEBEN SITE AND DATA SET

The Gorleben site is located near the community of Gorleben in the north-eastern part the federal state of Lower Saxony (Niedersachsen).

Currently the suitability of the site for the final disposal of all kinds of solid and solidified, especially heat-producing radioactive waste is investigated. The repository would be situated at a depth of about 850 m in the Gorleben salt dome which extends from a depth of about 3,500 m up to 260 m below the surface. The salt dome has a length of about 14 km and a width of about 4 km. Its tertiary clay cover has been partially removed by subglacial erosion forming a system of channels, one of which is the ”Gorleben Erosion Channel”. This channel has a length of more than 16 km and its width ranges between 1 and 2 km. Its erosional features extend to the caprock at a depth of about 250 m and in some locations they are in contact with the rock salt. The channel is filled with sandy and gravely sediments forming a system of two aquifers separated by clay layers.

Under the assumption of a scenario which leads to a release of radionuclides from the repository, these radionuclides would migrate through the aquifer system of the Gorleben channel to the surface and the biosphere. Therefore, the groundwater regime and a possible radionuclide transport through the channel has to be studied in a safety assessment.

Hydrogeological investigations are performed in an area of more than 300 km^2 around the salt dome. 340 borehole logs are compiled and partially re-interpreted in annex 6 of [8]. The compilation contains information about stratigraphic classification, petrographic classification, remarks concerning the genesis and colour of the kernels, and a classification into 34 hydrogeological units. In addition to this compilation, the following information concerning the geological and hydrogeological features of the site is available:

- geological and hydrogeological interpretation,
- results of pumping tests,
- results of salt concentration measurements,
- groundwater ages,
- seismic and geoelectrical data.

In Figure 1, the situations of the salt dome and of the erosion channel are given. In addition, the positions of exploration drillings and of the vertical cross-section used for the calculations described below are indicated.

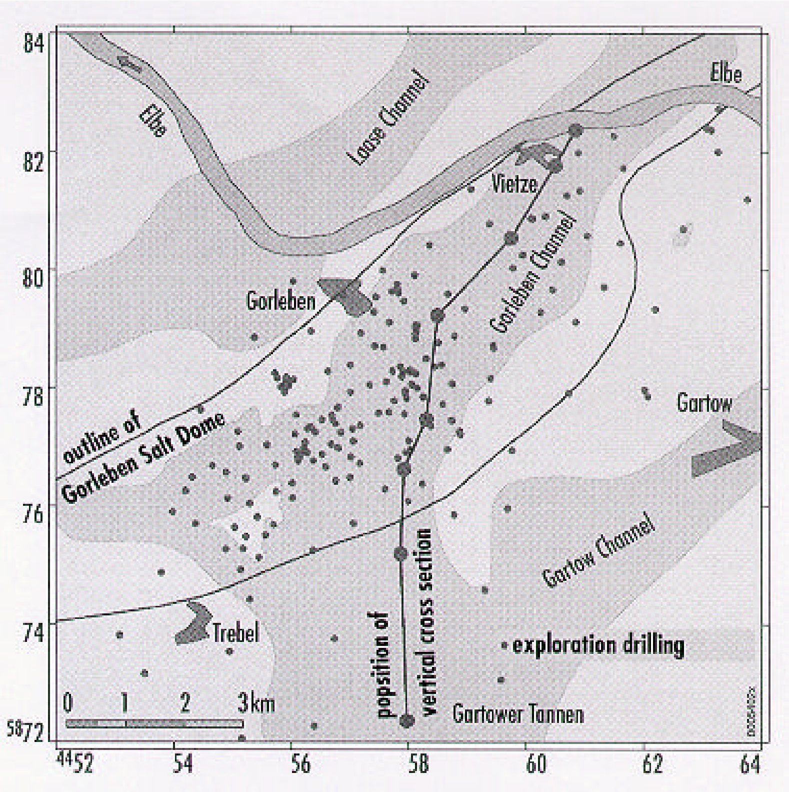

Figure 1. Gorleben: Situations of the salt dome, the erosion channel, exploration drillings and of the vertical cross-section.

