THEME 1: DEALING WITH CONTAMINATION OF SOIL, GROUNDWATER AND SEDIMENT

THS 1B.9 – RISK MODELING

IMPROVEMENTS WITH GEOSTATISTICS FOR LITHOLOGY REPRESENTATIVE FIELDS AND FLOW MODELS AT SELLAFIELD SITE

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ABSTRACT

Sellafield is the UK facility for Nuclear Fuel Reprocessing. It is a compact coastal site with an area of around 3 km^2. It is currently operational and is expected to remain licensed until 2120. Radioactive material has entered the sub-surface environment following accidental leaks during historical operations. This material is currently under active risk management prior to a final hazard reduction and remediation phase. Sellafield Ltd wishes to understand and control the legacy of ground contamination to ensure protection of the workforce, the public and the environment.

Previous work undertaken as part of the Sellafield Contaminated Land and Groundwater Management Project (SCL&GMP) led to the development of a conceptual model that described sources of ground contamination at Sellafield and the sub-surface soil and groundwater pathways through which the contaminants could migrate. This conceptual model was implemented in a numerical groundwater flow and transport model (in Amec Foster Wheeler's ConnectFlow modelling software). The current study has further developed this model by implementing an approach whereby a geostatistical description of lithologies within the Quaternary strata is used to generate permeability fields in ConnectFlow that take account of heterogeneity on a number of lengthscales. Pluri-Gaussian simulations are used to correctly describe the lithology heterogeneity (varying proportions curves, multi-scale spatial structures, punctually conditioned to data). Representations of the permeability field are then created and used to simulate groundwater flow and radionuclide transport.

INTRODUCTION

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In the work described in this paper, flow and transport modelling using parameter fields with a non-trivial second moment (a covariance) have been implemented to improve the representation of groundwater flow and radionuclide transport. The geological model has been enhanced in the "Inner Region" of the model (see Figure 1). The Inner Region contains the Sellafield site and the immediate surrounding area. Pluri-Gaussian simulations have been used to correctly describe the lithology heterogeneity (varying proportions curves, multi-scale spatial structures, punctually conditioned to data) in the Inner Region.

This paper describes how the improved geological model was built in the Inner Region.

DATA REVIEW

It is important to make a clear statement on the data sets used in the geological modelling phase. For example, it is necessary to recognise that data have been collected through a number of projects and that project-specific drivers for sampling may not always be the same.

This study has been based on several datasets:

- One MS Access database, which contains geological descriptions of material recovered from boreholes (lithology and stratigraphy as a function of depth)
- Two maps, in numerical format, corresponding to the topographic surface and to the top of the bedrock below the area of interest.

The two maps used for building the enhanced geological model correspond in Figure 1 to the square called "Inner Region"**.** It is a part of the existing ConnectFlow model, restricted to the area around the Sellafield buildings where most boreholes have been drilled. Outside the Inner Region, the initial coarser model has been used for flow simulations.

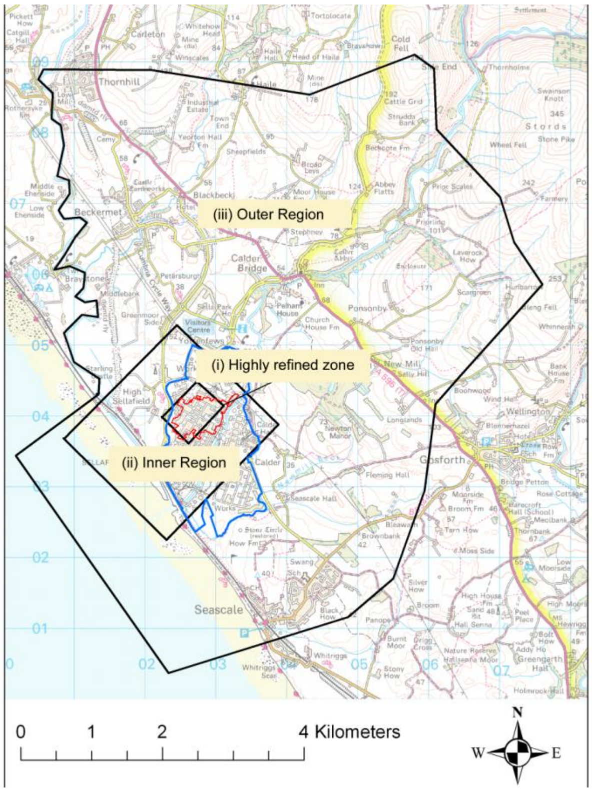

Figure 1: Location map of the nested areas in ConnectFlow.

