Direct multiple-point geostatistical simulation of edge properties for modeling thin irregularly-shaped surfaces

Abstract

Thin irregularly-shaped surfaces such as clay drapes often have a major control on flow and transport in heterogeneous porous media. Clay drapes are often complex curvilinear 3dimensional surfaces and display a very complex spatial distribution. Variogram-based stochastic approaches are often also not able to describe the spatial distribution of clay drapes since complex, curvilinear, continuous and interconnected structures cannot be characterized using only two-point statistics. Multiple-point geostatistics aims to overcome the limitations of the variogram. The premise of multiple-point geostatistics is to move beyond two-point correlations between variables and to obtain (cross) correlation moments at three or more locations at a time using "training images" to characterize the patterns of geological heterogeneity. Multiple-point geostatistics can reproduce thin irregularly-shaped surfaces such as clay drapes but is often computationally very intensive. This paper describes and applies a methodology to simulate thin irregularly-shaped surfaces with a smaller CPU and RAM demand than the conventional multiple-point statistical methods. The proposed method uses edge properties for indicating the presence of thin irregularly-shaped surfaces. This method allows directly simulating edge properties instead of pixel properties to make it possible to perform multiple-point geostatistical simulations with a larger cell size and thus a smaller computation time and memory demand.

1. Introduction

Thin irregularly-shaped surfaces, such as clay drapes, can greatly influence subsurface fluid flow and solute transport in heterogeneous porous media. Clay drapes may act as low-permeability barriers that compartmentalize fluid flow (Stright et al. 2006; Li 2008; Huysmans and Dassargues 2009). A realistic representation of the spatial distribution of clay drapes is therefore essential for reliable flow and transport predictions. Modelling these clay drapes is challenging because they are curvilinear 3-dimensional surfaces whose spatial distribution is very complex, as a result of geological processes that formed them. Their thicknesses may not exceed a few centimetres (Stright et al 2006), which is orders of magnitude smaller than the size of grid cells or elements commonly used in groundwater flow models. For common upscaling approaches (Renard and de Marsily 1997; Farmer 2002), the physical properties of thin clay drapes are assigned to the entire grid cell that contains them, which destroys their continuity as surfaces and their role as flow barriers.

Because of the complex spatial distribution of these thin irregularly-shaped surfaces and the lack of knowledge of their physical properties, deterministic models often fail to capture both their spatial distribution and the uncertainty associated with the distribution. Variogram-based stochastic approaches are not suited for complex, curvilinear, continuous and interconnected structures because they are based on two-point statistics (Koltermann and Gorelick 1996; Fogg et al 1998; Journel and Zhang 2006) and Huysmans and Dassargues (2009) clearly demonstrate that variogram-based methods are not suited to describe complex clay drapes. Multiple-point geostatistics aims to overcome limitations of variogram-based approaches by moving beyond two-point correlations between variables and simultaneously computing (cross) correlation moments between variables at three or more locations (Guardiano and

Srivastava 1993; Strebelle and Journel 2001; Strebelle 2000; Strebelle 2002; Caers and Zhang, 2004; Hu and Chugunova 2008).

Because of the limited direct well information from the subsurface, such statistical information cannot directly be obtained from samples. Instead, "training images" are used to characterize the patterns of geological heterogeneity. A training image is a conceptual explicit representation of the expected spatial distribution of hydraulic properties or facies types. The main idea is to borrow geological patterns from these training images and anchor them to the subsurface data domain. Several multiple-point simulation algorithms have been developed, such as snesim (Strebelle 2002), filtersim (Zhang et al 2006; Wu et al 2008), simpat (Arpat and Caers 2007) and hosim (Mustapha and Dimitrakopoulos 2010).

Multiple-point geostatistics is able to reproduce thin irregularly-shaped surfaces such as clay drapes. It is, however, computationally intensive because the training image requires that a small grid cell size be used to capture the thin surfaces. This results in large training images and a large search template size and thus large CPU times and memory requirements (Huysmans and Dassargues, 2009). Particularly in three dimensions, building field-scale simulations is computationally very intensive and improvements are needed (Hu and Chugunova 2008).