4. UNCERTAINTY AND SENSITIVITY ANALYSES

The borehole logs compiled in [8] contain a classification into petrographic units like "clay", "silt", "sand" and others. In earlier studies it was shown that the spatial distribution of the low-permeable clay layers is of significant influence on the groundwater movement. Therefore, firstly an analysis of this distribution was performed. Three-dimensional variography, kriging and conditional simulations for a categorical variable indicating the presence or absence of clay was carried out. Using co-ordinate transformations, additional stratigraphic information was taken into account. The analysis led to a "best estimate" for the distribution of the clay layers obtained by kriging and to a series of equally probable images for this distribution generated using conditional simulations [9].

The geostatistical analyses were performed in three dimensions for a domain (16 km x 16 km x 400 m) covering the southern part of the Gorleben erosion channel. Three series of uncertainty and sensitivity analyses for groundwater flow and solute transport models were performed:

1. For the first series a sequence of geostatistical simulation results was used to generate varying images of the spatial distribution of the clay layers whereas the hydrogeological parameters (conductivities, porosities, dispersion lengths) were left constant (reference values).
2. The second series was based upon one single spatial clay distribution model (a reference distribution obtained using kriging). The hydrogeological parameters were varied from realisation to realisation using Monte Carlo simulations.
3. For the third series, both geostatistical simulation results for the spatial clay distribution and Monte Carlo realisations for the input parameter sets were used.

Additionally, a reference calculation was performed using the kriging results for the facies distribution and the reference values for the parameters. The hydrogeological models used were freshwater models based on a vertical-plane (two-dimensional) cross section through the Gorleben channel (cf. Figure 1) which is regarded to be representative of the groundwater flow in this area. The uncertainty analyses were carried out for performance measures like groundwater travel times, time evolutions and maxima of nuclide fluxes. The uncertainties of the *advective groundwater travel time*, the *maximum* of the flux at the upper model boundary and the *arrival time* of the flux maximum caused by parameter variations (second series) are larger than the ones caused by facies distribution uncertainty (first series). As expected, the uncertainties for the third series (both parameter and facies distribution variation) are greater than the ones for the first and for the second one. Especially the third series is showing significant probabilities for more critical values (earlier arrival times, greater maxima). The sensitivity analyses were performed with respect to the hydrogeological parameters which were left constant within each of the clay layers on one hand and within the rest ("non-clay") on the other [10]. The conductivity of the clay layers, the ratio of the conductivities between clay and higher-conducting ("non-clay") layers, and to some extent the conductivity of the higher-conducting layers were identified as most sensitive with respect to *advective groundwater travel times*. In contrast, the *maxima* of the fluxes as well as the *arrival times* of these maxima are mainly determined by the conductivity of the "non-clay" layers and to some extent by the conductivity of the clay.

However, hydrogeological parameters usually change with position even within one single petrographic unit. Therefore, in a second step these images were superimposed with regionalised variables representing the (now position-dependent) hydrogeological parameters (Figure 2). Again, uncertainty analyses for the performance measures mentioned above were performed. As in the earlier calculations, the distributions obtained during the uncertainty analyses tend to more critical values than the reference case (Figure 3).

