Research paper/

An open, object-based framework for generating anisotropy in sedimentary subsurface models

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Abstract

The spatial distribution of hydraulic properties in the subsurface controls groundwater flow and solute transport. However, many approaches to modeling these distributions do not produce geologically realistic results, and/or do not model the anisotropy of hydraulic conductivity caused by bedding structures in sedimentary deposits. We have developed a flexible object-based package for simulating hydraulic properties in the subsurface – the Hydrogeological Virtual Realities (HyVR) simulation package which implements a hierarchical modeling framework that takes into account geological rules about stratigraphic bounding surfaces and the geometry of specific sedimentary structures to generate realistic

aquifer models, including full hydraulic-conductivity tensors. The HyVR simulation package can create outputs suitable for standard groundwater modeling tools (e.g., MODFLOW), is written in Python, an open-source programming language, and is openly available at an online repository. This paper presents an overview of the underlying modeling principles and computational methods, as well as an example simulation based on the MADE site in Columbus, Mississippi. Our simulation package can currently simulate porous media that mimic geological conceptual models in fluvial depositional environments, and that include fine-scale heterogeneity in distributed hydraulic parameter fields. The simulation results allow qualitative geological conceptual models to be converted into digital subsurface models that can be used in quantitative numerical flow-and-transport simulations, with the aim of improving our understanding of the influence of geological realism on groundwater flow and solute transport.

Introduction

Hydrogeologists typically need to characterize and represent the spatial distribution of hydraulic conductivity and porosity of recent (~ last 2 million years) geological material deposited in continental settings. Geological conceptual models can provide a framework for understanding subsurface heterogeneity (Anderson, 1989). Sedimentologists have also long recognized a hierarchy of bedding and structures within sedimentary deposits and have developed approaches to assist in the characterization of heterogeneous deposits that vary over large spatial and temporal scales (e.g., Miall, 1991; Aigner et al., 1999). Continental sedimentary deposits (e.g., glacial and fluvial sequences), and their associated hydraulic parameter distributions, can thus be represented at various scales, starting with stratigraphic contacts – these represent erosional events of depositional hiatuses that may form important hydraulic boundaries separating contrasting hydrostratigraphic units. Larger hydrostratigraphic units can be further sub-divided at various internal scales to better represent the spatial distribution of hydraulic properties that is controlled by smaller sedimentary depositional features. Variable sediment transport regimes can lead to the development of bedforms and sediment textures with varying orientation, which can cause these typically unconsolidated features to be hydraulically anisotropic. Previous studies have shown that variable anisotropy based on observed sediment bedding structures can affect groundwater flow (e.g., Borghi et al., 2015; Bennett et al., 2017) and solute transport and mixing (Bennett et al., 2017). It is therefore important to generate more realistic hydraulically anisotropic fields to further test hypotheses on the effects of heterogeneity and anisotropy in hierarchical sediments.

Numerous studies have applied hierarchical modeling frameworks to model aquifer materials (e.g., Scheibe and Freyberg, 1995; Weissmann and Fogg, 1999; Barrash and Clemo, 2002; Dai et al., 2004; Ritzi et al., 2004) using a variety of modeling approaches (see Koltermann and Gorelick, 1996). Object-based (or morphological) modeling approaches, which focus on the characteristic geometries of a sedimentary deposit, have been used in numerous hydrogeological studies (e.g., Jussel et al., 1994; Scheibe and Freyberg, 1995; Miller et al., 2000). In such approaches, the various sedimentary deposits observed are approximated by geometric forms and placed into the model domain. Within a hierarchical modeling framework, larger units are composed of smaller units (e.g., hydrofacies assemblages make up architectural elements). Object-based methods have not been well-utilized in groundwater research in the last twenty years, possibly due to the lack of available simulation packages. This paper presents an object-based simulation methodology where the full hydraulic conductivity tensor can be constructed at every grid cell using isotropic hydraulic conductivity, bedding parameters (dip and azimuth), and anisotropy ratios that are defined at every location within the domain. The simulation package we present fills the gap of an open-source object-based code for simulating geologically plausible realizations of anisotropic hydraulic conductivity fields.

The present study introduces a new framework for generating ensembles of hydrogeological conceptual models (or “virtual realities”). The key goals in the framework development are:

- The simulation of virtual spatial distributions of hydraulic parameters (particularly spatial distributions of full hydraulic-conductivity tensors) that are informed by sedimentary erosional and depositional concepts; and
- The development of an aquifer simulation platform that can be customized and extended by users to suit their particular research needs.

