

GEOSSAV: a simulation tool for subsurface applications

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Abstract

Well capture zone determination and site remediation has led to an increasing need of understanding how to quantitatively characterize both the heterogeneity of gravel aquifers and the influence of heterogeneity on groundwater flow and solute transport. Models play an important role in decision-making processes, especially in the context of better characterizing and in forecasting the behavior of a given coupled geological-hydrogeological system.

An example from the Rhine/Wiese aquifer near Basel, Switzerland, demonstrates the application of GEOSSAV on geostatistical data analysis and subsurface simulations based on ground-penetrating radar (georadar or GPR) and borehole data. Subsequent groundwater modeling of a well capture zone leads to a plane representation of the probability of a certain surface location belonging to the well capture zone, caused by hydrologic variations, water supply operation, and the uncertainty of subsurface heterogeneity.

The developed software GEOSSAV is a tool for the integration of hard and soft data in the stochastic simulation and visualization of distributions of geological structures and hydrogeological properties in the subsurface. It can also be used for other applications such as soil contamination, and ecology. GEOSSAV has been successfully tested on Microsoft Windows NT 4.0/2000/XP and on SuSE Linux 7.3. The current version is available at <http://www.unibas.ch/earth/pract>.

1 Introduction

For many practical hydrogeological problems such as determination of well capture zones or risk assessment of groundwater pollutants due to contaminated sites, not only statistical distribution of lithofacies is required but also site-specific structural information. The available information on heterogeneity, however, is mostly limited and typically of different quality (e.g., outcrop and core analyses, geophysical data). In addition, the quantitative integration of such diverse data types represents one of the major challenges in the field of subsurface characterization.

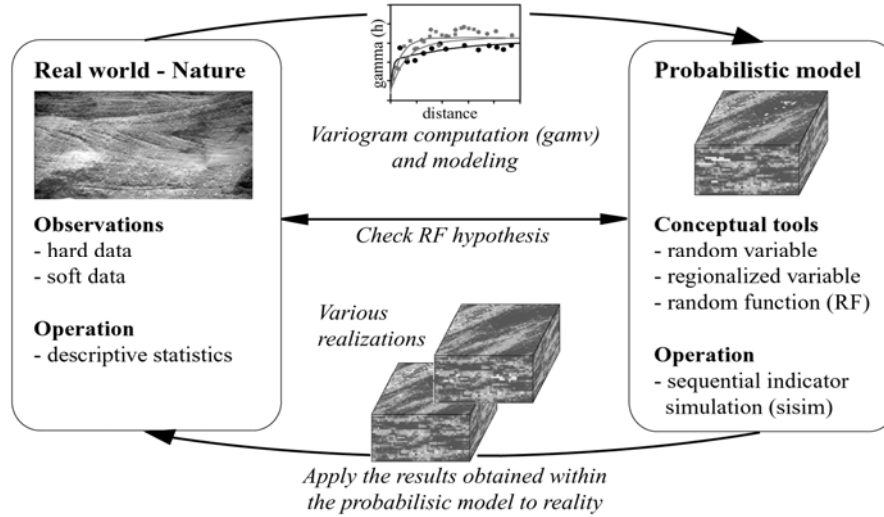


Fig. 1. Conceptual framework of the stochastic simulation approach, modified from Pannatier (1996). Based on the variogram modeling of the hard input data and the following stochastic simulation, various equiprobable realizations are generated and checked for consistency with the random function hypothesis. The results obtained within the probabilistic model should be checked by comparison of measured and calculated data.

Accurate modeling of subsurface parameter distributions depends both on the quantity and the quality of available data, which may be divided into two basic types: 'hard data' and 'soft data' (Poeter and McKenna, 1995). The technique used to model subsurface structures for a site-specific problem should be chosen specifically for the properties under consideration (e.g., lithofacies type, hydraulic conductivity, porosity), the knowledge of the subsurface, and the causes of uncertainty (Ayyub and Gupta, 1997).

In order to evaluate this uncertainty, data analysis and modeling spatial variability of data is the key to any subsurface simulation. Once spatial statistics is specified, multiple alternative realizations of the subsurface structures are created. Then subsequent process modeling (e.g., groundwater flow and transport modeling) can be used to compare modeled and field conditions (Fig. 1).

