Construction of high-resolution 3D stochastic geological models and optimal upscaling to a layer-type hydrogeological model

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Abstract This work has as main objective the implementation of a two-step methodology encompassing the construction of a high-resolution geological cellular model followed by an optimal upscaling to a layer-type hydrogeological model. In a first step a 3D high resolution geological model of the lithologies using the sequential indicator simulation (SIS) algorithm were constructed. SSI algorithm included simultaneously two constrains, which is one of the innovations of this work: i) correction for local means, respecting the geological complexity of the area and the vertical occurrence lithogroups, and ii) histogram of the vertical transitions between lithogroups, requiring that the transition between sections of the experimental data was honoured. In the second step the geological model is simplified to a layer-type model according an optimal procedure of Simulated Annealing. The proposed methodology was implemented to the underground area of the SPEL, in Seixal council.

Introduction

Geostatistical methods enable the spatial description of categorical or continuous variables of a particular phenomenon [1] and make possible the integration of several sources of data and resolution. In particular, a stochastic geological cellular model balance quantitative and uncertainty issues to surface survey data, geological knowledge and borehole depth data.

A well-known limitation of the detailed geological cellular models is the migration to compatible hydrogeological models. Typically, geological models encompass a grid of several millions of cells, and a hydrogeological model is a layer-type structure grid [2]. The simplification of the geological model according the hydrogeological issues can lead to unrealistic results especially in heterogeneous regions [3].

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This work has as main objective the implementation of a methodology that makes optimal integration between the geological models of stochastic high resolution (geostatistical models) and simulation models of groundwater (hydrogeological model) [4]. The solution presented is focused on achieving a high resolution geological model, taking advantage of geostatistical algorithms and subsequent optimal upscaling for a larger cellular mesh.

To this end, first we defined conceptually the main hydrogeological units. Therefore, the option of simplifying optimal stochastic geological model was carried out through an innovative software application developed, programmed and tested, based on the optimization method Simulated Annealing. Limits are obtained, for each of the hydrogeologic units, and an array of hydraulic parameters (transmissivity, storage coefficient and porosity), that can be used directly in the flow model.

The workflow encompasses the following steps [4]:

1. Borehole data analysis and selection of the major lithologies;
2. Resampling of irregular core data into constant core sizes and coding of borehole lithologies into an indicator vector;
3. Exploratory statistical analysis of the lithologies in terms of individual and two- and three-point template transition statistics, plus definition of regions (vertical and/or horizontal) and recalculation of statistics by region;
4. Calculation of experimental single or multiphase variograms of lithologies and fitting of theoretical models [5];
5. Stochastic simulation of N_s 3D high-resolution grids of lithologies with an enhanced version of sequential indicator simulation (SIS) [4][6], to better reproduce individual and transition statistics of lithologies by region, as well as variograms and experimental data;
6. Averaging the N_s grids into a most likely high-resolution grid of lithologies or select each of the simulated images for the following steps;
7. Optimal simplification or upscaling of the grid(s) of lithologies obtained in step 6 to a lower-resolution grid(s) using the Simulated Annealing (SA) procedure;
8. Taking into account the high and corresponding lower-resolution grid provided by SA and the reference hydraulic parameters of each hydrofacies, calculation of equivalent grid-block hydraulic parameters at low resolution.

Case study short description

The study area is an old explosive manufactory (SPEL) close to the Tagus river (Figure 1). During fifty years of activity, SPEL produces toxic organic compounds and potentially cancerigenous such as sulphuric acid, nitric acid toluene nitrates, trinitrotoluene (TNT) and dinitrotoluene (DNT) [7].