We have developed a new tool for modeling subsurface heterogeneity at a scale that cannot be practicably captured by aquifer-analog investigations and is relevant for groundwater studies at contaminated sites (~10^1-10^3 m). The Hydrogeological Virtual Realities (HyVR) simulation package can currently model sedimentary structures derived from fluvial hierarchical framework models. The ensembles of virtual realities generated can be used to investigate the effect of specific sedimentary structures on groundwater flow and solute transport dynamics.

In the following sections we introduce the modeling concepts and the computational methods implemented in HyVR; subsequently, the methods are applied in an example conceptual model based on the MADE site in Columbus, Mississippi, USA. Further details about computational methods and implementation of the HyVR simulation package can be found in the electronic repositories listed in the Supplementary Materials section.

Modeling concepts

The modeling approach used in the current study is underpinned by a hierarchical modeling framework that incorporates architectural element analysis; and by object-based modeling approaches. This section outlines these concepts as they apply to fluvial deposits, which constitute common and extensive aquifers.

Hierarchical modeling framework

We use a hierarchical modeling framework (e.g., Miall, 1991; Aigner et al., 1999) to characterize sedimentary features in the current study. We consider five hierarchical scales that we define as stratigraphic contacts, architectural elements, hydrofacies assemblages, hydrofacies, and microstructure.

Stratigraphic contacts are the largest scale of features (~10^2 to 10^4 m in lateral extent) that we consider here. In recent (~ last 2 million years) fluvial deposits, stratigraphic contacts represent allocyclic changes to depositional settings that are controlled by tectonic or climatic changes (e.g., Milankovitch cycles, Fischer, 1986). Examples of major strata bounded by stratigraphic contacts include deposits from glacial and fluvial systems.

Architectural elements (see Miall, 1985) are three-dimensional sedimentary features (e.g., channels) that are formed by autocyclic processes that occur within depositional systems (Beerbower, 1964). They are often superimposed on allocyclic sequences by higher frequency events that occur over periods of tens to thousands of years (Miall, 2013). Different fluvial systems will have their own characteristic architectural elements, and these may range from 10^1 to 10^2 m in lateral extent (Miall, 1985). Architectural elements are recognized by their outer bounding surfaces, which are often erosional, as well as by their internal facies assemblages (Allen, 1983).

Each architectural element is filled with sediment which may also exhibit internal structures that have a predictable or coherent spatial arrangement and relationship; these have been extensively studied in both modern environments (e.g., Heinz et al., 2003) and ancient deposits (e.g., Allen, 1983). For example, a tabular body formed of amalgamated gravel bars (a type of architectural element; see below) can consist of cyclical (i.e., interstratified) layers or assemblages of massive gravel, openwork gravel, and various crossbeds (e.g., Heinz et al., 2003). Each cycle would represent one assemblage. These assemblages often form hydraulically distinct zones, referred to as hydrofacies assemblages (e.g., Atkinson et al., 2014), that may have a lateral extent of ~10^0 to 10^2 m.

Finally, these assemblages are made up of individual sediment facies such as openwork gravel and massive sand, which may correspond to hydrofacies – units of similar hydraulic properties (Anderson, 1989). These may vary laterally on the order of 10^{-1} to 10^1 m. Within hydrofacies, the hydraulic conductivity and porosity may vary – which we denote microstructure, representing variations at scales ranging between ~10^{-3} and ~10^{-1} m. The hierarchical modeling framework is summarized in Figure 1.

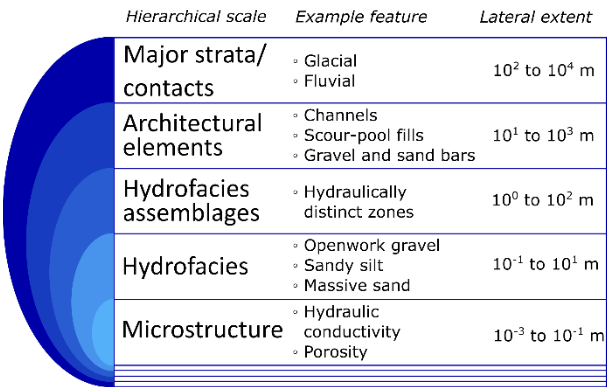

Figure 1: Hierarchical modeling framework diagram

The HyVR simulation package described in this study focuses on selected fluvial architectural elements and their associated hydrofacies assemblages. In its current state of development, the package can simulate geometries that can be used to represent several fluvial architectural elements, including (but not limited to): channels (CH), scour-pool fills (HO), gravel and sand bars (GB, SB), and laminated sand (LS) or laminated fines. Table 1 lists the architectural elements along with their typical geometries.