The objective of this paper is to develop a methodology to simulate thin irregularly-shaped surfaces that reduces CPU times and memory requirements compared to conventional multiple-point statistical methods. The methodology is based on the idea proposed by Stright et al (2006) of using edge properties for upscaled flow simulations without losing information about thin irregularly-shaped flow barriers. The edge of a model cell is a continuous or

categorical value associated with the cell face. This idea was extended to not only use edge properties in the flow simulation step but also in the multiple-point geostatistical facies simulation step. This work explores the idea of directly simulating edge properties instead of pixel properties, which allows using a larger cell size for multiple-point geostatistical simulations and thus reduces computational time and memory requirement. The theory and implementation of multiple point geostatistics is first reviewed. The new methodology for directly simulating edge properties is then explained and it is then demonstrated by applying it to two realistic examples. The first example is for pollutant transport in a channelized aquifer and the second example considers the simulation of clay drapes in a real case study of a cross-bedded aquifer in Belgium.

2. Multiple point geostatistics

This section first briefly reviews the mathematical basis behind multiple-point geostatistics and the single normal equation simulation (SNESIM) algorithm (Strebelle 2002). Consider an attribute S that can have N possible states $\{s_j, j=1...J\}$. Attribute S can be a categorical property, such as a facies, or a continuous value such as porosity or permeability, with its interval of variability divided into J classes. A data event d_n of size n centered at location \mathbf{u} is constituted by (1) the data geometry defined by the n vectors $\{\mathbf{h}_{\alpha}, \alpha=1...n\}$ and (2) the n data values $\{s(\mathbf{u}+\mathbf{h}_{\alpha}), \alpha=1...n\}$. A data template τ_n comprises only the data geometry. The categorical transform of variable S at location \mathbf{u} is defined as:

$$I(\mathbf{u}; j) = \begin{cases} 0 & \text{if } S(\mathbf{u}) = s_j \\ 1 & \text{if } S(\mathbf{u}) \neq s_j \end{cases}$$

The multiple-point statistics are probabilities of occurrence of the data events $d_n = \{S(\mathbf{u}_{\alpha}) = s_{j,\alpha}, \alpha = 1...n\}$, which is equivalent to the probabilities that the n values $s(\mathbf{u}_1) \ldots s(\mathbf{u}_j)$ are jointly in the respective states $s_{j,1} \ldots s_{j,n}$. For any data event d_n , that probability is also the expected value of the product of the n corresponding indicator data:

$$\operatorname{Prob}\left\{d_{n}\right\} = \operatorname{Prob}\left\{S\left(\mathbf{u}_{\alpha}\right) = s_{j,\alpha}; \alpha = 1...n\right\} = \operatorname{E}\left[\prod_{\alpha=1}^{n} I\left(\mathbf{u}_{\alpha}, j_{\alpha}\right)\right]$$

Such multiple-point statistics or probabilities cannot be inferred from sparse field data because they require a densely and regularly sampled training image depicting the expected patterns of geological heterogeneities. Training images merely reflect a prior geological concept and do not need to carry any locally accurate information. Training images can be obtained from observations of outcrops, geological reconstructions and geophysical data that are processed with Boolean simulation techniques if needed (Strebelle and Journel 2001; Maharaja 2008).

The single normal equation simulation (SNESIM) algorithm (Strebelle 2002) allows borrowing multiple-point statistics from the training image to simulate multiple realizations of facies occurrence. SNESIM is a pixel-based sequential simulation algorithm that obtains multiple-point statistics from the training image, exports it to the geostatistical numerical model and anchors it to the actual subsurface hard and soft data. For each location along a random path, the data event d_n consisting of the set of local data values and their spatial configuration is recorded. The training image is scanned for replicates that match this event to determine the local conditional probability that the unknown attribute S(u) takes any of the J possible states given the data event d_n , as

$$\operatorname{Prob}\left\{S\left(\mathbf{u}\right)=s_{j}\left|d_{n}\right\}=\frac{\operatorname{Prob}\left\{S\left(\mathbf{u}\right)=s_{j} \text{ and } S\left(\mathbf{u}_{\alpha}\right)=s_{j,\alpha};\alpha=1...n\right\}}{\operatorname{Prob}\left\{S\left(\mathbf{u}_{\varepsilon}\right)=s_{j,\alpha};\alpha=1...n\right\}}$$

The denominator can be inferred by counting the number of replicates of the conditioning data event found in the training image. The numerator can be obtained by counting the number of those replicates associated to a central value $S(\mathbf{u})$ equal to s_k . A maximum data search template is defined to limit the geometric extent of those data events. SNESIM requires reasonable CPU demands by scanning the training image prior to simulation and storing the conditional probabilities in a dynamic data structure, called the search tree. The theory and algorithm behind SNESIM are described by Strebelle (2002). Descriptions of standard SNESIM parameters are given by Liu (2006).