To bridge this inherent gap in terms of resolution and coverage that exists between nature and probabilistic models, we developed the software package GEOSSAV (Geostatistical Environment fOr Subsurface Simulation And Visualization) that combines geostatistical analysis, simulation, visualization, and data export for groundwater simulation systems (Regli et al., 2004). The paper starts by summarizing integrated methods in GEOSSAV. Then an application is given to illustrate site-specific considerations of heterogeneity in subsurface modeling. The paper concludes with a description of hardware and software requirements for running GEOSSAV, planned new developments, and information for acquiring the software.

2 Methods

GEOSSAV, as an interface to selected geostatistical programs from the Geostatistical Software LIBrary, GSLIB (Deutsch and Journel, 1998), allows the modeler to: (1) import hard and soft field data or data from a pre-existing database, (2) update soft data using a bivariate calibration method, (3) compute and visualize spatial variability of data by variogram analysis, (4) generate distributions of structure types and structure properties of the subsurface using sequential indicator simulation based on a choice of kriging techniques (simple, ordinary, and Bayesian), and (5) visualize the data and the modeled spatial distributions in two- and three-dimensions by 3D rendering and slicing perpendicular to the main coordinate axis. Furthermore, export options for finite-difference groundwater models allow either files that characterize single model layers (which are saved in ASCII matrix format) or files that characterize the complete 3D flow model set-up for MODFLOW-based groundwater simulation systems (which are saved in block-centered flow package files (Harbaugh and McDonald, 1996)).

3 Example of the Rhine/Wiese aquifer

GEOSSAV was applied to generate the aquifer structures of a well capture zone (in the order of several hundreds of meters). The structures were simulated on a 550 m x 400 m x 21 m grid and subsequently exported to a finite-difference groundwater flow and advective transport model to simulate a river restoration pilot project in the region of Basel, Northwestern Switzerland. Particularly, the groundwater simulation of this portion of the Rhine/Wiese aquifer, described in Regli et al. (2003), includes simulation of changing well capture zones depending on subsurface heterogeneity, hydrologic variations, water supply operation, and progress of river restoration.

3.1 Site description

The study site is located in the area of the ancient confluence of the main river Rhine (with flow to the Northwest) and its tributary Wiese (with flow to the Southwest). The average discharge of the river Rhine over the last 110 years amounts to 1'052 m³/s and is therefore around 90 times larger than the average discharge of the tributary Wiese with 11.4 m³/s over the last 68 years.

Detailed drill-core descriptions of five boreholes and georadar data from 14 vertical georadar sections (total length of all sections 3'040 m) have been examined. The unconfined aquifer consists of Quaternary unconsolidated coarse alluvial deposits. Tertiary marls underlie these gravels and are considered impermeable for the purposes of the model. The aquifer thickness varies between 13 and 18 meters. The lower 80% of the aquifer consists of Rhine gravel and the upper 20% of Wiese gravel (Zechner et al., 1995). This may be explained as due to the

reworking of the Wiese gravel by the river Rhine under landscape-shaping conditions whereby the top sequence of Wiese gravel would be preserved until the next shift of the active channel area of the river Rhine. The Rhine and Wiese sediments are easily distinguished lithologically because the sediments come from different source areas with distinct geological units. Also, within these two stratigraphic units a number of sedimentary structures are recognized that were generated by sedimentary processes in the braided fluvial system. Lithofacies types associated with the sedimentary structures for this area include (Regli et al., 2002): open-framework gravel (OW), open-framework/bimodal gravel couplets (OW/BM), gray gravel (GG), brown gravel (BG), alternating gray and brown gravel layers (GG/BG), horizontally layered or inclined, silty gravel (SG), sand lenses (SA), and silt lenses (SI).

For the georadar investigations, described in Regli et al. (2002), a pulseEKKO IV georadar system with a 1'000 V transmitter was used (Sensors & Software Inc., 1993). The transmitting and receiving antennae were separated by 2 m and the recording step size was 0.25 m. The 50 MHz antennae used for this study allow recognition of the basal aquiclude surface, the main erosion boundaries within the coarse alluvial deposits, and the larger sedimentary structures down to the aquiclude at approximately 13-18 m depth. According to Jol and Smith (1991) and Huggenberger (1993), the vertical resolution depends on the georadar-wave frequency and is equal to a quarter of the wavelength, or 0.5 m in this case. Due to the relatively long wavelengths of the 50 MHz antennae, few transitions of alternating sequences of open-framework and bimodal gravel may be distinguished on the georadar sections. However, the main sedimentary structures as described above could be delineated.