Table 1: Selected architectural elements generated using the HyVR simulation package

Architectural element	Object geometry
Channels	Extruded parabolas
Scour-pool fills	Truncated ellipsoids
Gravel and sand bars	Sheets
Laminated sand	Sheets
Clay lenses	Truncated ellipsoids

Object-based modeling approaches

Object-based methods have been implemented widely in subsurface simulation (e.g., Jussel et al., 1994; Scheibe and Freyberg, 1995; Deutsch and Tran, 2002) as they can preserve the three-dimensional forms of geobodies, are generally computationally efficient, and can be parameterized using geometric constraints and probabilistic rules derived from geological observations (Koltermann and Gorelick, 1996). Therefore, we use an object-based approach for simulating hydrofacies assemblages within architectural elements. The HyVR simulation package can simulate three simplified geometries: extruded parabolas, truncated ellipsoids, and sheets (see Figure 2); these can then be used to build a variety of architectural elements and hydrofacies assemblages (see Table 1). The implementation of this approach in the HyVR algorithm is outlined in the following section.

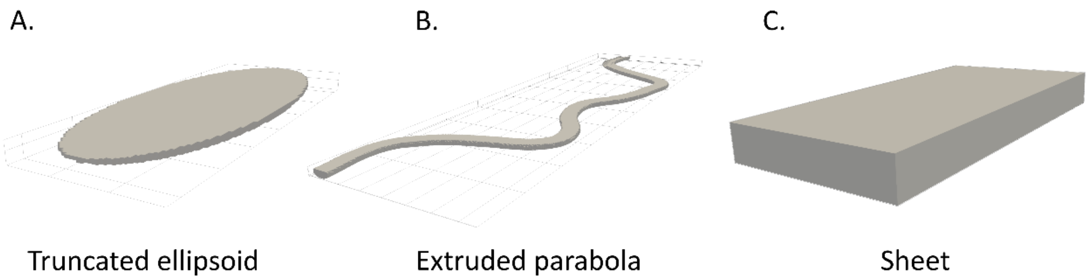

Figure 2: Object geometries currently implemented in HyVR.

Extruded parabolas

Parabolas extruded along arbitrary curves with variable sinuosity are useful to represent channels, which are ubiquitous in fluvial systems. Channels are preserved in the sedimentological record following some disturbance to the flow regime (e.g., channel avulsion). While they often contain channel deposits, they can also be filled by various types of material including fines and organics due to channel abandonment (e.g., oxbow lakes). In some depositional systems (e.g., glaciofluvial systems) the flow and sediment transport may be too dynamic for continuous channels to be preserved in the stratigraphic record. However, in lower energy environments (e.g., meander systems), channels are often preserved and may represent important controls (both barriers or conduits) to groundwater flow.

Truncated ellipsoids

Truncated ellipsoids are discrete features that have concave-up lower contact surfaces and generally flat top contact surfaces. They have been used in a number of studies (e.g., Jussel et al., 1994; Huber and Huggenberger, 2015; Bennett et al., 2017) to represent trough features (i.e., scour-pool fills) present in braided river deposits. Siegenthaler & Huggenberger (1993) presented a conceptual model in which these features are formed at stable channel confluences where scour occurs. Changes in the discharge regime of surface water flow may cause migration of the pool, and/or infilling of the scour pools. The former process can produce sets of cross-bedded troughs. Their persistence in sedimentary deposits is likely due to their low position within the stratigraphic record (Siegenthaler and Huggenberger, 1993). Truncated ellipsoids can also be used to represent discrete lenses embedded in a matrix of different material.

Sheets

Tabular, laterally extensive depositional units can be approximated as sheets. Sheet-type features are found with many different grain sizes, including fine-grained overbank deposits, laminated lacustrine bed deposits, and poorly sorted gravel traction sheets. The three-dimensional forms of these features depend on the flow regimes in which they were deposited and are therefore highly heterogeneous. They are often difficult to characterize, and it may therefore be appropriate to approximate these forms as sheets with more complex internal structures, such as approximating certain architectural elements (such as gravel bars and bedforms) as sheet geometries with dipping internal structure. This approach is used in the present study.

Generating hydrogeological virtual realities

To achieve our modeling aims we have developed a new algorithm for the simulation of hydrogeological parameter fields, denoted the Hydrogeological Virtual Reality simulation package (HyVR). The most important aspects of the HyVR package are summarized in this section. HyVR has been written in Python and is openly available online, facilitating user customization of the program.

During HyVR simulations, properties are assigned to regular model grids of three-dimensional, cuboid cells. The workflow of simulations follows the sequence of hierarchical units, from largest to smallest (see Figure 1). Simulations begin with the generation of major stratigraphic contact surfaces, followed by simulating the initial contact surfaces of architectural elements. Hydrofacies assemblages and associated hydrofacies are then simulated within each architectural element. Finally, the microstructure of the generated features is generated. Thus, each model grid cell is assigned a value for each hierarchical level. The computational methods used in the HyVR algorithm are briefly described in the rest of this section. For more detailed information about the computational methods implemented in HyVR, please refer to the online technical documentation (https://driftingtides.github.io/hyvr/).