3. Direct multiple-point geostatistical simulation of edge properties

The proposed method is based on the idea proposed by Stright et al (2006) of using edge properties for simulating fluid flow in porous media containing fine-scale thin flow barriers that cannot be accurately represented in current pixel-based flow models. To preserve these fine-scale features at the block scale, Stright et al (2006) introduced the edge of a model cell as an additional modelling variable. The edge of a cell is a continuous or categorical value associated with the cell face and is defined in conjunction with the cell centered property which is often reserved for facies type and/or flow properties. The cell edge and cell-centered property jointly define an edge model to capture the behaviour of the barriers for flow simulations through a simple translation into transmissibility multipliers. The option to assign tansmissibilities already exists in commercial flow simulators. The edge properties can in this way be inserted in finite element of finite difference flow simulators by building a mesh along the constructed edges. The edges are not necessarily perpendicular surfaces, but can also be

incorporated in irregular grids. Edge properties can be used in a large variety of simulation and modelling methods.

In this paper, this idea is extended to not only use edge properties for the flow simulation step but also for the multiple-point geostatistical facies simulation step. This section explains the method of directly simulating edge properties instead of pixel properties in the SNESIM algorithm, which allows performing SNESIM simulations with a larger cell size and thus requires smaller computation time and memory. The method is illustrated in this section with a small and simple training image showing a few clay drapes. In the following section, the method is applied to two more realistic examples: (1) pollutant transport in a channelized aquifer and (2) a real case study of a cross-bedded aquifer in Belgium.

The method starts from a training image depicting the thin irregularly-shaped surfaces of interest. The grid scale of this training image should be fine enough such that the thin surfaces can be represented by pixels. This training image can be obtained from observations of outcrops, geological reconstructions and geophysical data, if necessary processed with Boolean simulation techniques (Strebelle and Journel 2001; Maharaja 2008). The training image should be representative of the geological heterogeneity and must be large enough such that the essential features can be characterized by statistics defined on a limited point configuration (Hu and Chugunova 2008). Moreover, training images are bound by the principles of stationarity and ergodicity (Caers and Zhang 2004). To illustrate the method, a simple training image of sand bodies separated by a few horizontal and inclined clay drapes is shown in Fig 1a.

After the training image has been created, each large scale facies body in the image is indexed individually, from 1 to the number of facies bodies, such that the thin irregularly-shaped surfaces of interest separate the individual facies bodies. In our example, each sand body is assigned a number from one to eight (Fig 1b).

After image training, a model grid size for simulation is chosen. This grid should be chosen such that flow simulations preserve the flow behaviour and connectivity of the relevant structures of the fine scale training image, without requiring exceedingly long computational time. This model grid, which is coarser than the resolution of the training image, is superimposed over the training image and grid nodes are placed at the center of each grid cell (Fig 1b).

In the next step of the method, the grid is searched in the x, y and z-direction for the presence of clay drapes between grid nodes of the coarser grid (Stright et al 2006). If the index values of the two nodes differ, the edge between the two nodes is flagged as "1", indicating that a clay drape is present. Otherwise the edge between the two nodes is flagged as "0", indicating that no clay drape is present (Fig 1c). After this process, the edge properties can be represented by two matrices (or three 3D matrices in 3D) with the same size as the coarse grid: matrix B displaying the edge properties at the bottom of a grid cell (Fig 1d) and matrix R displaying the edge properties at the right side of a grid cell (Fig 1e). The edge properties at the top and left side of a cell are not stored since they can be obtained from the edge properties at the bottom and right side of neighbouring cells.

In the last step of the method, matrices B and R are combined into one matrix E by applying the coding shown in Table 1 describing the four different possibilities for each cell. This

allows obtaining a single training image displaying all edge properties. If, for example, a cell displays no flow barrier, this cell is coded "0". If, for example, a cell displays a flow barrier at the right and not at the bottom, this cell is coded "1". The E-coded training image of our simple example is shown in Figure 1f.

The E-coded training image can be used as input training image to perform SNESIM simulations with 4 categories, which represent the four possible outcomes for E. This E-coded training image (Fig 1f) is much coarser than the original training image depicting thin irregularly-shaped surfaces of interest using pixels (Fig 1a), while still preserving all relevant information about the presence of the clay drapes. If facies other than the thin clay barriers are present, a combined upscaled edge and facies training image can be built where the number of categories is 4 times the number of facies besides the clay drapes.