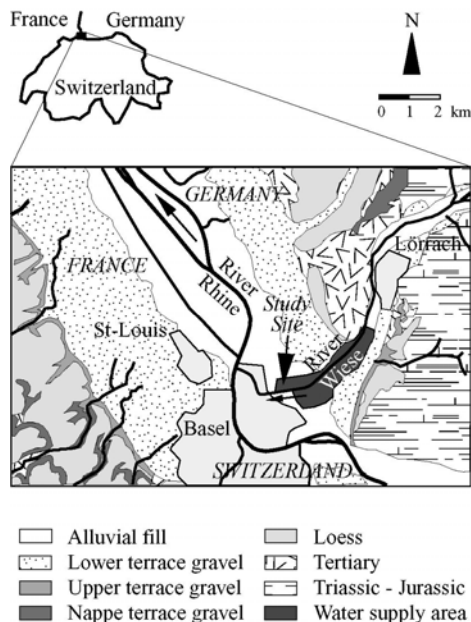


Fig. 2. Simplified geological overview of the Basel area, Switzerland, and location of study site – at the lower end of the city's water supply area Lange Erlen – within the ancient confluence of main river Rhine and its tributary Wiese.

The drill-core and georadar data are interpreted based on Regli et al. (2002). This lithofacies-based interpretation of outcrop, drill-core and georadar data considers differences in data uncertainty and provides lithofacies type probabilities for points along boreholes and grid nodes with arbitrary mesh sizes in horizontal and vertical direction along georadar sections. The sampled data from the georadar sections are at nodes of grids separated by 5 m x 1 m.

3.2 Variogram computation

The variogram computation is based on the drill-core and georadar data. The indicator transform at grid node location is set to 1 for the lithofacies types with the greatest probability values, 0 otherwise. The directional variograms, given for specified azimuth and dip, characterize the geometric anisotropy of the sedimentary structure types. They indicate orientations and ranges corresponding to maximum and minimum horizontal and vertical distances of spatial correlation. Variogram information for the nine sedimentary structure types in the study area is given in Table 1. The lithofacies proportions are based on the data density representing a specific structure type. The values written in italics are estimated because the corresponding structure types never have the greatest probabilities and, therefore, the indicator transform is always set to 0 by default for these structure types.

Table 1. Variogram information of Rhine and Wiese gravel used for the sequential indicator simulation to define the geometric anisotropy of the sedimentary structure types: OW: open-framework gravel, OW/BM: open-framework/bimodal gravel couplets, GG: gray gravel, BG: brown gravel, GG/BG-horizontal: alternating gray and brown gravel, horizontally layered, GG/BG-inclined: alternating gray and brown gravel, inclined, SG: silty gravel, SA: sand, SI: silt. Isotropic nugget constant, dip, and plunge of the sedimentary structure types are 0; the variogram models of the sedimentary structure types are exponential.

	Sedimentary structure type	OW	OW/BM	GG	BG	GG/BG		SG	SA	SI
						horizontal	inclined			
Wiese gravel	Variogram parameter									
	Probability density function	<i>0.02</i>	0.05	0.16	0.05	<i>0.50</i>	<i>0.05</i>	0.02	0.14	<i>0.01</i>
	Sill	<i>0.13</i>	0.12	0.18	0.115	<i>0.13</i>	<i>0.13</i>	0.045	0.18	<i>0.13</i>
	Azimuth [°]	<i>240</i>	240	240	240	<i>240</i>	<i>240</i>	270	200	<i>240</i>
	Max. horiz. range [m]	<i>3</i>	24	60	34	<i>50</i>	<i>7</i>	14	50	<i>3</i>
	Min. horiz. range [m]	<i>1.5</i>	18	24	24	<i>18</i>	<i>3</i>	18	16	<i>1.5</i>
Rhine gravel	Vertical range [m]	<i>0.5</i>	4	6	5	<i>6</i>	<i>1</i>	4	3	<i>0.5</i>
	Probability density function	<i>0.02</i>	0.06	0.12	0.05	<i>0.50</i>	<i>0.05</i>	0.03	0.16	<i>0.01</i>
	Sill	<i>0.1</i>	0.095	0.155	0.055	<i>0.1</i>	<i>0.1</i>	0.04	0.17	<i>0.1</i>
	Azimuth [°]	<i>310</i>	320	315	300	<i>310</i>	<i>310</i>	300	300	<i>310</i>
	Max. horiz. range [m]	<i>5</i>	54	60	40	<i>70</i>	<i>8</i>	30	60	<i>5</i>
	Min. horiz. range [m]	<i>2</i>	22	19	22	<i>30</i>	<i>4</i>	17	22	<i>2</i>
	Vertical range [m]	<i>1</i>	10	5	11	<i>10</i>	<i>2</i>	10	8	<i>1</i>