Simulating contact surfaces of major strata and architectural elements

Major strata are defined by their upper mean elevations and the architectural elements that are to be included within them. In this way, they act as scaffolds for subsequent smaller-scale simulation of heterogeneity. Once the mean top and bottom system elevations have been defined, the top contact surface is generated; all model cells between the lower and upper contact surface are assigned to the strata. Contact surfaces can either be "flat" or "random", where the deviation from the mean plane is modeled using a multivariate standard normal dependence model. We used Gaussian covariance models in the present study to represent smoothly varying contact surfaces.

Architectural elements are initially defined using a lookup table that lists: the average bottom and top elevations of the unit, its name, and a stratum identifier. The lookup table can be specified by the user or randomly generated using input parameters defined for each stratum. The random generation of lookup tables begins with the random choice of an architectural element from those defined for an individual stratum; the probability of each architectural element being chosen is defined in the model parameter file. The thickness of the architectural element is then drawn from an independent random normal distribution defined for each stratum. To account for the erosive nature of many contact surfaces, the algorithm may erode the underlying elements – here the 'avulsion' thickness is subtracted from the bottom and top of the architectural element. Once the architectural element lookup table has been populated, architectural element contact surfaces are generated using the same procedure as used for major strata contact surfaces. When the architectural elements have been generated, external hydrofacies assemblage geometries and hydrofacies are simulated.

Simulating the geometry of hydrofacies assemblages and hydrofacies

The generation of hydrofacies assemblages and internal hydrofacies occurs stratum- and architectural-element-wise, beginning with the lowest architectural element in the lowest stratum. The simulation of hydrofacies assemblages is object-based, with random placement of geometric shapes within the architectural element. Currently, three shapes are supported: truncated ellipsoids, extruded parabolas, and sheets (see Figure 2). Truncated ellipsoids and extruded parabolas are "erosive" features – they are able to erode underlying units, and therefore the architectural element (and strata) boundaries may be altered during the course of the simulation.

Hydrofacies assemblages are assigned to each architectural element starting from the lowest depth of the element. Simulation proceeds layer-wise, with the thickness of each layer determined by an aggradation input parameter; the number of assemblage assigned in each layer is an input parameter. Assemblage outer boundaries are generated, and model grid cells that fall within these boundaries are assigned corresponding values. Five properties are assigned to each model grid cell during hydrofacies assemblage simulation: the unique identifier of the individual hydrofacies assemblage generated and its type; the hydrofacies code; and azimuth κ and dip ψ, properties denoting the angle of the bedding plane from the mean direction of flow and from the horizontal plane, respectively.

Truncated ellipsoids represent trough-like features. The method for generating the boundaries of these features has been described previously by Bennett et al. (2017). The center of the truncated ellipsoid (x, y coordinates) and the "paleoflow" angle α (i.e., the orientation of the major ellipsoid axis) are drawn from a random uniform distribution with bounds stipulated by the user. The boundary of the truncated ellipsoid is simulated using the geometry lengths from the input parameters. The internal structure of truncated ellipsoids can be defined in the following ways: (1) trough-wise homogeneous, with constant azimuth and dip; (2) bulb-dip-type, with azimuth and dip values based on the three-dimensional gradient at the ellipsoid boundary; (3) bulb sets, comprising nested alternating hydrofacies with azimuth and dip values generated as for bulb-dip-type; and (4) dip-set internal structure, where the features have a constant azimuth and dip but the assigned hydrofacies alternate throughout the truncated ellipsoid. Figure 3 shows the internal structures of truncated ellipsoid assemblages that can be generated. Alternating hydrofacies that comprise the internal structure have a set thickness.

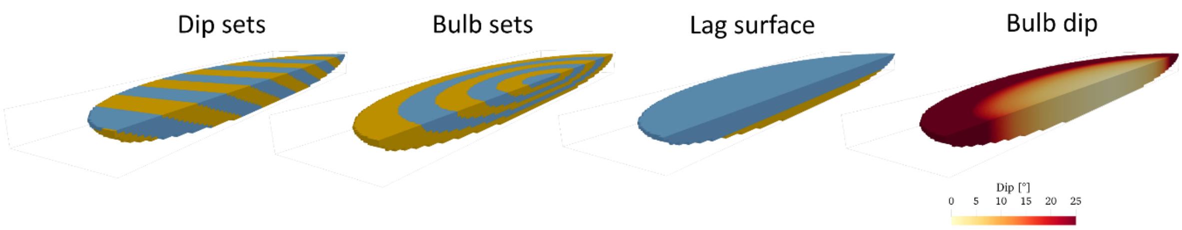

Figure 3: Internal structure of truncated ellipsoid geometries.