The horizons limiting the units, restricted to the Inner Region are shown in Figure 2.

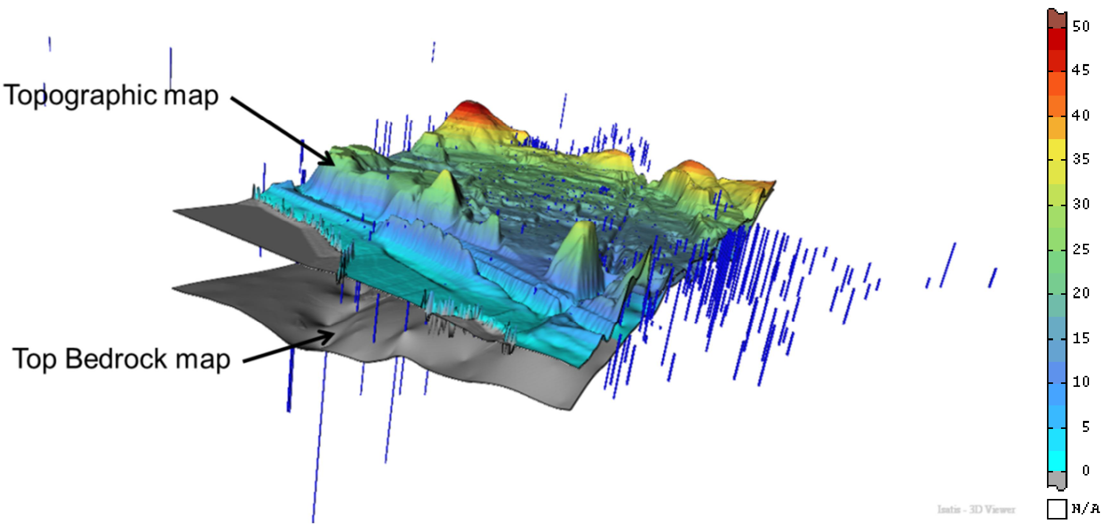

Figure 2: 3D view of the wells (blue lines), top and bottom horizons within the area of interest. A vertical exaggeration of 10 has been applied.

The Inner Region grid has been populated with rock properties in order to define a simplified and numerical representation of the geological environment. The rock properties considered in this section are the lithologies of Quaternary strata. In order to allow further calculations, these boreholes data have been discretized into the 3D Inner Region grid.

RESULTS AND DISCUSSION

Architecture of the Quaternary strata

For geostatistical simulations, an intermediate grid has to be defined from this Inner Region grid, which must take into account the geological correlation lines. It means that the grid layers must be consistent with the geological sequences organization to avoid mistakes and to ensure that the final model will be realistic enough. Therefore, the grid building process first requires a flattening step which places the information back in the sedimentation time where correlation can be calculated meaningfully. Several flattening options are available, as illustrated in Figure 3.