The main outcome of the variogram analysis is the orientation of the sedimentary structure types representing the main flow direction of the river Rhine in the lower part of the aquifer and the tributary Wiese in the upper part of the aquifer.

The relatively large ranges of spatial correlation of a few meters up to a few 10s of meters for the different sedimentary structure types may be significantly influenced by the resolution of the georadar system and the density of the sampled data taken from the georadar sections. The sedimentary structures of the Rhine gravel are modeled as geostatistical structures that are horizontally around 20% and vertically around 45% larger than the structures of the Wiese gravel.

3.3 Sequential indicator simulation

The aquifer is simulated by sequential indicator simulation (Deutsch and Journel, 1998). The sequential indicator simulation principle allows conditioning by including all data available within the neighborhood of a model cell, including the original data and all previously simulated values. The steps in the sequential indicator simulation are as follows: In the first step, a grid network and coordinate system is established. In the second step, the existing data is assigned to the nearest grid node. If there is multiple data available, only the closest data is assigned to the nearest grid node. In the third step, a random path through all grid nodes is determined. For a node in the random path: (1) the nearby data and previously simulated grid nodes are searched, and (2) the conditional distribution is estimated by indicator kriging (Deutsch and Journel, 1998). From this distribution (3) a simulated lithofacies is randomly drawn and set as hard data. Then the next node in the random path is selected and the steps (1) – (3) are repeated. This way, the simulation grid is built up sequentially. In the last step, the results are checked. The data and the global proportions (random function hypothesis: limited deviations of the input and output probability density functions of the sedimentary structure types) have to be honored, and the orientations and sizes of the sedimentary structures have to be in accordance with the observed sedimentary structures.

In Fig. 3 one realization of the sequential indicator simulation is shown with separate realizations for the lower and the upper parts of the aquifer. The regular model grid is defined by 110 x 80 x 10 cells for the lower part and by 110 x 80 x 1 cells for the upper part, respectively. Cell sizes are 5 x 5 x 1.5 m for the lower part, and 5 x 5 x 6 m for the upper part, respectively. The saturated thickness of the topmost layer, however, is about only 1-2 m.

A total of ten combinations of sedimentary structure-type distributions were simulated, each called an aquifer realization. The resulting probability density functions of the sedimentary structure types deviate less than $\pm 10\%$ from the initial probability density functions. For determining statistical moments and their confidence limits by a Monte Carlo type modeling more than 100 or 1000 realizations are needed. However, to qualitatively examine the effects of subsurface heterogeneity in this boundary condition dominated model (changes in river discharge and permeability of riverbed; see section 3.4), a smaller number of aquifer realizations already produces the main trends of groundwater flow and transport behavior.