Extruded parabolas are assigned along arbitrary curves (or centerlines). Extruded parabola centerlines in HyVR are parameterized using the disturbed periodic model implemented by Ferguson (1976); we use the second-order autoregressive model approximation described in Equation 16 of that work. Two-dimensional "channel" velocities $\vec{v}$ are evaluated at the centerline and then interpolated to grid cells using an inverse-distance-weighted interpolation; azimuth values are derived from these velocities. Dip values of grid cells within the extruded parabola are assigned based on input parameters. If alternating hydrofacies are to be simulated, these are constructed by creating dipping planes that are evenly spaced along the extruded parabola centerline. To account for the multiple channels that are often concurrently present in many river systems, multiple extruded parabolas can be generated at each simulation depth. Note that in HyVR there is no interaction of extruded parabolas, and subsequent extruded parabolas will supersede – or "erode" – those previously generated. Once the predefined number of extruded parabola has been simulated, a three-dimensional migration vector may be added to the extruded parabola centerlines and the extruded parabola assignment to model grid cells begins again.

For erosive hydrofacies assemblages (i.e., truncated ellipsoids and extruded parabolas), generation starts at $z_{AE\,unit}^{bot} + AE_{depth} \cdot \beta$ where β is a buffer term that allows the user to control how much of the underlying unit is eroded. Lag surfaces can also be simulated at the bottom of erosive features and assigned a different hydrofacies value.

Sheets are comparatively simple to generate as they are laterally extensive within major strata boundaries. The internal structure of sheet features may be homogeneous (i.e., without internal structure), or laminations can be generated. In the HyVR algorithm, laminations are simulated sequentially by assigning all model grid cells between a specific elevation interval the appropriate hydrofacies codes. Dipping set structures can also be incorporated into these features; these structures may vary in orientation.

Hydrofacies assemblages may be populated with dipping hydrofacies structures. Such structures are generated by creating planes at regular intervals within individual assemblages that fill architectural elements. In truncated ellipsoids, the planes are constructed along the centerline of the assemblage, perpendicular to the paleoflow angle α. In extruded parabola assemblages, the planes are constructed along the centerlines and are perpendicular to $\vec{v}$. The distance from the center of each model grid cell to all planes is calculated and then the model grid cells between planes are assigned a hydrofacies value. To account for cyclicity of hydrofacies, it is possible to control the sequence of hydrofacies assignment within internal structures (e.g., by juxtaposing openwork gravels with sandy gravels). The HyVR package also allows for linear trends in hydrofacies assemblage geometry sizes with increasing elevation or horizontal direction (x-direction only). Such trends may be set for each architectural element included in the model parameter input file.

Simulating hydraulic parameters

Spatially distributed hydraulic parameters are simulated once all hydrofacies assemblages (and hydrofacies) have been generated. The hydraulic parameter outputs of HyVR are: the porosity $\theta(x, y, z)$ and an isotropic hydraulic conductivity $K_{iso}(x, y, z)$ value (later used as the within-bedding conductivity), the ratio of within-bedding to across-bedding hydraulic conductivity $K_{\parallel}/K_{\perp}$, and the associated full hydraulic-conductivity tensor $\mathbf{K}(x, y, z)$ in each model grid cell.

The internal heterogeneity of hydraulic parameters is first generated for each individual hydrofacies assemblage simulated in the previous steps. Spatially varying $\ln(K_{iso})$ and θ fields are generated for each hydrofacies present in an assemblage using spectral methods to simulate random multi-Gaussian fields with exponential covariance functions (Dietrich and Newsam, 1993). These methods are identical to those used simulating contact surfaces, but in three dimensions. An anisotropy ratio is also assigned to each model grid cell according to the hydrofacies present; these ratios are globally constant for each hydrofacies. A background internal heterogeneity is simulated for model grid cells that are not within assemblages using values defined for each architectural-element type. The associated simulation methods for these are the same as for the within-element internal heterogeneity. Once isotropic hydraulic-conductivity values have been assigned to all model grid cells, spatial trends may also be applied. As for trends in hydrofacies assemblage geometry, K_{iso} trends are assigned using a linearly-interpolated factor in the x- and/or z-direction. The K_{iso} value of each model grid cell is then multiplied by these trend factors.

