Qualitative and Quantitative 3D Modeling of Surficial Materials at Multiple Scales

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INTRODUCTION

An understanding of the distribution of surficial materials is key to many problems in geological engineering, mineral-resource inventory, and environmental remediation. However, for most states the zone between the surface (usually represented by surface glacial geology and the cooperative soil survey) and bedrock is unmapped. In Ohio, regional-scale maps of soil, surface glacial geology, and bedrock have been available for over 100 years, but concentrated mapping of the full sequence of surficial materials did not begin until 1998. The Ohio Division of Geological Survey (ODGS) is conducting three-dimensional (3D) mapping and modeling of surficial materials at the 1:100,000 scale. Currently, over one-third of the state has been mapped (concentrating on glaciated areas) at the 1:100,000 scale using qualitative methods based on geologic interpretation and drafting on Mylar (for an example of a completed product, see Swinford et al., this volume). Surficial materials are represented by two-dimensional (2D) polygons, which are assigned alphanumeric sequences describing sediment type, thickness, and lateral distribution ("stack" maps, Kempton, 1981), providing information in the third dimension. Mapping is conducted from the surface to the bedrock interface using soil maps, legacy geologic maps, water wells, bridge borings, and detailed site studies (mainly from environmental remediation). Envisioned applications for the GIS data and maps include surface/ground water simulations, mineral-resource inventory, and geologic engineering (seismic hazards, landslides, etc.).

As part of this mapping work, quantitative methods based on geostatistics are also being investigated. Lithology (clay, silt, sand, gravel) is modeled using sequential indicator simulation (Journel, 1983; Deutsch and Journel, 1998) to investigate methods for modeling stratigraphic and facies-scale variability at the 1:24,000-scale. Simulation is based on the same principles as kriging, but Monte Carlo techniques are used to develop multiple models (realizations) or configurations from one data set rather than obtaining a single, optimized estimate of lithology. Geostatistic simulation provides a range of statistically possible configurations of the subsurface that are faithful to the well data and statistical structure. While useful in themselves as 3D models, geostatistical models can give guidance to stack mapping by exposing consistent configurations of lithology. The amount of horizontal continuity in the models can give some measure of the uncertainty or appropriateness of assigning a stack sequence to potentially complex sediments of buried glacial valleys.

The goal of this paper is to illustrate the application of both methodologies being pursued at the ODGS to map unconsolidated sediments. Results are compared to enhance the understanding of the strengths and weaknesses of both approaches, and to discern how information from one technique can be used to improve the other. Geostatistical simulation has much to offer as a technique for 3D modeling. Output is in a 3D grid format ("voxel") and ready for volumetric (inventory) calculations or input into numerical models such as flow simulations for groundwater. There are scientific advantages as well; model parameters and procedures are completely traceable, so the maps are more "scientific" in that they meet the requirement of repeatability. While subjectivity is reduced, such modeling still requires much interpretation and "trade craft." A key advantage of simulation is the generation of multiple versions ("realizations") of the model that obey the data and the spatial structure. This aspect of simulation provides myriad possibilities for the assessment of uncertainty, ranging in complexity from generating basic statistics to describe variations between simulation runs to full analysis of the effect of uncertainty on all model parameters. Uncertainty assessment is key to evaluating risks when using the models for real world decisions. However, simulation techniques are not a way to generate maps quickly (good geostatistical practice requires careful, time-consuming investigation), nor map large areas (computation demands are limiting). Reconnaissance mapping over large areas is still the realm of traditional geologic mapping due to the limitations of the data (interpretation is needed over interpolation) and computation limits of large 3D voxel grids. This study proposes that both traditional mapping and geostatistical simulation have important and complementary roles in surficial mapping and characterization.