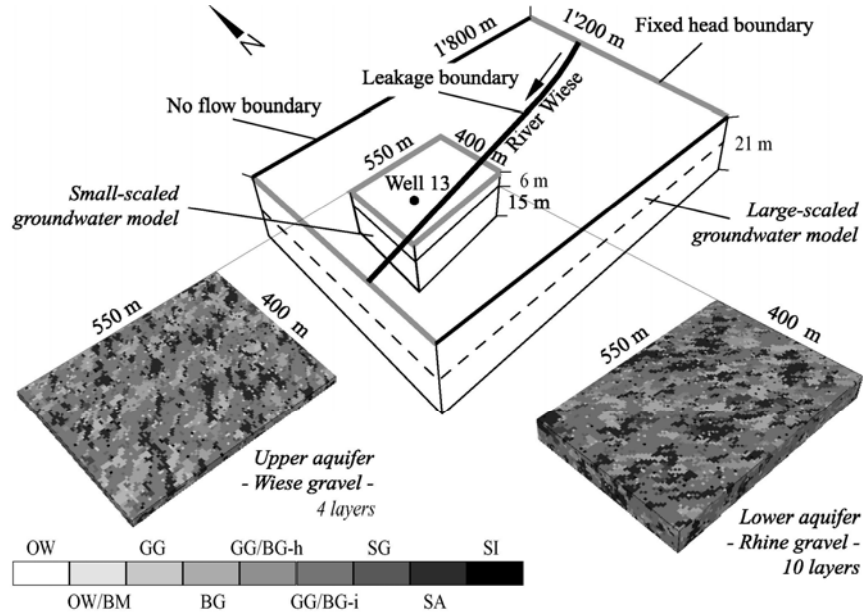


Fig. 3. Situation of the small-scaled groundwater model, which relies on stochastically generated aquifer properties. OW: open-framework gravel, OW/BM: open-framework/bimodal gravel couplets, GG: gray gravel, BG: brown gravel, GG/BG-h: alternating gray and brown gravel, horizontally layered, GG/BG-i: alternating gray and brown gravel, inclined, SG: silty gravel, SA: sand, SI: silt.

The changes in orientation and ranges of the sedimentary structures, caused by the above-mentioned interactions of the two rivers over time, are recognized and included in the model by partitioning the aquifer vertically into two hydrostratigraphic units. The generated sedimentary structures are characterized by randomly selecting hydraulic conductivity and porosity values given by means and variances in Rauber et al. (1998). Then, files with the distributions of the hydraulic parameters are generated and exported into PMWIN (Chiang and Kinzelbach, 2001) to perform steady-state groundwater flow and transport simulations.

3.4 Results of the small-scaled groundwater model

For each aquifer realization, a flow model computation was performed and the capture zone for drinking water well 13 was approximately defined by particle tracking. By superposition of all produced capture zones a probability distribution is obtained that describes the probability of a point on the ground surface belonging to the capture zone. This probability is given by the fraction of capture zones among all realizations containing the point.

Fig. 4 shows probability distributions of the capture zone of drinking water well 13 for conditions before and after river restoration as well as for low river discharge, moderate and high floods. Fig. 4a represents the calibrated groundwater model. The average of the mean squared deviations of observed versus calculated heads over the 10 flow simulations is 0.10 m². In Fig. 4b-f, predictions under changed boundary conditions are given, with each probability distribution representing the result of 10 flow and advective transport simulations.

The probability distribution of the well capture zone is strongly influenced not only by changing river discharge and riverbed structure, but also by subsurface heterogeneity. Preferential flow paths can be detected to some extent. In particular, zones along the riverbank with increased infiltration rates of river water can be recognized. River restoration is simulated by increasing the leakage factor by a factor of 10 and 100, respectively, within the restored river channel, assuming moderate and strong increase of the hydraulic conductivity of the riverbed.

The small-scaled groundwater model produces probable well capture zones depending on the uncertainty of the available data representing sedimentary structure types and the variability of hydraulic conductivity and porosity values for each.