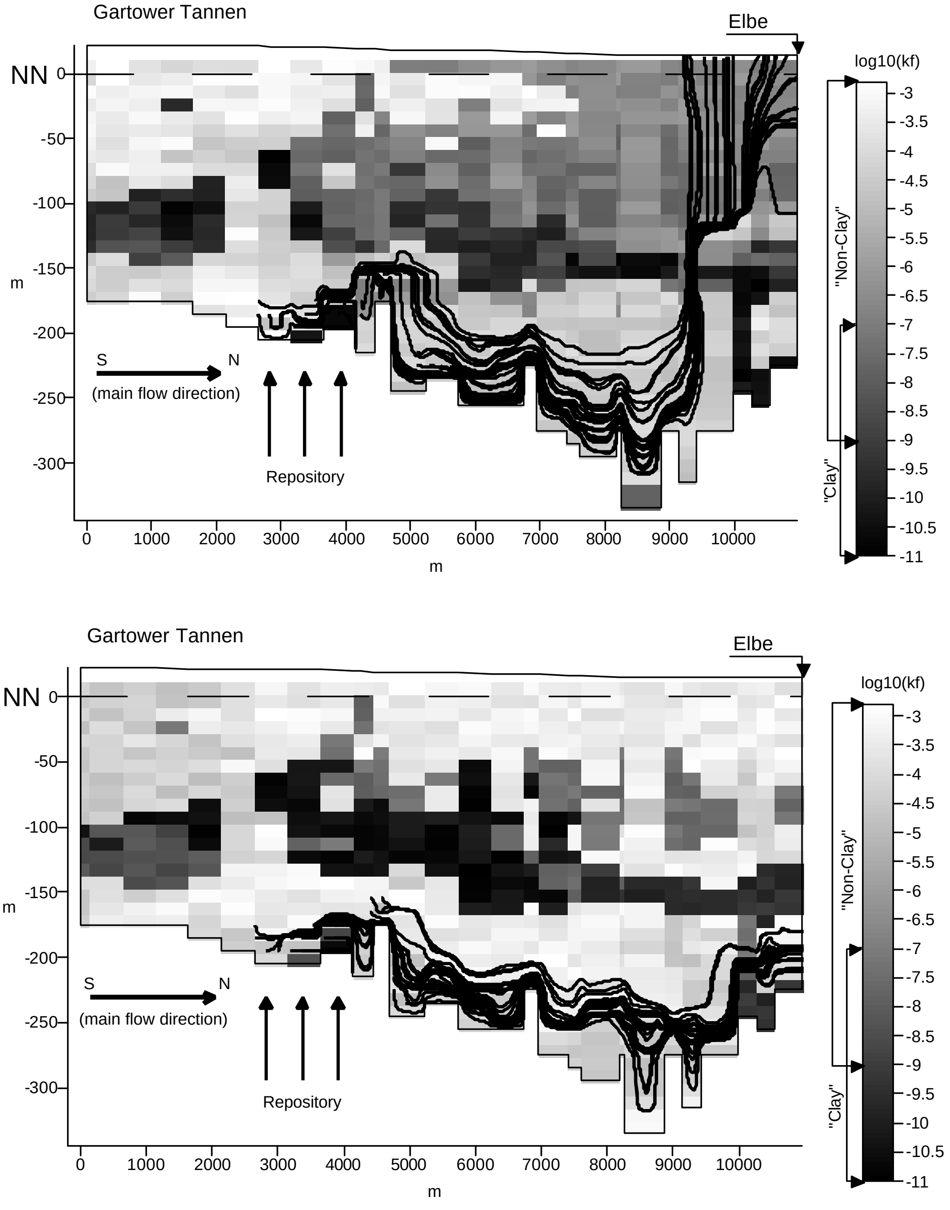

Figure 2. Vertical-plane hydrogeological model: conductivity distribution and calculated (advective) pathlines for two realisations.