The full hydraulic-conductivity tensors $\mathbf{K}$ for each model grid cell are then approximated by rotating the diagonal tensor of principal hydraulic-conductivity values to the orientation of the local bedding structure, represented by dip ψ and azimuth κ (see Bennett et al., 2017, or the technical documentation, for further details). Lateral hydraulic conductivity in the bedding plane is assumed to be isotropic (i.e., $K_{xx} = K_{yy}$) and vertical conductivity is calculated by dividing the lateral conductivity by the anisotropy ratio K_h/K_v. Once $\mathbf{K}$ has been calculated, the simulated parameter files are saved and can be used for groundwater flow and solute transport simulations.

Model inputs and outputs

Model input parameters are contained in `*.ini` files which can be easily customized using a text editor. This format was chosen for its readability and the ability to be used with numerous programing languages.

It is an important goal of the development of the HyVR simulation package that outputs should be suitable for hydrogeological applications. Therefore, HyVR simulation outputs can currently be saved in a variety of formats including: native Python and MATLAB data files; VTK rectilinear grid files, to facilitate visualization in ParaView (Ayachit, 2015); HydroGeoSphere input files (Aquanty, 2012); MODFLOW-2005 layer property flow input files (Harbaugh, 2005); and MODFLOW 6 node property input files (Hughes et al., 2017), allowing for the use of the XT3D option (Provost et al., 2017). Due the restriction of the finite volume method, simulation outputs in MODFLOW-2005 format are restricted to the isotropic hydraulic-conductivity values and the anisotropy ratios $K_{\parallel}/K_{\perp}$ at each model grid cell.

An example simulation

To demonstrate the HyVR simulation package, we provide an example parameter field simulation mimicking the Macrodispersion Experiment (MADE) site at the Columbus Air Force Base, Mississippi, USA. The MADE site has been the focus of numerous hydrogeological investigations (e.g., Boggs et al., 1990; Bowling et al., 2005; Bohling et al., 2016).

HyVR input parameters

Based on the geological conceptual model of Bowling et al. (2005, Fig.13), we divided the stratigraphy of the MADE site into four major strata with approximate mean elevations below ground surface (see Table 2): Meandering fluvial stratum (0-3 meters below ground surface); braided fluvial stratum (3-8 mbgs); transitional sand stratum (8-9.5 mbgs); and marine sand stratum (9.5-11 mbgs). The meandering fluvial stratum consists of horizontally stratified floodplain clayey silts that are interspersed with channels filled with finer-grained silty clay and a coarse sandy gravel lag (Bowling et al., 2007). The braided fluvial stratum below comprises a sandy gravel matrix (Boggs et al., 1990) that includes cross-bedded dipping units (Bowling et al., 2007) which we interpret as discrete scour-pool fill architectural elements (cf. Siegenthaler and Huggenberger, 1993). The transition stratum is expressed as fine-grained sands with occasional silt and clay laminations (Boggs et al., 1990). The lowermost stratum included in this subsurface model is the Cretaceous Eutaw Formation that consists of marine clays.

Table 2: Selected strata simulation input parameters.

Major strata	Mean elevation of contact surfaces [m below ground surface]	Architectural elements
Meander	0.0-3.0	Meander channel
		Silt sheet
Glaciofluvial	3.0-8.0	Cross-bedded scour
		Sandy gravel
Transition	8.0-9.5	Sand sheet
		Clay lens
Clay	9.5-11.0	Clay sheet

Seven architectural elements have been identified for the example simulation. Laterally continuous features were modeled as sheet-type architectural elements. These elements are assigned one lens thickness and hydrofacies. Discrete hydrofacies assemblages within clay lenses and scour architectural elements were modeled as truncated ellipsoids. For the clay lenses, the dimensions of the assemblages were estimated; for the cross-bedded scour-pool fills, dimensions were derived from similar features observed in gravel pits in northeastern Switzerland by Jussel et al. (1994). The meander channel was simulated using extruded parabolas, with parameters were derived from outcrop analogs described by Bowling et al. (2007, Fig.8a). Selected architectural element input parameters are summarized in Table S1 of the Supporting Information.

Hydrofacies for the MADE site example simulation are: Sandy gravel, sandy clayey gravel, openwork gravel, sand, fine sand, clay, and silty clay. The first four hydrofacies in this list were categorized by Rehfeldt et al. (1992) in the braided fluvial system and we have used the hydraulic-conductivity values that are reported therein. Additional hydrofacies were necessary for the other systems present at the site, based on the characterization of Bowling et al. (2005). Hydraulic conductivity and other hydraulic parameter values for these hydrofacies were derived from a variety of sources (Mitchell, 1956; Witt and Brauns, 1983; Jussel et al., 1994). Selected simulation input parameters for hydrofacies have been included here (see Table 3). More information about the hydrofacies parameters and their derivation, as well as the parameter file with all simulation input parameters is included in the Supporting Information.