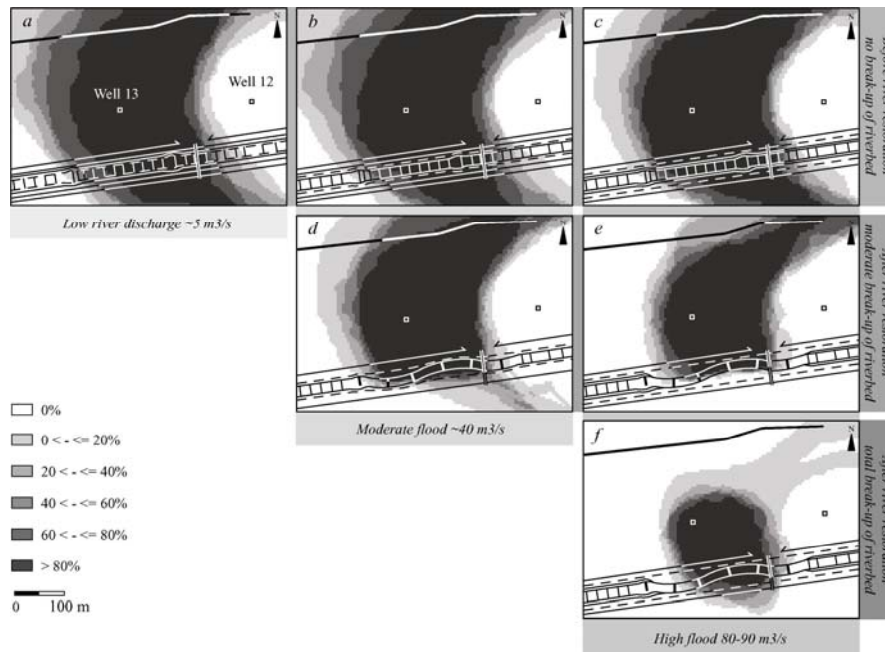


Fig. 4. Changes of the capture zone distribution of drinking water well 13 depending on river discharge, river restoration, water supply operation, and subsurface heterogeneity: (a,b,c) before river restoration; (d-f) after river restoration (increasing the leakage factor by a factor of 10 (d,e) and 100 (f)); (a) low river discharge ($\sim 5 \text{ m}^3/\text{s}$); (b,d) moderate flood ($\sim 40 \text{ m}^3/\text{s}$); (c,e,f) high flood ($80\text{-}90 \text{ m}^3/\text{s}$). Each capture zone distribution is based on 10 aquifer realizations and describes the probability of a point on the ground surface belonging to the capture zone. Groundwater extraction at well 13 is constant at $0.046 \text{ m}^3/\text{s}$.

4 Integration platform and software resources

GEOSSAV consists of an integration platform and individual simulation, visualization, and export modules, as shown in Fig. 5. The software integration platform and development environment for GEOSSAV is Tcl (Tool command language) and its graphical user interface Tk (Toolkit; (Ousterhout, 1995)). In addition, some of the Tcl/Tk extensions (Harrison, 1997) such as [incr Tcl], [incr Tk], [incr Widgets], and TkTable are integrated into GEOSSAV. Tcl/Tk was chosen because of its speed of use, breadth of functionality, flexibility for cross-platform deployment, and ease of integrating new extensions such as rendering 3D graphics through the OpenGL API (application programming interface). In addition, Tcl/Tk and its extensions allow the integration of diverse software resources irrespective of the programming language (e.g., Fortran, C/C++) in which they are written.

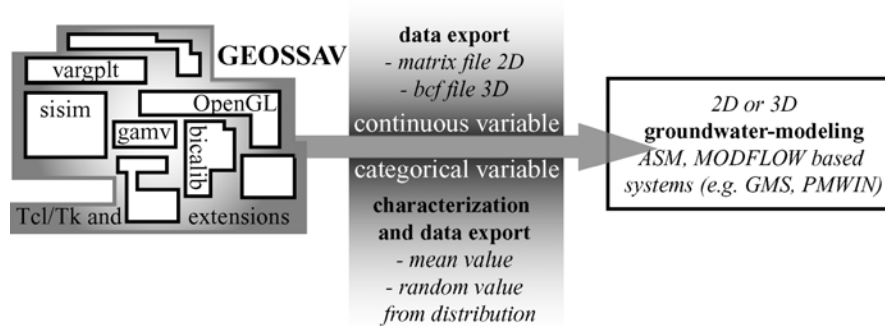


Fig. 5. The various modules integrated within GEOSSAV. Gamv computes the spatial variability of irregularly spaced data. Sisim is used for the sequential indicator simulation of categorical and continuous variables, and bicalib is used for considering soft data in the indicator formalism. OpenGL supports visualization of data and results in 2D and 3D. Export options allow files to be generated in data formats for use in other applications.

