HYBRID DETERMINISTIC AND STOCHASTIC HYDROSTRATIGRAPHIC MODELING OF A COMPLEX GLACIAL AQUIFER SYSTEM
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1. INTRODUCTION

At the Pall Life Sciences (formerly Gelman Sciences) site in Ann Arbor, Michigan, USA, wastewater containing 1,4-dioxane was discharged into unlined seepage lagoons and spray irrigated across a 15-acre field from 1967 to 1985. 1,4-Dioxane is readily soluble in water but resistant to microbial degradation and adsorption to soil particles (USEPA 2006). Mapped contaminant plumes (Figure 1) extend several kilometers in different directions from the original source area and provide a tracer-like record of solute transport through 80 m of glacial drift underlying the site and surrounding area. Despite substantial attempts to contain and remove the 1,4-dioxane following its discovery nearly three decades ago, remediation activities continue to this day along with efforts to characterize and model the aquifer system beneath a groundwater Prohibition Zone established in 2005. An array of more than 175 monitoring wells and 20 extraction wells has been drilled in the area, where the deepest known plume appears to be advancing toward a municipal water supply well and the Huron River. The experience at this site underscores the need for improved models of complex glacial aquifer systems. This study employs hybridized models incorporating stochastic variability within a deterministic hydrostratigraphic framework to model spatial variability of physical hydrogeologic properties in western Ann Arbor. Such a hybrid approach, described below, is expected to expand the space of uncertainty associated with model-generated contaminant transport predictions in this complex glacial aquifer system.

Figure 1. Location of PLS Site and monitoring well distribution, Ann Arbor, MI. Recessional moraine [surface geology after Kunkle (1960)]
1 ppb
85 ppb
500 ppb
Composite 1,4-dioxane plume map circa 2004
PLS Property

Figure 1. Location of the Pall Life Sciences study site and monitoring well distribution. 1,4-Dioxane concentrations shown as mapped in 2004.

2. APPROACH

The Pall Life Sciences (PLS) site is a natural laboratory for investigating solute transport in a complex glacial aquifer system. It sits on the northwest flank of the northeast-southwest trending Fort Wayne terminal glacial moraine (Leverett and Taylor 1915). Multiple aquifers with contrasting hydraulic head gradients lie directly beneath the PLS property and glaciotectonic sediment deformation appears to be minimal there. Data include abundant subsurface well control along with more than two decades of static water level and 1,4-dioxane concentration data. A two-step approach was employed to model the distribution of aquifer materials and their physical properties in the study area.
First, a deterministic hydrostratigraphic framework was developed from an allostratigraphic interpretation defining the three-dimensional distribution of aquifer and aquitard units, constrained by available hydraulic head and contaminant concentration data. The resulting hydrostratigraphic architecture was transferred to a numerical flow and transport (MODFLOW) model. Second, stochastic modeling was employed to generate an ensemble of realizations defining three-dimensional hydraulic conductivity fields within that deterministic hydrogeologic framework.

2.1 Deterministic Hydrostratigraphic Modeling

The glacial stratigraphy is exposed within local sand and gravel pits located on the flank of the Fort Wayne Moraine (Figure 1). Ten stratigraphic sections were measured along the east and south face of a quarry across a composite thickness of approximately 30 meters (Frahm 2011). The measured sections were correlated using an exposed till contact as a datum. The base of the till is sharp, subhorizontal, and laterally continuous across 260 m of exposure. This surface delineates a macroscopic change from the fine-textured till above to coarse, clastic aquifer below. Below the contact, stratigraphic units were defined by erosive surfaces, abrupt changes in particle size, and 1-6 m thick fluvial fining-upward sequences. Most units contain coarse grained particles and are poorly sorted, ranging from fine sand to boulder size. Occasional lenses of moderately- and well sorted medium grained sand may provide preferential pathways for transmission of groundwater.

Monitoring wells, most of which were gamma logged, provide the basis for detailed subsurface correlation across the study area. In addition, available head and concentration time series data provide an important constraint on hydrogeologic interpretations. In contrast to a more conventional lithostratigraphic correlation methods, an allostratigraphic approach was employed to identify and correlate bounding surfaces that divided the glacial sediments into mappable ‘allohydrostratigraphic’ units. Based initially on gravel pit exposure observations, and subsequently upon correlation of identified allostratigraphic surfaces into the subsurface, recognition criteria were developed to identify discontinuities within the glacial sediments (Frahm 2011). These criteria included: 1) changes in gross lithology; 2) changes in texture; 3) changes in gamma response; and 4) truncation geometries of correlated surfaces. For example, abrupt vertical or horizontal changes in sediment textural lithology (coarse-grained to fine-grained, fine-grained to coarse-grained) were indicative of potential allostratigraphic surfaces. Sharp, laterally continuous basal diamicton contacts are associated with glacial readvance, and represent a distinct change in depositional energy. The incision and fill of large scale channelized sand and gravel units, including the presence of basal lag gravels suggest amplification of the flow regime and represent discontinuities within the glacial deposits. When they can be correlated across gravel pit exposures or subsurface cross sections, contacts like these are well suited for allostratigraphic definition of major hydrostratigraphic units.