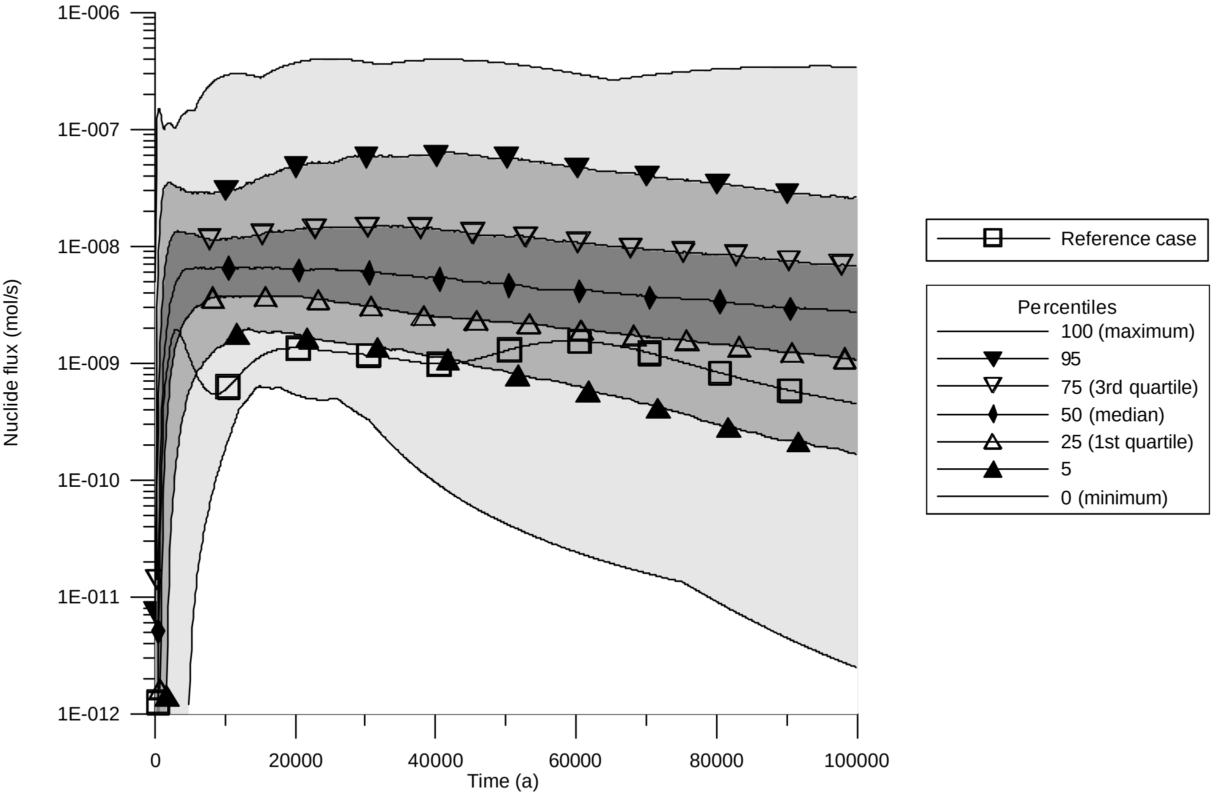

Figure 3. Uncertainty analysis: percentiles for the time evolution of nuclide fluxes across the upper model boundary.

In addition, a method to localise regional sensitivities for variables varying with position has been developed and tested. For facies, obtained by kriging, the conductivities in the clay cover between the two aquifers are of importance (Figure 4), whereas for facies obtained by simulation the importance of areas in the lower aquifer which are mainly "non-clay" increases.

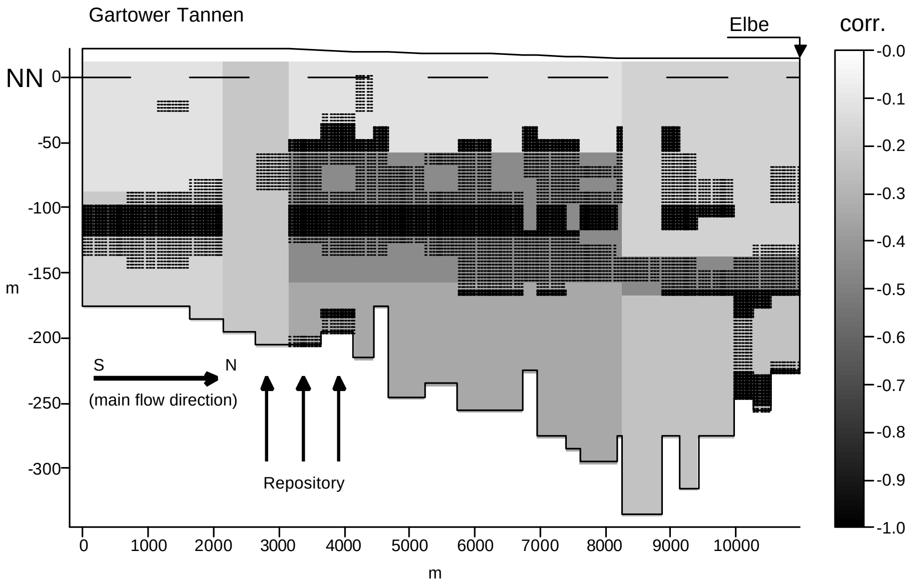

Figure 4. Correlation coefficients between logarithms of conductivities in 10 areas of interest and logarithms of groundwater travel times (facies obtained by kriging, dark background areas = clay).