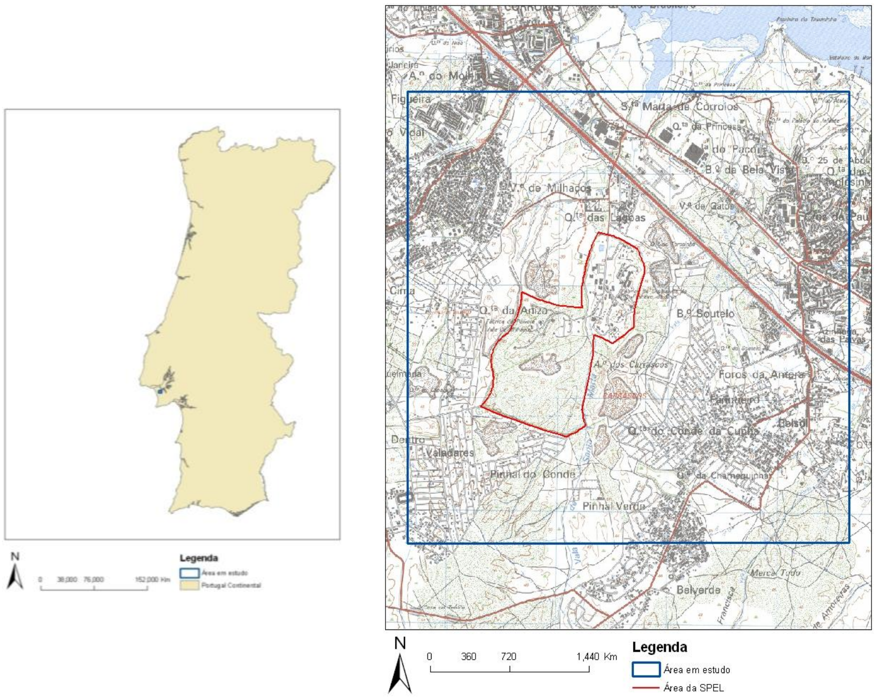

Figure 1 Location of the study area in Portugal

The geology and geomorphology of the area have been studied by several authors [8][9]. The Paleogene deposits are essentially a succession of sandstone arches, conglomerates, mudstones, and marly limestones. The Miocene marine facies are situated closer to the estuary, and consist of two sets: a sandy shale, and an older sandstone-marl. As a whole, the Miocene is represented mainly by alternating shale and sand toward the top, and by sandstone and marl units toward the base. The Pliocene deposits are mainly continental, although a marine episode is represented in Placenciano, and are almost exclusively composed of sands interspersed with thin shale layers.

The aquifer system consists mainly of Paleogene and Neogene terrain, partly covered by Quaternary units. The structure of the basin is sub-horizontal, composed of continental detrital Paleogene and Neogene units, interspersed with brackish and marine formations, corresponding to the maximum of the Miocene transgression. In this stratigraphic interval, a complex multi-layer hydrogeological system has been generated. It consists of an irregular, heterogeneous, and anisotropic sequence of confined, semiconfined, and unconfined aquifers in conglomerates, sands, sandstones, and limestones, interlaid by aquitards and aquicludes in discontinuous layers of silts, shales, and marls.

Within the aquifer system aquifer units alternate with sandstone, carbonate rocks (calc-sandstone, marl, limestone), and low permeability units, such as shales and marls. The aquifer system is composed of a free upper aquifer, consisting mainly of fine sand, interspersed with shale and/or sandy shale, overlying a confined aquifer (locally semi-confined) composed of sandstones, calc-sandstones, and marls of Mio-Pliocene age. Both aquifers have equipotential behaviour to porous media, although, mainly in the Miocene carbonate, permeability can also be controlled by fissures. Finally, separated from the aquifer above by marly formations, there is a confined multi-layered aquifer, composed of calc-sandstone layers of the basal Miocene.

The aquifer system has been extensively exploited for groundwater, which has led to great socioeconomic benefits in terms of agricultural production, industrial use, and urban water supply.

Data analysis

Data used in the present study were provided by 81 boreholes logs within a square of 4 by 4 km square. First an expedite analysis to the logs descriptions were conducted leading to the identification of five main litologies: i) sands, ii) limestones, iii) sandstones, iv) shales and v) marls.

Figure 2 represents the proportions of the five litologies in depth, and shows clearly a zonation in depth. Thus, for indicator simulation conditioning purposes it was decided to subdivide the entire volume in four vertical regions of 50m each, those statistics are presented in Table 1.