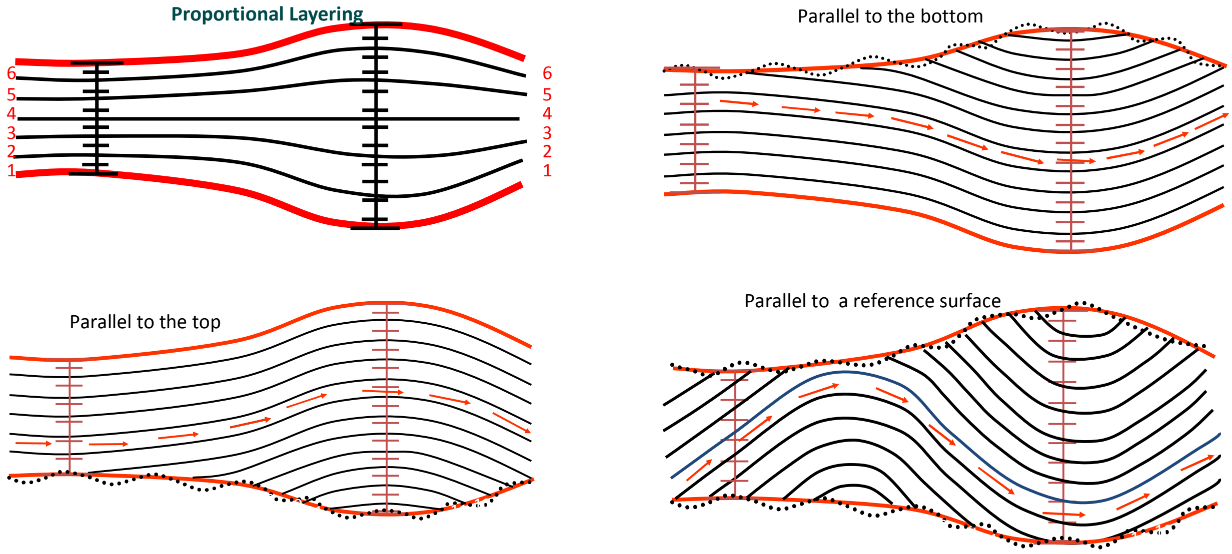

Figure 3: Different layering options corresponding to different correlation hypotheses.

In this particular case, the flattening has been made with a horizontal reference marker. Therefore, the intermediate grid for geostatistical simulations and the final Inner Region grid to be used for further flow simulations have the same geometry.

Six classes of lithology coming from boreholes analysis have been used (Figure 4). Each lithology corresponds to different flow behaviour.

	Ground	*Natural Quaternary data disturbed as a result of construction, excavation, etc.*
	Clay	*Clay to Gravel represent Quaternary strata sorted by the predominant grain size in the material. Clay corresponds to very fine grains when Gravel is made of coarse grains.*
	Silt	
	Sand	
	Gravel	
	Bedrock	*Permo-Triassic strata that underlie the region. No attemp has been made to sub-divide these rocks into different lithology categories.*

Figure 4: Classes of Lithology definition.

Geological model

There are many mathematical methods for calculating the distribution of rock properties in space from boreholes data. Often, these data are not numerous enough to ensure that the results are realistic. In this study, the central area of the Inner Zone is very well sampled, but its peripheral area is under-sampled and some hypotheses are required to model this area appropriately.

For the categorical variables (lithology) simulations, the 3D distribution of lithology proportion represents the numerical version of the conceptual geological model elaborated by the geologist. It is a numerical representation of the regional geological trend, which must be accounted for by the lithology simulation methods. Such a constraint is extremely useful for modelling under-sampled areas.

The 3D distribution of facies proportion is built from a basic tool, the vertical proportion curve, which simply represents the vertical evolution of the proportion of each lithology within each layer of the unit. This curve is calculated from borehole data and helps in characterizing the lithological distribution. Its calculation process is summarized in Figure 5.