5. CONCLUSIONS AND FUTURE WORK

In its present stage, the study has demonstrated that geostatistical analyses are promising as a first step towards an integrated assessment of the impact of spatial variability of the geological features of repository sites covered or surrounded by sedimentary systems on safety indicators. This holds especially for sites like Gorleben where detailed data are given at a high density.

The analysis showed that performance indicators calculated using geostatistical simulations might tend to more critical values in comparison to the ones obtained using "traditional" approaches. A method for the localisation of key uncertainties has been developed and tested.

Future work should include the use of more sophisticated geostatistical simulation techniques as well as a further development of the approach in order to include more of the available information. Especially, a distinction between more than two facies types seems to be promising. Furthermore, the integration of information coming not from the drillings but from other sources (hydrogeological tests, salt concentration measurements, groundwater ages, geophysical data) is envisaged. The integration of data related to the groundwater flow regime would lead to an information flow not only from the site-describing work to the hydrogeological modelling as in the present stage but also vice versa. This would also require the use of more sophisticated (saltwater, possibly three-dimensional) hydrogeological models.

6. REFERENCES

1. Gomit J. M., Marivoet J., Raimbault P., Recreo F.: EValuation of Elements Responsible for the effective Engaged dose rates associated with the final STorage of radioactive waste: EVEREST project. Volume 1: Common aspects of the study. Final report. EUR 17449/1 EN. EC, Luxembourg, 1997.
2. Marivoet J., Wemaere I., Escalier des Orres P., Baudoin P., Certes C., Levassor A., Prij J., Martens K.-H., Röhlig K.-J.: The EVEREST project: sensitivity analysis of geological disposal systems. In *Reliability Engineering and System Safety* 57 (1997) 79-90.
3. Becker A., Fischer H., Hofer E., Kloos M., Krzykacz B., Martens K.-H., Röhlig K.-J.: EValuation of Elements Responsible for the effective Engaged dose rates associated with the final STorage of radioactive waste: EVEREST project, Volume 3a: Salt Formation, site in Germany. EUR 17449/3a EN, EC, Luxembourg, 1997.
4. Martens K.-H., Fischer H., Hofer E., Krzykacz-Hausmann B.: Stochatic and deterministic analyses for a generic repository in rock salt in the EU-Project SPA. BMU-Schriftenreihe Reaktorsicherheit und Strahlenschutz 2000, BMU 2000-550.
5. Martens K.-H.: Deterministic and Stochastic Methods in Long-Term Safety Assessments in the Framework of EU's SPA Project. DisTec 2000. International Conference on Radioactive Waste Disposal. September 4-6, 2000, Berlin.
6. Koltermann C. E.; Gorelick S. M.: Heterogeneity in sedimentary deposits: A review of structure-imitating, process-imitating, and descriptive approaches. In *Water Resources Research*, vol. 32, No. 9, pp. 2617-2658, September 1996
7. Olea R. (ed.): Geostatistical glossary and multilingual dictionary. Oxford University Press, New York, Oxford, 1991
8. Ludwig R.: Projekt Gorleben. Hydrogeologische Grundlagen für Modellrechnungen. BGR-Archiv No. 112 002. BGR Hannover. Unpublished report, 1994.
9. Röhlig K.-J.: Geostatistical Analysis of the Gorleben Channel. GeoENV98. Second European Conference on Geostatistics for Environmental Applications. November 18-20, 1998, Valencia. Kluwer Academic publishers, Dordrecht, Boston, London, 1999
10. Röhlig K.-J; Pöltl B.: Investigation of parameter and model uncertainties for groundwater and solute transport models based on conditional indicator simulations. A case study using data from the Gorleben site. StatGIS 99 – Geostatistik und GIS. St. Georgen, Österreich, 20./21.9. 1999. In Mathematische Geologie 2000 (in print).