Figure 2. Subsurface cross section locations. Base map produced by Environmental Health Division, Department of Public Health, Washtenaw County, Michigan (Sources: MiGDL Pall/MDEQ Database, Washtenaw County GIS).
Eight hydrostratigraphic cross sections (Figures 2, 3) were interpreted based on geologists’ logs and gamma logs for lithological control. Available hydrogeologic data including hydraulic head and contaminant concentration data from the monitoring wells was used to interpret connectivity of aquifer units. Concentration data used were available through December 2010, and comparative hydraulic head data were drawn from the September 2010 comprehensive annual sampling event. Data were compiled into an extensive database and uploaded into RockWorks15 geological modeling software. The database includes well locations, depths, and relevant elevations, the depth of well screens, drillers’ and geologists’ logs describing the sediments encountered. Where available, contaminant concentrations or Simulprobe data were included, as well as digitized natural gamma logs. The Rockworks database was used to construct a 3D model of the hydrostratigraphic architecture based on the interpreted allostratigraphic surfaces. The resultant model constitutes an internally consistent hydrostratigraphic architecture for the aquifer system in the west Ann Arbor region.

![Figure 3. Hydrostratigraphic cross section G-G’ (see Figure 2 for location). Interpreted aquifer units are shown in yellow, aquitard units green, bedrock surface gray. Allostratigraphic bounding surfaces are numbered 0 through 8.](image)

The elevation of bounding surfaces was mapped using Surfer software. Adjacent surfaces were subtracted using grid arithmetic to generate isopach maps of succeeding aquifer and aquitard units. Isopach and structure contour map grids were then transferred to MODFLOW to define explicitly deterministic aquifer and aquitard units that were subsequently populated by stochastic realizations of hydraulic conductivity distributions.

### 2.2 Stochastic Modeling

Geostatistical simulation of aquifer properties (conditioned to gamma log observations) was employed to model smaller scale hydraulic conductivity variability within the larger deterministic hydrostratigraphic framework using a three step process. First, continuous random fields of natural gamma radiation response recorded in monitoring well logs located throughout the site were generated (Pappas and Lemke 2011). Natural gamma radiation counts were normalized to account for variation introduced by different logging and drilling equipment. Gamma values were also analyzed for variability related to changes in sediment texture and separate variograms were constructed for vertical and horizontal (omnidirectional) gamma variation. One hundred stochastic realizations of gamma values were then constructed using a Sequential Gaussian Simulation algorithm and conditioned to natural gamma radiation measurements for 77 wells in the study area. Depth intervals in each well were classified as aquifer or aquitard based on their position within the deterministic allohydrostratigraphic interpretation. Aquifer and aquitard simulations were generated separately (using independent variograms and conditioning data).

Second, an empirical relationship was used to transform simulated gamma values to K values (Figure 4). This relationship was established using laboratory hydraulic conductivity measurements on samples taken from a continuous rotosonic core at monitoring well MW-96. Hydraulic conductivity was assigned to 30x30x3m model cells throughout a 14km² area embedded within a regional groundwater model.
Figure 4. Empirical correlation of hydraulic conductivity as a function of natural gamma radiation log values for samples taken from corresponding depths in MW-96.

Finally, individual cells were extracted from paired aquifer and aquitard realizations in locations corresponding to the distribution of aquifer and aquitard units within the 3D hydrostratigraphic model and merged into a single 3D model honoring the original allohydrostratigraphic interpretation. In this way, 100 composite realizations containing spatially distributed parameters representative of aquifer and aquitard materials were generated (Figure 5). These procedures required the creation of two computer programs, DETERMINE.for, which interrogates the hydrostratigraphic model surface grids to determine which VMODFLOW grid cells correspond to aquifer/aquitard material; and GSL2VMF.for, which constructs the aquifer/aquitard composites and writes an output file in .VMP property file format for insertion into the MODFLOW model.

Figure 5. Distributions of hydraulic conductivity property values for: (a) aquifer material in model layer 20; and (b) aquitard material in model layer 20 in the study area in the central portion of the MODFLOW model. Note that VisualMODFLOW does not have the capacity to display K property colors along a color spectrum (i.e., from low to
high values); rather, property color values are assigned randomly. Thus the complimentary distribution of aquifer and aquitard units is shown separately here for a single layer to illustrate the stochastic infill of K values within the deterministic hydrostratigraphic architecture.

3. FUTURE INVESTIGATIONS

A priori ranking of the 100 stochastic realizations is underway using K value distributions for flow paths along the primary migration direction between the source area and the Huron River, a potential groundwater discharge location at the site. Relevant transport metrics (e.g., first arrivals and breakthrough times at the river calculated using MODPATH and MT3D) will be compared among realizations to evaluate the degree to which stochastic variability influences transport and whether a priori rankings can be used to identify realizations representing the range of transport behavior uncertainty predicted using the full ensemble.

4. REFERENCES


Pappas, L.K. and L.D. Lemke, 2011, Connecting stochastic and deterministic hydrostratigraphic models of the Quaternary Fort Wayne Moraine glacial aquifer system, Ann Arbor, Michigan, USA; Geological Society of America Abstracts with Programs, 43(5) p. 80.