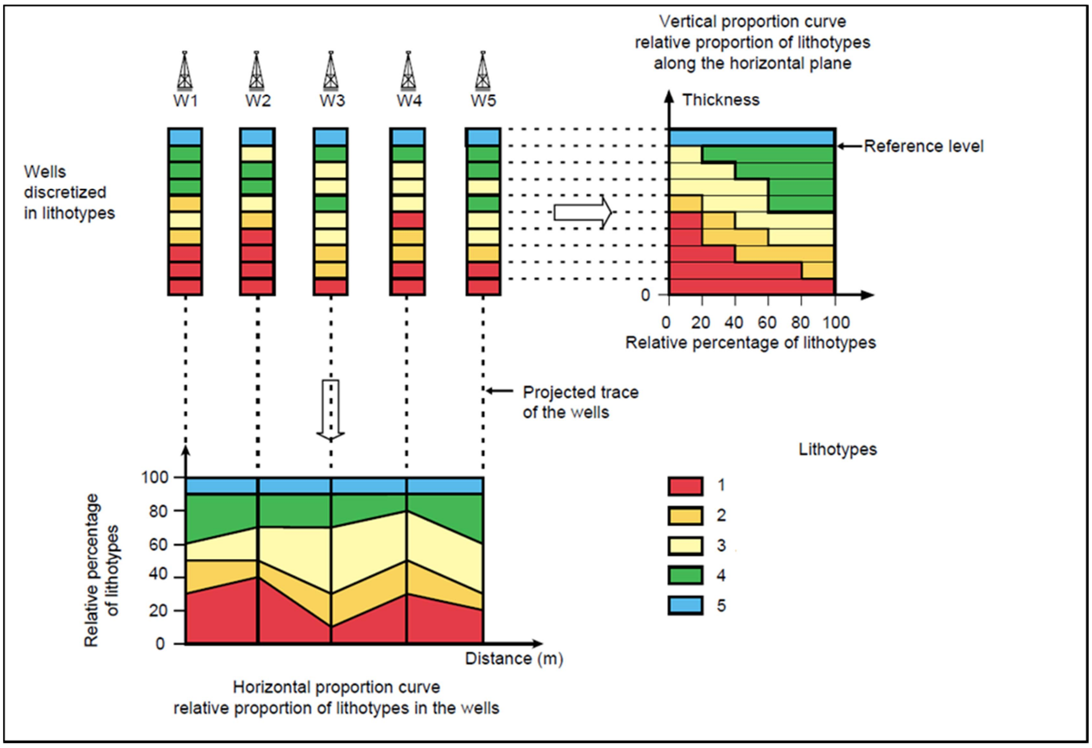

Figure 5: Vertical Proportion Curve calculation.

The global proportion curve (calculated from all the boreholes, in the flattened grid) for Sellafield Inner Region is shown in Figure 6. It indicates that the wells are properly correlated and that the layering type is accurate (i.e. no spurious facies cycle is encountered). The vertical sequence of the different lithologies is consistent with the observed distribution of sediments in the study area. In this figure, the vertical scale corresponds to the elevation from the reference level (sea level). The red lithology (ground) corresponding to excavations and artificial soil is obviously above sea level. The remaining few percents of bedrock correspond to local discrepancies between the horizons at flow simulation scale and recent boreholes. The horizons have not been modified for preserving the consistency with the flow simulation grid and the few samples of bedrock at the bottom of the stratigraphic unit have been kept, to avoid any bia in the geological model. It can be noted that significant shale intercalations can be found near the top of the structure.

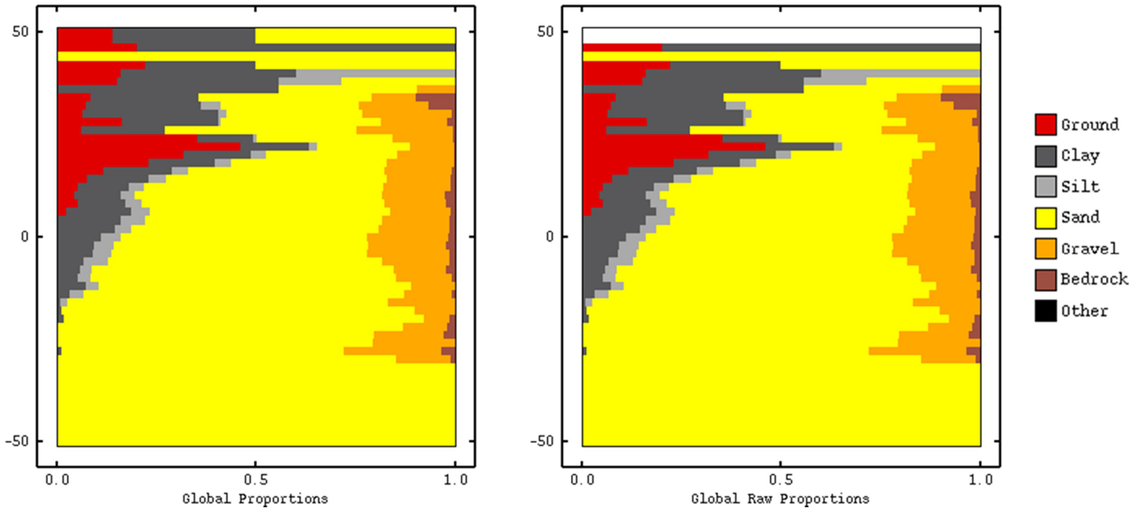

Figure 6: Global Vertical Proportions Curves (VPC) used for simulations. On the left is the global VPC after completion of empty layers and on the right is the raw VPC.