Table 3: Selected simulation input parameters for hydrofacies

Hydrofacies	ID	K_h [m/s]	$\frac{K_h}{K_v}$	ϕ
Sandy gravel	0	1×10^{-5} [a]	1 [d]	0.20 [d]
Sandy clayey gravel	1	1×10^{-7} [a]	0.25 [d]	0.17 [d]
Openwork gravel	2	1×10^{-1} [a]	0.025 [d]	0.35 [d]
Sand	3	1×10^{-4} [a]	1 [d]	0.43 [d]
Fine sand	4	1×10^{-5} [b]	2.3 [e]	0.43 [d]
Clay	5	2×10^{-9} [c]	2.3 [c]	0.52 [c]
Silty clay	6	3×10^{-9} [c]	1.7 [c]	0.45 [c]

[a](Rehfeldt et al., 1992)
[b](Freeze and Cherry, 1979, Table 2.2)
[c](Derived from Mitchell (1956), see supplementary material)
[d](Jussel et al., 1994)
[e](in Chapuis and Gill, 1989; Witt and Brauns, 1983)

Model results

The results of the HyVR simulation of the MADE site example look similar to the geological conceptual model from which the input parameters were derived (Figure 4). The cross-bedded structures observed by Bowling et al. (2005) are visible in the example realization depicted in Figure 4. The isotropic hydraulic-conductivity, porosity, dip and azimuth parameter fields vary based on their location within (and outside of) the simulated architectural elements. The HyVR simulation package takes approximately 60 minutes to generate a parameter model with a model domain size of $\ell \times w \times d = 200\text{ m} \times 70\text{ m} \times 11\text{ m}$ and a model grid resolution of $\Delta x \times \Delta y \times \Delta z = 0.5\text{ m} \times 0.5\text{ m} \times 0.1\text{ m}$.