Table 1 Proportions of the lithologies by regions.

Depth (m)	*Sand*	*Limestone*	*Sandstone*	*Shale*	*Marl*
0;50	0,694	0,004	0,054	0,246	0
51;100	0,512	0,023	0,282	0,173	0,004
101;150	0,031	0,023	0,630	0,108	0,206
151;200	0	0,039	0,205	0,162	0,593

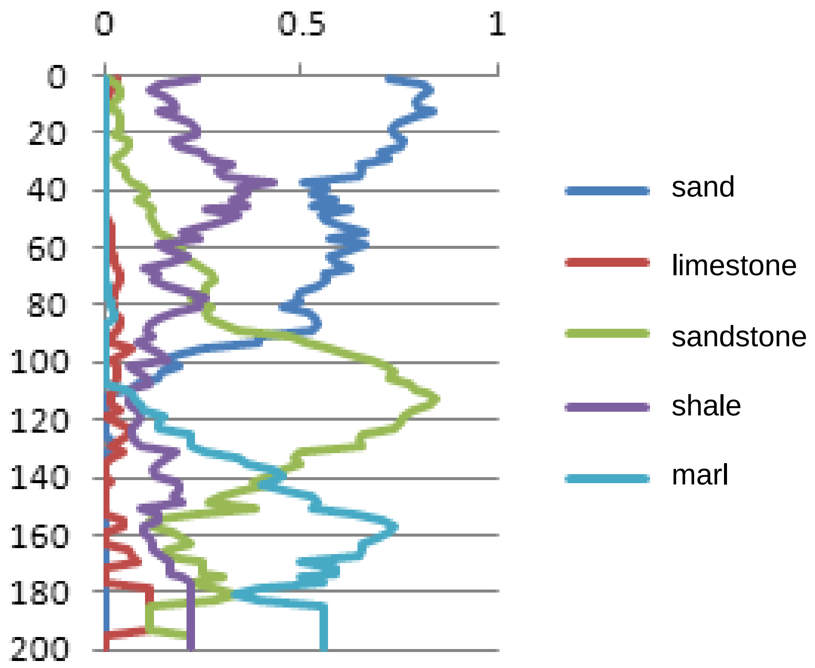

Figure 2 Litologies proportions in depth

In a second step, transition statistics of the litologies in vertical were computed for simulation conditioning purposes. Table 2 shows an extract of those statistics.

Table 2 Experimental two-point template proportions of lithologies for region 0-50m (only for illustration purposes).

	Sand	**Limestone**	**Sandstone**	**Shale**	**Marl**
Sand	0,918	0,001	0,005	0,075	0,000
Limestone	0,000	0,800	0,000	0,200	0,000
Sandstone	0,050	0,000	0,882	0,067	0,000
Shale	0,219	0,000	0,035	0,745	0,000
Marl	0,000	0,000	0,000	0,000	0,000

Simulations and results

Multi-phase variograms were computed and fitted for the five lithologies as displayed in figure 3.