In general, a global VPC is not enough, as the proportions of each lithology often vary laterally. In such a case, local VPCs are calculated from groups of neighbouring boreholes. The 3D distribution of lithology proportions is then interpolated in the 3D grid from these local VPCs. The interpolator is kriging and no additional 2D constraint (i.e. trend) is used. This technique allows us to take into account lateral changes (i.e. non-stationarity) in lithology proportions.

The boreholes projected on the horizontal plane and the local proportion curves corresponding to this study are illustrated in Figure 7. The area contains many wells so the local VPCs were constructed using regular polygons defined by 10 nodes on a rotated grid with an overlay ratio of 1.2 (to increase robustness).

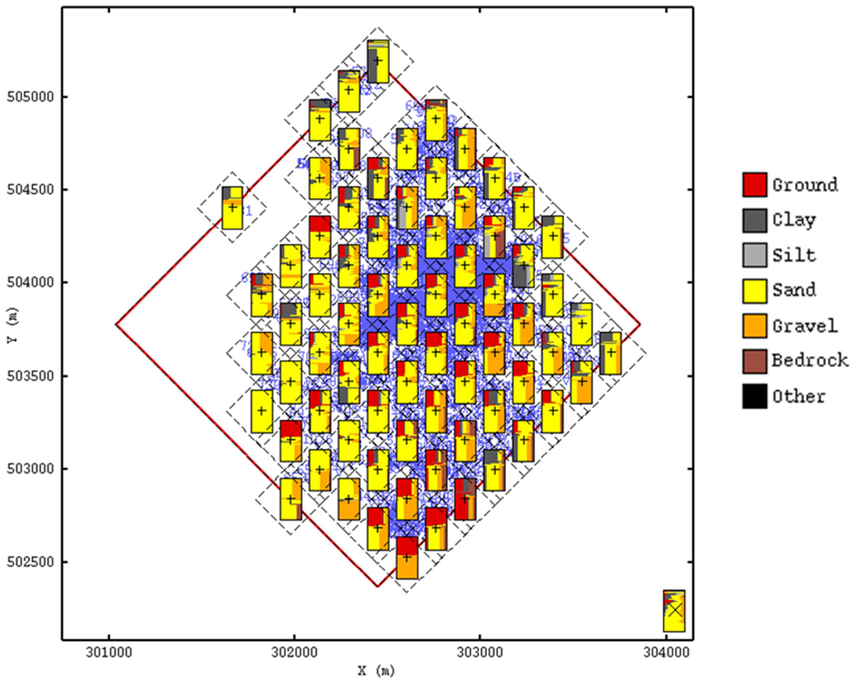

Figure 7: Local Vertical Proportions Curves used for simulations with regular polygons (dashed lines).

The VPCs show that sand and gravel are the dominant lithologies in the central and south-west parts of the area, which are underlain by a valley feature (the Sellafield Buried Channel) filled with Quaternary sediments. In the north, north-west and eastern parts of the area, there is a general fining upward of the grain size (i.e. going from sand and gravel at depth to silt and clay nearer the surface. In the non-sampled areas (mainly the South-West end), the proportions have been extrapolated by kriging, following the trend observed further east.

Note that the lithology proportions are very important for subsequent lithological simulation and flow behaviour. As an example, the proportion of sand is shown in Figure 8.

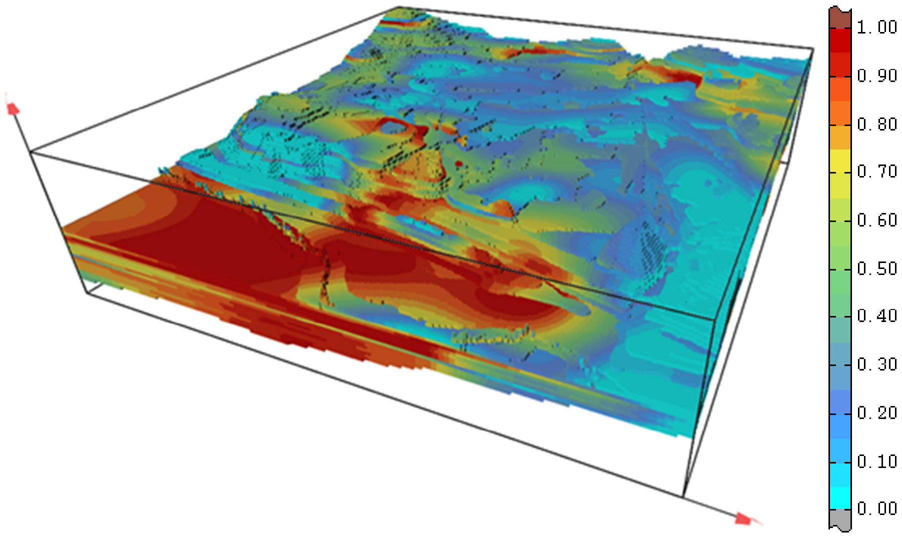

Figure 8: 3D proportion of Sand.