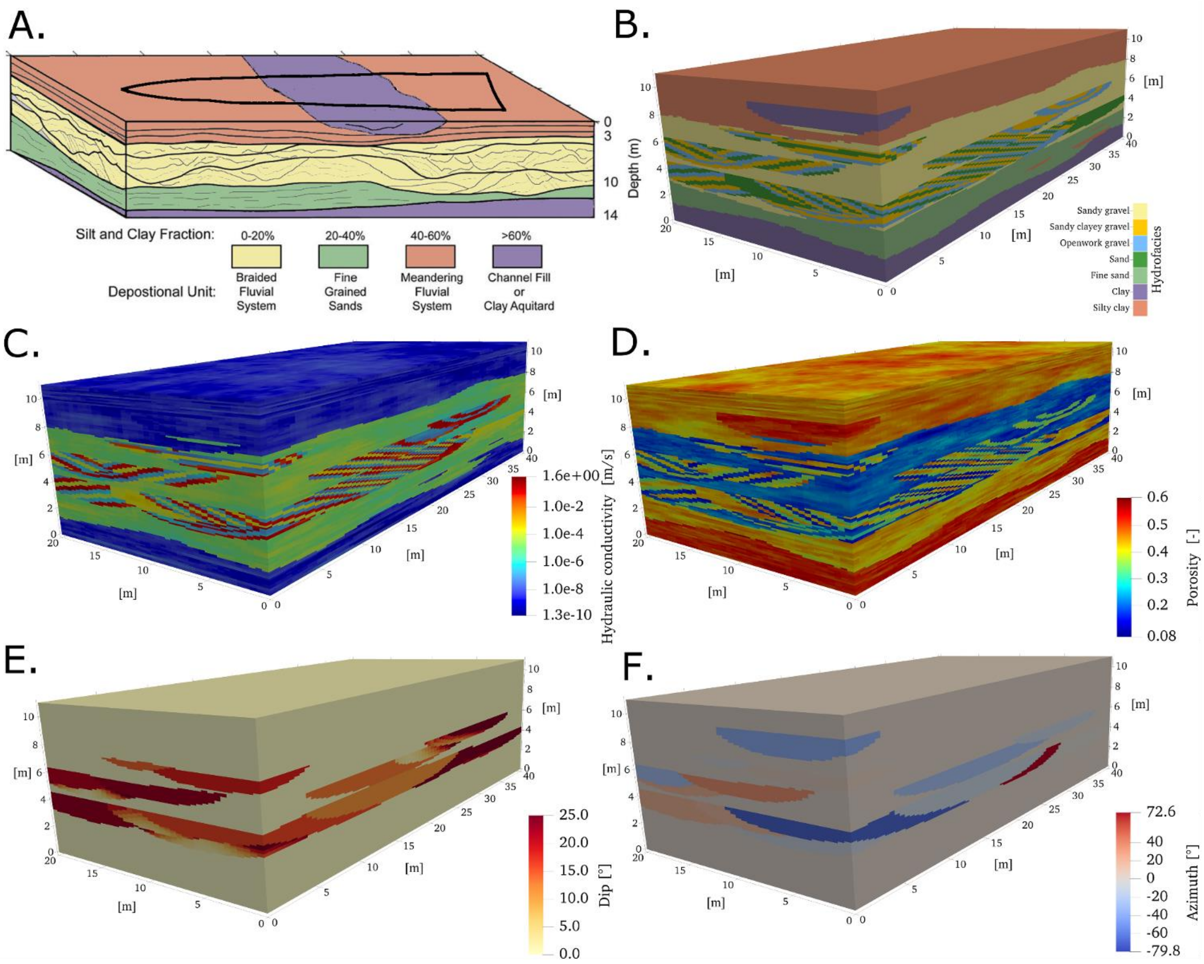

Figure 4. Panel A: Geological conceptual model of the MADE site amended from Bowling et al., (2005, Fig.13, p.901). Panels B-F: Distributed parameter fields from a single realization of the HyVR simulation using input parameters derived from characterization of the MADE site.

Discussion

The HyVR package has been developed with the goal of simulating clastic sedimentary deposits, with a focus on fluvial systems. Apart from the current suite of geometries possible in HyVR (channels, truncated ellipsoids, and sheets) there are numerous other geometries that could be implemented (e.g., lobes, wedges, ribbons) to represent additional fluvial architectural elements (e.g., lateral accretion units, levees, crevasse splays). The key requirement for simulating these features is that their form can be parameterized and applied to the simulation model grids. There is also scope for deriving input parameters from geostatistical analysis of site observations. For example, Markov chains or transitional probabilities (Carle and Fogg, 1996) based on borehole information could be used to constrain the probability of an architectural element being generated, or the mean geometry of simulated hydrofacies assemblages. The HyVR simulation package has been developed to be flexible, has extensive code commenting and documentation, and is openly available so that it can be extended according to the specific research needs of users.

The intent of HyVR is to generate sedimentary deposits that mimic a specific site with respect to the sedimentary features found there. Geological conceptual models can thus be converted from qualitative drawings to digital subsurface models that can be assessed quantitatively in numerical simulations of groundwater flow and solute transport, allowing the influence of sedimentary structures on these processes to be explored. Although the fields simulated with HyVR cannot honor direct measurements at given sites (e.g., borehole information), other site data (e.g., mean system boundaries, mean assemblage geometries, hydrofacies present) and associated statistics (e.g., mean and variance of hydraulic conductivity) can be incorporated to develop site-specific conceptual models in data formats that are suitable for groundwater flow and solute transport simulations. We do not expect that such flow-and-transport simulations will match site measurements of hydraulic head and concentrations – the latter would require calibration and conditional simulations (see below). However, HyVR allows users to build ensembles of plausible conceptual models that can be used for hydrogeological scenario testing.

Process-based sedimentological models (e.g., Nicholas et al., 2013; MINES ParisTech / ARMINES, 2017) provide increasingly detailed models of fluvial stratigraphy. The adaptation of these existing process-based models for hydrogeological studies provides an alternative way forward in the goal of simulating parameter fields that resemble observed deposits, albeit more computationally demanding. Currently, the lack of bedding structure outputs (i.e., dip and azimuth) from many process-based sediment deposition models is a barrier to their ability to simulate full hydraulic-conductivity tensors. One option would be to derive the necessary bedding structures from the simulated contact surfaces. Such a method could be used with a variety of existing models in order to simulate the full hydraulic-conductivity tensor.

The HyVR algorithm may also be a useful tool for the generation of three-dimensional training images for multiple-point geostatistics algorithms that allow for conditioning to hydraulic-conductivity observations (e.g., Mariethoz et al., 2010). The creation of suitable three-dimensional training images is an ongoing challenge for implementing multiple-point geostatistics, and conditioning training images to measurements of dependent quantities, such as hydraulic heads or concentrations, is a much more complex task than conditioning on conductivity measurements (Linde et al., 2015).

Conclusion

In the present study we have introduced a new framework for simulating subsurface models that are informed by geological depositional concepts. The HyVR simulation package produces spatially distributed parameter models, including full hydraulic-conductivity tensors and porosity. The parameter fields generated are suitable for standard flow-and-transport simulation packages, such as the MODFLOW family of programs. HyVR is openly available so that it forms a codebase that can be used by hydrogeological researchers and practitioners to explore subsurface heterogeneity in clastic sedimentary systems and its influence on groundwater flow and solute transport.

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Supplementary Materials

The most current versions of the simulation package and technical documentation are available at https://github.com/driftingtides/HyVR and https://driftingtides.github.io/hyvr/ respectively.

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