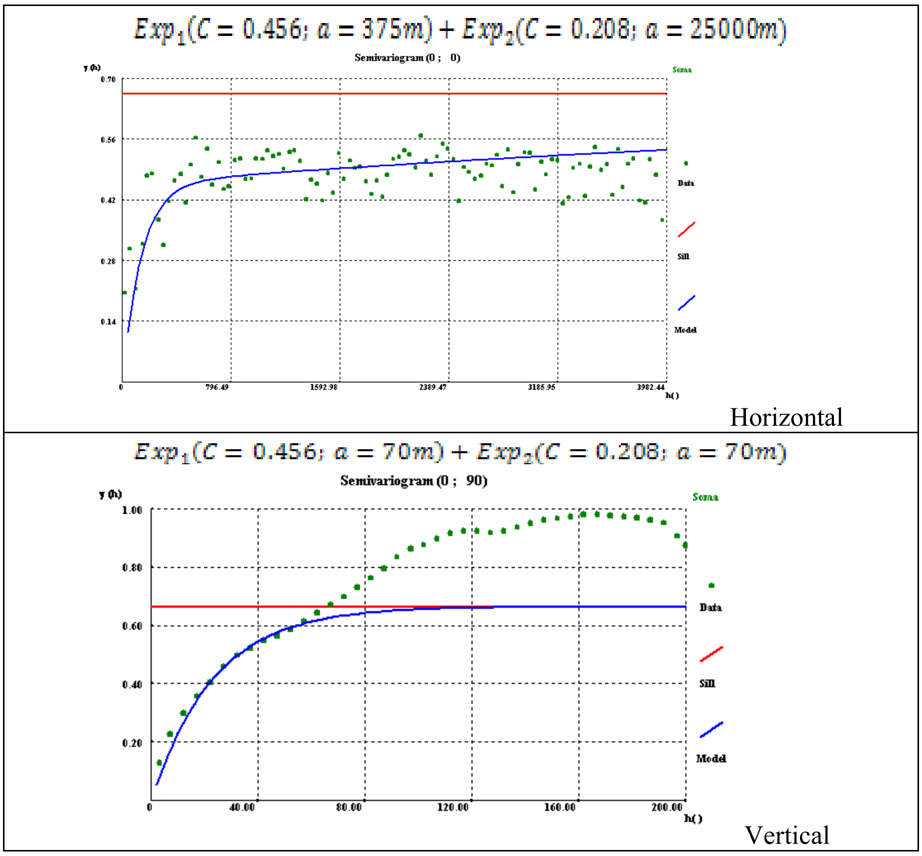

Figure 3 Multi-phase variograms of the lithologies

Results were obtained first through simulation of 30 images of lithologies via SIS with conditioning to local proportions and transition histograms by region. An average image was also computed (Figure 4).

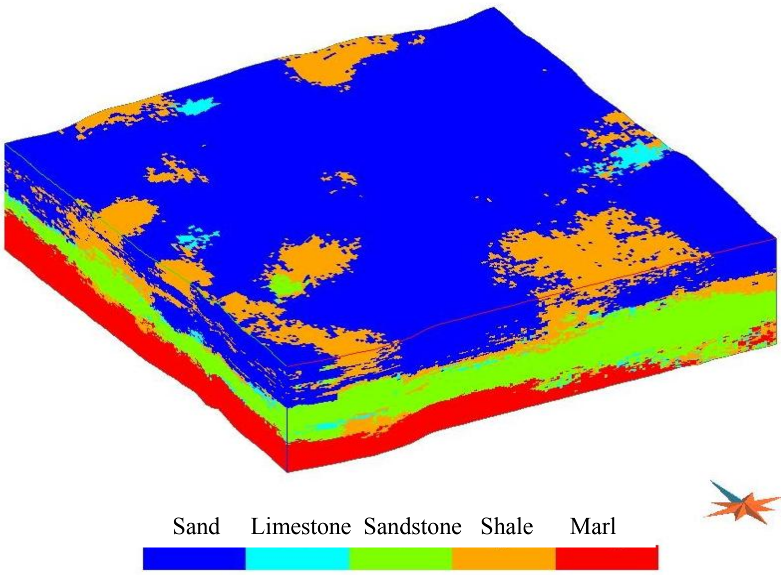

Figure 4 Average image of the simulated lithologies (3D geological model)

As said before, hydrogeological models are limited concerning the number of cells and layers. Therefore, it is necessary to reduce the number of cells from several millions and dozens in vertical of the 3D stochastic geological models to a layer-type model of hundreds of thousands cells. The solution can be provided by an optimal upscaling, minimizing information losses.

Based on [8], from top to bottom, five hydrogeological units were recognized and were used for simplification purposes via SA:

I) Sands on top, an unconfined aquifer;
II) Intercalation of shales, the first impermeable layer;
III) Sandstone, the thirst hydrogeological unit, a confined aquifer;
IV) Again, intercalation of shales;
V) Marls at bottom.

Final results are presented at 2D grids layer by layer with transmissivity, porosity and storage (figure 5, 6). Those outputs can be inputted directly into a flow simulator as *MODFLOW* (figure 7). Results were evaluated through a set of dynamic tests with particle tracking.