The 3D spatial distribution or lithology proportions can be used for constraining many simulation methods, such as:

- SIS (Sequential indicators simulation);
- Gaussian based algorithms (Truncated Gaussian and Pluri-Gaussian methods);
- MPS (Multi-Points Statistics method);
- Genetic algorithms.

The Gaussian based approach has been used in this study. The idea of gaussian based simulation techniques is to generate categorical variables distributions by thresholding a Gaussian distribution, as detailed in Armstrong and Galli et al. 2011. Such techniques rely on the simulation of Gaussian underlying variables which can be performed using one of the many algorithms available (2). In the simplest case, the Truncated Gaussian simulation technique, one Gaussian Random Function, characterized by its variogram model, is thresholded to provide random sets corresponding to each lithology. The thresholds are defined from the lithology proportions, as shown in Figure 9. At a given location (a layer in the Figure), the proportion of each lithology is reported on the ordinate of the Gaussian cumulative density function. The corresponding abscissas correspond to the thresholds. Applying such thresholds on Gaussian Random Function ensures that the simulated lithology proportion will be in agreement with the experimental proportions at each location in the studied zone.

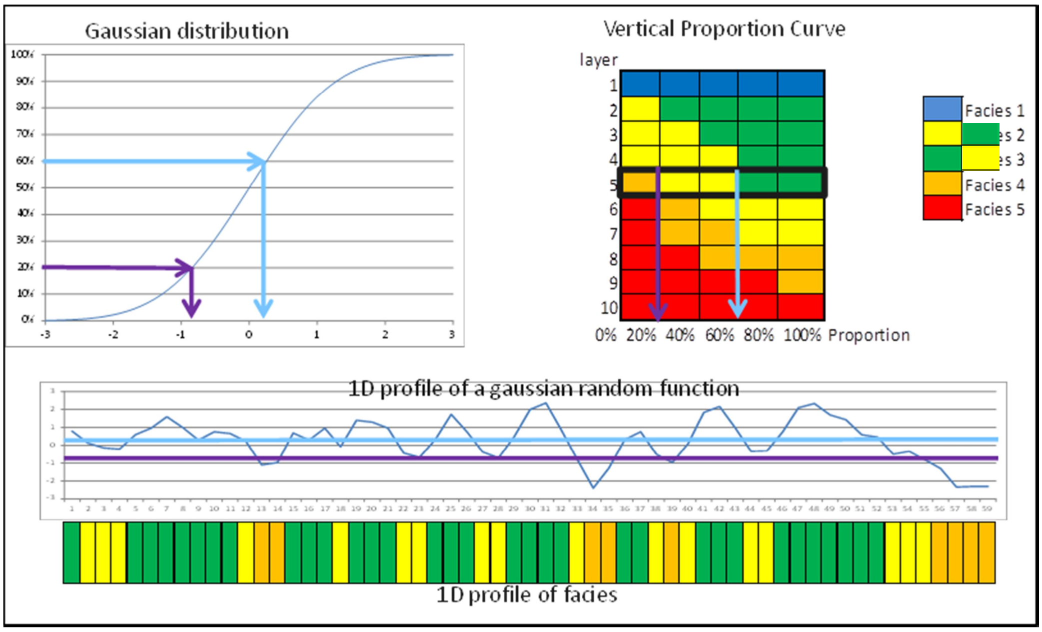

Figure 9: Thresholds determination from lithology proportion and principle of thresholding.