4. Applications

In this section, the method of direct multiple-point simulation of edge properties is applied to two realistic examples to illustrate its use and advantages. First, the method is applied for a flow and transport simulation in a synthetic channelized aquifer. The simulated solute plume obtained after upscaling using direct multiple-point simulation of edge properties is compared to the plume simulated with a full fine-scale approach and from a standard upscaling approach. This comparison allows validating the approach for flow and transport problems. In a second example, the method is applied to the real case study of the cross-bedded Brussels Sands aquifer in Belgium. This example illustrates the reduction in computation time for a problem with a real training image with realistic dimensions and patterns.

4.1 Pollutant transport in a channelized aquifer

To validate the proposed approach for a groundwater flow and transport simulation, an example of pollutant transport in a synthetic channelized aquifer is considered and results are compared to a full fine-scale approach and two standard upscaling approaches. It is assumed that the base of each channel is a clay or shale drape flow barrier that may potentially compartimentalize flow in the aquifer. Figure 2 shows a 2D horizontal training image for this geological setting. It consists of 250 x 250 cells of size 0.2 m x 0.2 m. This training image was obtained after processing a training image from Caers and Zhang (2004). This fine-scale training image was used as input to SNESIM for simulating pixel-based realizations of the clay and sand facies. Computational time and pattern reproduction quality of SNESIM realizations are strongly dependent on the input parameters selection (Liu 2006). A sensitivity analysis of the input parameters was carried out. The simulation grid consists of 100 x 100 cells of 0.2 m x 0.2 m. Optimal pattern reproduction for this case was found for simulations using a circular template of 11 by 11 nodes, 6 multi-grids, a re-simulation threshold of 15 and 2 re-simulation iterations. Figure 3 shows the 2D SNESIM realization that is used as input to the groundwater flow and transport model to calculate plume shapes and extents in a finescale model.

The groundwater flow and transport model (Figure 4) is 20 m by 20 m 2D horizontal model, discretised into grid cells of 0.2 m by 0.2 m in the fine-scale model. Constant heads are applied to the east and west boundaries so that the hydraulic head gradient is 1 m/20 m. The north and south boundaries are impermeable. Hydraulic conductivities of the sand facies and the clay facies are 10^{-4} m/s and 10^{-6} m/s, respectively. The effective porosity of sand and clay facies is 10%. Three sources of an inert contamination are located at 5 m from the west

boundary with an arbitrarly chosen source concentration of 1000 mg/l. A low longitudinal dispersivity value of 0.02 m was chosen, based on the small grid cell dimension. Transverse dispersivity was assumed to be one order of magnitude smaller than longitudinal dispersivity (Zheng and Bennett 1995). The differential equations describing groundwater flow are solved by PMWIN (Chiang and Kinzelbach 2001), which is a pre- and post-processor for the MODFLOW model (McDonald and Harbaugh 1988), a block-centered finite-difference method based software package. Transport by advection and dispersion is simulated with MT3DMS (Zheng and Wang 1999).

Figure 4 shows the contaminant plumes calculated with the fine-scale model after 10 days. Contaminant plume shapes and extent are largely influenced by the clay drapes present in the model. The clay drapes clearly act as barriers for flow and contaminant transport. These calculated contaminant plumes of the fine-scale model are compared to the calculated plumes of three upscaled models: an upscaled model using direction simulation of edge properties and two upscaled models using standard cell-based upscaling methods.

In the direct edge simulation approach, the small grid cell size training image (Fig. 2) is converted into an edge training image with a larger grid cell size by first indexing each sand body of the initial training image from 1 to the number of sand bodies, so that the clay drapes separate the individual facies bodies (Fig. 5). Next, the simulation grid size is defined as 1 m, which is five times larger that the grid cell size of 20 cm of the pixel training image. This upscaled cell size is chosen because it roughly corresponds to half of the shortest distance between separate clay drapes, which preserves individual clay drapes in the upscaled model. This coarser grid is superimposed on the indexed training image and grid nodes are placed at the center of each grid cell. The coarser grid is searched for the presence of clay drapes

between the grid nodes. If the pixel value of two nodes differs, the edge between the two nodes is flagged as "1". After visualization of the edges, this results in the edge training image shown in Figure 6. This edge training image is as training image to perform SNESIM simulations with 4 categories. Figure 7 shows the SNESIM edge realization that is used as input to the upscaled groundwater flow and transport model, which has a grid cell size of 20 cm. The edges are inserted in the model using the "horizontal flow barrier package" of PMWIN, where the barrier thickness and barrier hydraulic conductivity are equal to 20 cm and 10⁻⁶ m/s, respectively. All cells in the model have a uniform hydraulic conductivity of 10⁻⁴ m/s. All other properties and input parameters of the model are identical to those of the fine-scale flow and transport model.