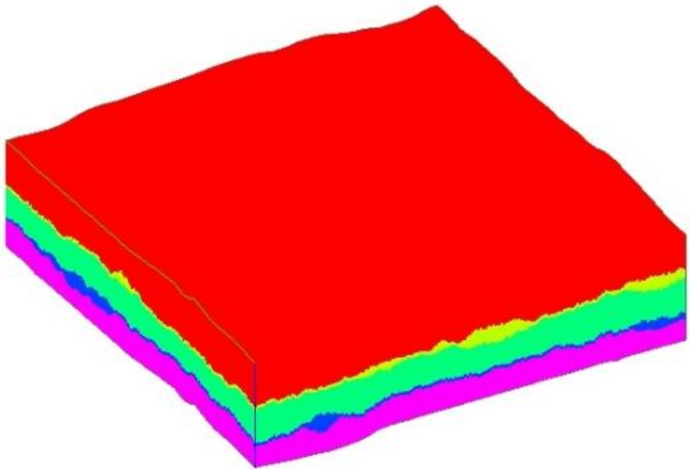

Figure 5 Results of the post processing by simulated annealing (simplified 3D geological model of 5 layers).

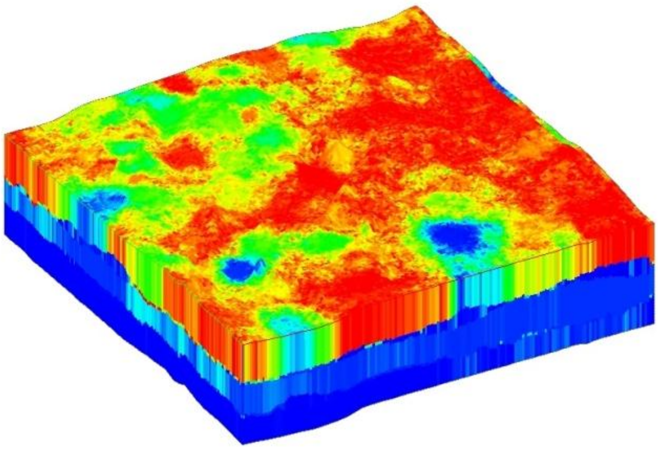

Figure 6 Permeability output layer by layer (simplified 3D geological model of 5 layers).

Results of the methodology are realistic mainly in what concerns the low continuous layers of shales. Incomplete layers models are incompatible with flow simulators such as MODFLOW, and this methodology shows a solution for reconciliation between complexes morphology and layer-type models.

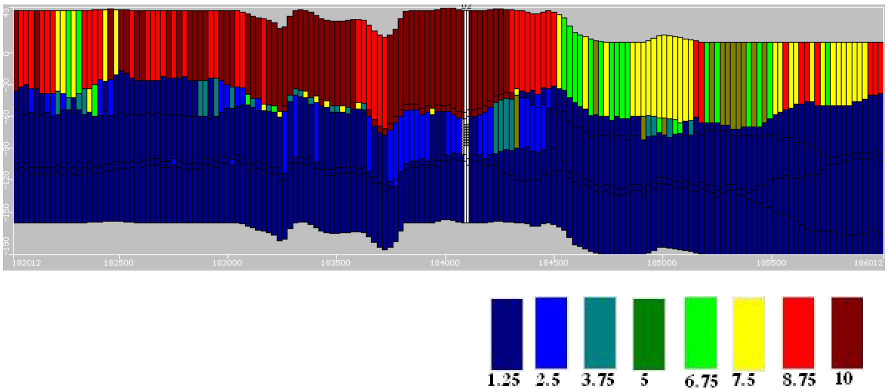

Figure 7 Cross-section of permeability (m/d) layer by layer (simplified 3D geological model of 5 layers).

Properties of the layer-type model are computed via harmonic and arithmetic means of homologous small cells, and therefore the lateral extension of the layers are compensated via properties calculations.

In summary, all results are promising highlighting the SIS conditioning with vertical transition statistics and the upscaling to a layer-type model.

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