The thresholding method can be applied with three lithologies or more (two levels of truncation) to the simulation of an anisotropic underlying Gaussian variable. It can be noticed that the lithologies are subject to an order relationship. As illustrated in Figure 9, this lithology ordering is related to the continuity of the underlying Gaussian random function. Due to this continuity, going from a low Gaussian value at a given point to a high Gaussian value at another point implies crossing intervals or areas with intermediate Gaussian values, which may correspond after thresholding to intermediate lithologies. The lithology ordering also depends on the proportions of the lithologies. If, at a given location in the field, a lithology disappears (null proportion), then unusual lithology transitions occur in all the directions. For example, with Lithologies 2, 3 and 4, if Lithology 3 is not present there will be a contact between Lithology 2 and Lithology 4 (contact green / orange in Figure 9. In practice, such a configuration is quite frequent.

Discretization effects related to the ratio between grid cells size and underlying Gaussian random function variogram range may also lead to unexpected lithology transitions. In general, such occurrences are quite rare, especially when the grid cells size is low, as in this study.

The lithology ordering implied by the TGS technique is very compatible with commonly observed depositional sequences, where lithology ordering is related to granulometry. Coarse material is generally deposited first, leading to vertical and lateral changes from coarser-grained to finer-grained lithologies. Therefore, this technique often leads to realistic outcomes.

Complex lithology organizations can be found in nature, which cannot be simulated with a simple TGS. In such cases, more complex constructions are required. It can be handled by the (truncated) Pluri-Gaussian method, which requires the definition of two underlying Gaussian variables. Each of the underlying Gaussian simulated variables is truncated using its own proportion curves. The relative organization of the two sets of proportions is provided by the truncation scheme.

In practice, the statistical inference of the underlying Gaussian variable structures is controlled by the fitting of a variogram model to the experimental lithology indicators variograms. In the truncated Pluri-Gaussian simulations mathematical framework, there is a (complex) formula which relates experimental lithology indicator variograms and the underlying Gaussian random functions variograms. This formula includes the thresholds applied on all the underlying Gaussian random functions, therefore the lithology proportions and the truncation rules, the correlation coefficient between these random functions and their variograms. The fitting exercise consists in adjusting the variogram type, ranges and sills of each underlying Gaussian random function in order to get a good match between experimental lithology indicators variograms and the theoretical curves, the proportions and the truncation rules being defined. All the lithology indicators variograms are fitted simultaneously, and the goal is to find the best compromise between all the facies.

In this study there are two distinct groups, one corresponding to the fining upward of sediments (i.e. from gravel to clay) within the Quaternary strata, the other to the unconformity between the bedrock and overlying Quaternary strata. This is summarized in the lithotype rule definition illustrated in Figure 10.

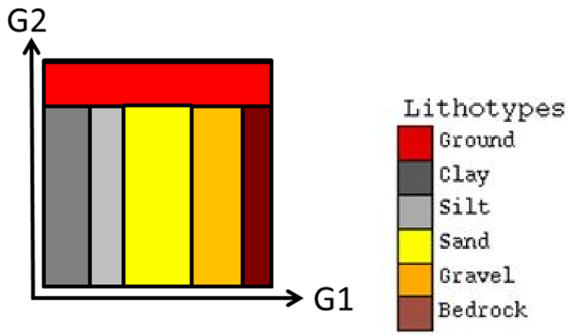

Figure 10: Definition of lithotype rules.

The fitted variograms of the lithologies controlled by the two underlying Gaussian functions are shown in Figure 12 and Figure 13. The fitting is pretty good, ensuring that the model parameters are adequate.

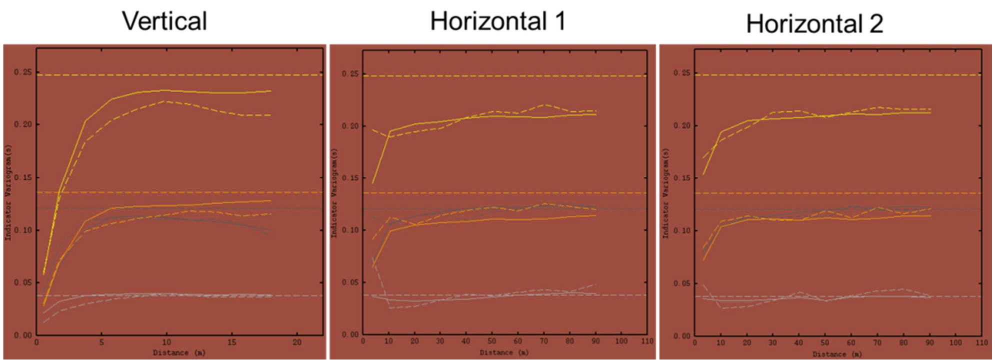

Figure 11: Variograms of indicators for Gaussian 1 (dash point for experimental and lines for model).