In the standard upscaling approaches, a SNESIM realization calculated with the same parameters as the reference realization is upscaled by (1) calculating the geometric mean hydraulic conductivity of every cell and (2) the effective hydraulic conductivities in the x- and y- direction for flow calculated by FLOWSIM (Deutsch 1987). Figure 8 shows the SNESIM realization and the upscaled hydraulic conductivity fields that are inserted in an upscaled flow and transport model. The second upscaled model was run with the Visual Modflow pre- and post-processor from Schlumberger Water Services instead of PMWIN (Chiang and Kinzelbach 2001), because Visual Modflow allows defining separate anisotropic hydraulic conductivities in the x- and y-direction cell-per-cell.

Figure 9 and 10 show the resulting contaminant plumes simulated with the three upscaled models. Figure 9 shows the results for an upscaled model using direction simulation of edge properties. Figure 10 shows the results for the upscaled models using standard upscaling methods. These results should be compared to figure 4. Figure 9 shows that the contaminant

plumes calculated with the edge approach display characteristics similar to those of the plumes calculated with the full fine-scale model. Contaminant plume shapes and extent are largely influenced by the clay drapes present in the model. Figure 10 shows that in the other upscaled models that assign the clay drapes to the entire grid cell, the clay drapes do not act as flow barrier. As a result, the contaminant plumes in these models are barely influenced by the clay drapes. This shows that this the direct edge simulation method allows much better preservation of all relevant information about the presence of thin irregularly-shaped surfaces compared to cell-based upscaling methods.

4.2 Application on the cross-bedded Brussels Sands aquifer (Belgium)

To illustrate savings in computational time for a simulation based on a real training image with realistic dimensions and patterns, the proposed method is applied to the cross-bedded Brussels Sands aquifer in Belgium. The Brussels Sands formation is an early Middle-Eocene shallow marine sand aquifer in Central Belgium. The aquifer displays complex geological heterogeneity and anisotropy that complicates pumping test interpretation, groundwater modelling and prediction of pollutant transport (Huysmans et al 2008). In order to investigate the effect of small-scale sedimentary heterogeneity on groundwater flow and transport in this aquifer, a training image was constructed based on photographs, field sketches and measurements of the small scale sedimentary structures (Fig. 11). At this scale, the features most important for groundwater flow and transport are relatively thin clay-rich horizontal and inclined clay drapes that may act as flow barriers. These structures were simulated using SNESIM from SGems (Remy 2004). The 2D SNESIM simulations (Fig. 12) had large CPU times and RAM requirements because of the small grid cell size of 5 cm, which is needed to capture the thin clay drapes, compared to the larger scale of groundwater flow and transport.

This led to a large training image (600 by 600 nodes) and large template sizes (192 nodes) which resulted in a large CPU times and RAM requirements (Huysmans and Dassargues 2009).

To reduce computational time while preserving the features important for groundwater flow and transport, the approach proposed in this paper is applied to the case study of the Brussels Sands. The small grid cell size training image (Fig. 11) is converted into an edge training image with a larger grid cell size by first indexing each sand body of the initial training image from 1 to the number of sand bodies, so that the clay drapes separate the individual facies bodies (Fig. 13). Next, the simulation grid size is defined as 30 cm, which is six times larger that the grid cell size of 5 cm of the pixel training image. This cell size is chosen because it roughly corresponds the shortest distance between separate clay drapes, so that individual clay drapes can be preserved in the upscaled model. This coarser grid is superimposed on the indexed training image and grid nodes are placed at the center of each grid cell. The coarser grid is searched for the presence of clay drapes between the grid nodes. If the pixel value of two nodes differs, then the edge between the two nodes is flagged as "1". After visualization of the edges, this results in the edge training image shown in Figure 14a. The E-coded training image is shown in Figure 14b.