Compiled GSLIB modules without any enhancements are integrated into GEOSSAV: The sequential indicator simulation module 'sisim' (Deutsch and Journel, 1998) requires information about the spatial variability of the regularly or irregularly spaced data, which can be computed with the variogram module 'gamv' and then visualized with the module 'vargplt' and a PostScript display device (Deutsch and Journel, 1998). The indicator kriging approach allows the modeling of single property classes, represented by indicators, using single indicator variograms. In addition, the sisim algorithm is able to account for soft data. The integration of soft data in the indicator formalism is made possible by the Markov-Bayes option for cokriging using the module 'bicalib' (Deutsch and Journel, 1998).

The open, standardized API OpenGL (Open Graphics Library; (Fosner, 1997; Wright and Sweet, 2000)) has been integrated in the Tcl/Tk environment and is used for rendering of the 3D data distributions and for slicing perpendicular to the main coordinate axis. Export formats are compatible with widely used finite-difference groundwater modeling environments (e.g., ASMWIN (Chiang et al.,

1998); GMS (Environmental Modeling Systems Inc., 2002); PMWIN (Chiang and Kinzelbach, 2001)). Also data may be exported as individual files for single model layers (saved in ASCII matrix files) or as data files characterizing the complete 3D model set-up for MODFLOW-based groundwater simulation systems and saved in block-centered flow (bcf) package files (Harbaugh and McDonald, 1996). Groundwater flow and transport simulation is external to GEOSSAV.

4.1 Hardware and software requirements

GEOSSAV may be operated on Windows and on most kinds of Unix based operating systems. The following hardware components are required: (1) PC with at least a Pentium II processor running Windows NT 4.0 or higher, or SuSE Linux 7.3 or higher; (2) 24-bit color graphics card or better; (3) 64 MB or more Ram; and (4) 5 MB or more hard disk space.

Tcl/Tk is the software environment that embeds the implemented applications for hydrogeological analysis and allows an integrated use of them. The distributed GEOSSAV executable (which is platform dependent with different versions for the Win32 and Linux platform but sharing the same code base for all platforms) automatically calls all the necessary Tcl/Tk scripts.

4.2 Distribution information

GEOSSAV is distributed electronically at no cost. The current version is available at <http://www.unibas.ch/earth/pract>. The package includes everything needed to run GEOSSAV including the current version of GEOSSAV and all the necessary open-source Tcl/Tk interactive-environment software. Although the authors cannot provide any professional support service, they welcome comments and will attempt to respond to questions regarding the software and its application. The authors neither guarantee the integrity nor the proper performance of the software.

4.3 Further developments

GEOSSAV is useful for many earth sciences applications and other subsurface investigations because its main target is the simulation and visualization of heterogeneous subsurface properties using hard and soft data. Consequently, we are about to upgrade GEOSSAV with: (1) additional methods for data analysis (e.g., change of coordinate systems, declustering of data); (2) interactive curve fitting for selecting variogram models based on experimental variograms generated from field data; (3) subsurface characterization (e.g., Monte Carlo analysis); (4) the option to export additional data files for finite-difference groundwater flow and transport systems; and (5) the possibility to control and execute groundwater simulations, which are external to GEOSSAV. In addition, we anticipate the implementation of a design tool in GEOSSAV that will allow fully object-oriented

visualization of model data and simulated structures, which can be added in any order to the display.

5 Conclusions

GEOSSAV is described with an application as a tool for the integration of hard and soft geological and geophysical data in the stochastic simulation and visualization of hydrogeological properties of the subsurface. The implemented software packages support subsurface characterization from data processing through simulation and visualization to model verification and data export to external finite-difference groundwater simulation systems. In particular GEOSSAV allows to model categorical and continuous variables such as lithofacies types and distributions of hydraulic properties. The distinguished lithofacies can be explained based on depositional processes (e.g. fluvial sediment sorting processes).

Although the given example includes a characterization of the simulated geological structures by hydraulic parameters, GEOSSAV can definitely be used for other applications such as groundwater and/or soil contamination, site remediation, and ecology. In fact, whenever stochastic solutions are preferred to solve site-specific heterogeneity problems, GEOSSAV can be used as a user-friendly and adequate software solution.

Due to the Tcl/Tk integration platform and development environment as well as the modular set-up, GEOSSAV can be easily upgraded and adapted to specific problems, which may be solved using geostatistical methods.

Acknowledgments

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