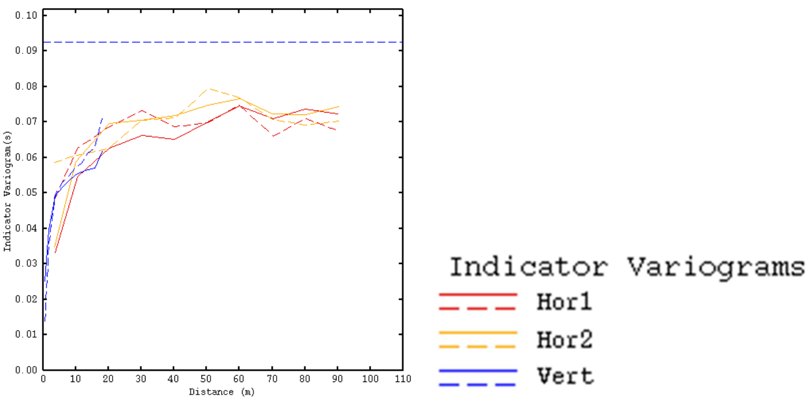

Figure 12: Variograms of indicators for Gaussian 2 in all directions (dash point for experimental and lines for model).

The optimal match of the lithology indicators variograms has been obtained with only two cubic structures for each of the two Gaussian random functions.

In this study, 100 simulations have been performed. It means that 100 different 3D distributions of lithologies are available, which are all equivalent, no one being more probable than the others. All the realizations honor the lithology proportions distribution and the lithology distribution interpreted along the boreholes. An example of a lithofacies distribution 3D view is shown in Figure 13.

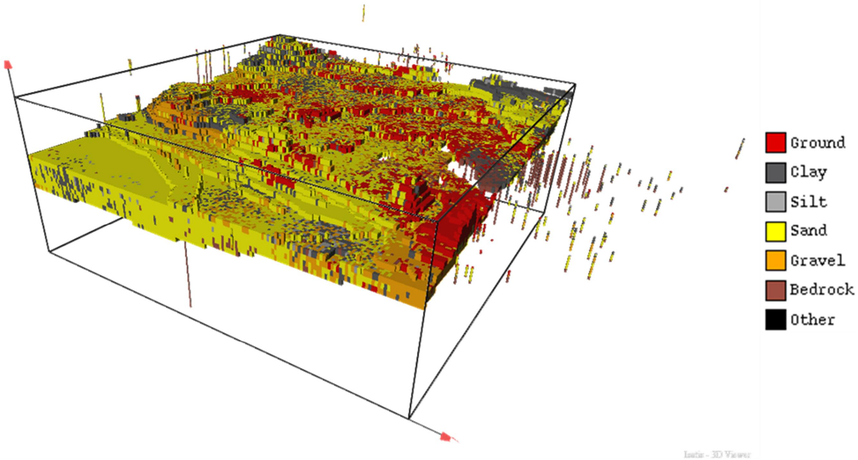

Figure 13: One lithology simulation result in structural space.

CONCLUSIONS

Geostatistical processing is a relevant method for characterizing a radiological contamination by integrating the advanced spatial evaluation of collected samples from boreholes. Pluri-Gaussian simulations that have been used to correctly describe the lithology heterogeneity (varying proportions curves, multi-scale spatial structures, punctually conditioned to data) allow an accurate flow modelling, able to reproduce digitations of the pollution front, which is not possible with a very continuous geological model. In addition, several equiprobable realizations of the facies distribution can be generated, leading to several representations of the permeability field. Therefore, several possible realizations of the flow and transport model can be generated, based on these different representations of the permeability field. It allows quantifying the uncertainty on pollution movements in the aquifer and better characterizing the risk for the population to be exposed to this pollution.

ACKNOWLEDGMENTS

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All geostatistical calculations and graphics are performed using ISATIS software (Geovariances). All flow and transport calculations are performed using ConnectFlow software (Amec Foster Wheeler).

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