Fig. 14b is used as training image to perform SNESIM simulations with 4 categories. To optimally choose the input parameter values, a sensitivity analysis of the input parameters to pattern reproduction and computation time is carried out. Optimal results are found with an elliptical search template of 20 by 7 nodes and 3 multi-grids. Fig. 15 shows three realizations after visualization of the edge properties. From visual inspection of the simulated realizations, patterns seem to be satisfactorily reproduced. The three pixel SNESIM simulations (Fig. 12)

contain 5 to 8 continuous horizontal clay drapes, 6 to 10 discontinuous horizontal clay drapes and 19 to 26 inclined clay drapes. The three edge SNESIM simulations (Fig. 15) contain 6 to 11 continuous horizontal clay drapes, 8 to 10 discontinuous horizontal clay drapes and 19 to 26 inclined clay drapes. Both techniques simulate equal numbers of horizontal and inclined clay drapes, while the direct simulation of edge properties is significantly faster.

Computational time for three direct edge realizations is smaller than 10 s while it is about 600 s. for the three realizations shown in Fig.. The direct SNESIM simulation of edge properties is therefore 60 times faster than ordinary SNESIM simulation of facies, which represents significant savings in CPU time.

Discussion and conclusion

This paper describes and applies a method for direct multiple-point geostatistical simulation of edge properties for modeling thin irregularly-shaped surfaces such as clay drapes. Instead of pixel values, edge properties indicating the presence of irregularly-shaped surfaces are simulated using SNESIM. This allows very significant computation time reductions while preserving all relevant information about the presence of thin irregularly-shaped surfaces, much better than conventional cell-based upscaling methods. The simulated edge model can be used as input to flow simulations through a simple translation into transmissibility multipliers. The option to set transmissibilities already exists in commercial flow simulators. The edge properties can in this way be inserted in finite element of finite difference flow simulators by building a mesh along the constructed edges. The edges are not necessarily perpendicular surfaces, but can also be incorporated in irregular grids.

This method is particularly valuable for three-dimensional applications of multiple-point geostatistics, which remain one of the most important challenges for multiple-point geostatistics (Huysmans and Dassargues 2009). Building reservoir or aquifer-scale simulations in three dimensions with multiple facies is still computationally intensive and requires further improvement (Hu and Chugunova 2008). This method allows building reservoir or aquifer models with significantly reduced computational time for the case where thin irregularly-shaped surfaces are an important feature for flow and transport.

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Tables

Table 1 Definition of E-coding

В	R	E
0	0	0
0	1	1
1	0	2
1	1	3

Figure captions

Figure 1 Methodology for translating the initial training image to an coarser E-coded training image: (a) initial training image; (b) indexed training image and coarser grid; (c) visualization of edges; (d) B-matrix; (e) R-matrix; (f) E-matrix

Figure 2 Horizontal 2D training image of 50 m x 50 m (white = sand facies, black = clay facies)

Figure 3 Reference SNESIM facies realization (white = sand facies, black = clay facies)

Figure 4 Calculated contaminant concentrations for t = 10 days for the realization of Figure 3.

Figure 5 Indexed training image of the channelized aquifer

Figure 6 (left) E-coded edge training image (blue = 0, cyan = 1, yellow = 2, red = 3) and (right) edge training image

Figure 7 (left) SNESIM edge property realization after visualization of the edge properties and (right) E-coded SNESIM edge property realization

Figure 8 (left) Upscaled hydraulic conductivity values by geometric mean approach, (middle) effective horizontal conductivity in x-direction using FLOWSIM (Deutsch, 1987) and (right) effective horizontal conductivity in y-direction using FLOWSIM (Deutsch, 1987)

Figure 9 Calculated contaminant concentrations for t = 10 days for the direct edge property realization of Figure 7.

Figure 10 Calculated contaminant concentrations for t = 10 days for the upscaled realizations of Figure 8.

Figure 11 Vertical 2D training image of 30 m x 30 m in N40°E direction (white = sand facies, black = clay-rich facies) (adapted from Huysmans and Dassargues, 2009)

Figure 12 Example SNESIM facies realizations (white = sand facies, black = clay-rich facies) (adapted from Huysmans and Dassargues, 2009)

Figure 13 Indexed training image

Figure 14 (a) Edge training image and (b) E-coded edge training image (blue = 0, cyan = 1, yellow = 2, red = 3)

Figure 15 (up) Example SNESIM edge property realizations after visualization of the edge properties and (below) E-coded SNESIM edge property realizations (blue = 0, cyan = 1, yellow = 2, red = 3)