Mapping work for the 2006 fiscal year National Cooperative Geologic Mapping Program-STATEMAP component project is located in the Ashtabula and Youngstown 1:100,000 scale quadrangles located in northeast Ohio. This project area is the focus of this contribution. The area is heavily glaciated with extensive deposits of Wisconsinan- and Illinoian-age drift. Near Lake Erie, ice proximal (till, kames, outwash) and lake deposits (lacustrine, beach ridges) cover the Portage escarpment (Brockman, 1998). Further inland, the depositional environment changes to till plains and buried valleys. A key feature of most of the buried valleys in this region (Bagley, 1953) is that they were ice-dammed (to the north), which resulted in a greater portion of fine sediments (lacustrine deposits) than is found in buried valleys that drain to the south (Ritzi et al., 2000). A buried valley in the southwest corner of the 1:24,000 Ashtabula South quadrangle is the subject of both qualitative stack mapping and geostatistical modeling (Figure 1).

METHODOLOGY

A key component of both mapping techniques is the collection of base maps and boring data. A GIS/ digital database approach (based on ESRI ArcGIS and Microsoft Access) to data compilation is adopted for efficient distribution and storage. Detailed discussion of specific software modules and file formats used in the GIS data management is beyond the scope of this paper. Software used for geostatistical modeling is given a more thorough treatment.

The 1:100,000-scale "stack" maps (for this study, the USGS Ashtabula and Youngstown quadrangles) are initially drawn on 1:24,000-scale Mylar maps using (underlying) several different paper base maps and a light table. Interpretations are based on maps of soil parent materials, drift thickness, bedrock geology, and legacy geology maps. In addition, boring data from water wells (Ohio Division of Water, ODW), bridge borings (Ohio Department of Transportation, ODOT), and environmental studies (Ohio Environmental Protection Agency, OEPA) provided key information for mapping below the surface. The general data sources and procedures for making stack maps are described in the following sections.

Soils Maps

Whereas a major innovation of these maps is the inclusion of information in the subsurface, surface information remains critical and has a large impact on the appearance of the final map. Surface mapping units (lithologies) are largely derived from county-scale soil surveys. Soil survey information (1:15,840 scale) is used to make maps of parent material. Teams of pedologists use field investigations, soil sampling, and air photo interpretation to divide the landscape into polygons of like soils. The suite of soil mapping units and the rules for delineation on the landscape are based on a mutually agreed upon conceptual model. Mapping units are organized on major transitions in soil type, often those of significance to the management of the land. At the county scale, these transitions between soil units are usually due to changes in geomorphology and, therefore, provide a potentially high-resolution data source for surface lithology.

The primary source of digital soil data is the Natural Resource Conservation Service (NRCS) Soil Survey Geographic, commonly known as SSURGO (Soil Survey Staff, 2006). SSURGO GIS databases provide the mapping polygons as GIS files and extensive tabular data that describe soil horizonation, chemical/ physical properties, and descriptions of soil suitability for a wide range of land uses. The tables do not, however, explicitly define parent materials for each soil type. They are assigned to the polygons by creating a lookup table of interpreted (by this author) parent materials for each mapping unit. The tables are based on the detailed soil profiles and interpretive descriptions found in the written soil survey report. 1:24,000-scale maps of parent material are generated for each quadrangle (Figure 2). The stack model is much more accurate for layers near land surface than at depth because the level of detail in the soil survey is far greater than available well and boring data. However, the main intended use for soil mapping is land management. Therefore, there are often discrepancies between parent materials determined from soil polygons and the actual parent material (verification is conducted from boring data and by geomorphic interpretation). Parent material maps created in this fashion must be used with caution and interpreted with care.

Drift-Thickness Map

A second piece of mapping information is drift thickness (DT) (Powers and Swinford, 2004). DT maps are calculated from the surface digital elevation model (DEM) and the bedrock-topography map (Figure 3) (the bedrock topography map is usually updated and revised during the stack mapping process, past versions available as Mylar basemaps, contour shapefiles (vector), and grids (ODGS, 2003)). A key issue for DT maps is "flying outcrops" where the elevation of the bedrock topography (BT) exceeds that of the DEM. Such areas are not unexpected, as there are significant inaccuracies in both datasets. The accuracy of USGS DEMs is in the range of 5 to 10 feet Root Mean Squared Error (RMSE) (Venteris and Slater, 2005; Smith and Sandwell, 2003). The accuracy of BT within the Ashtabula and Trumbull quadrangles was estimated as

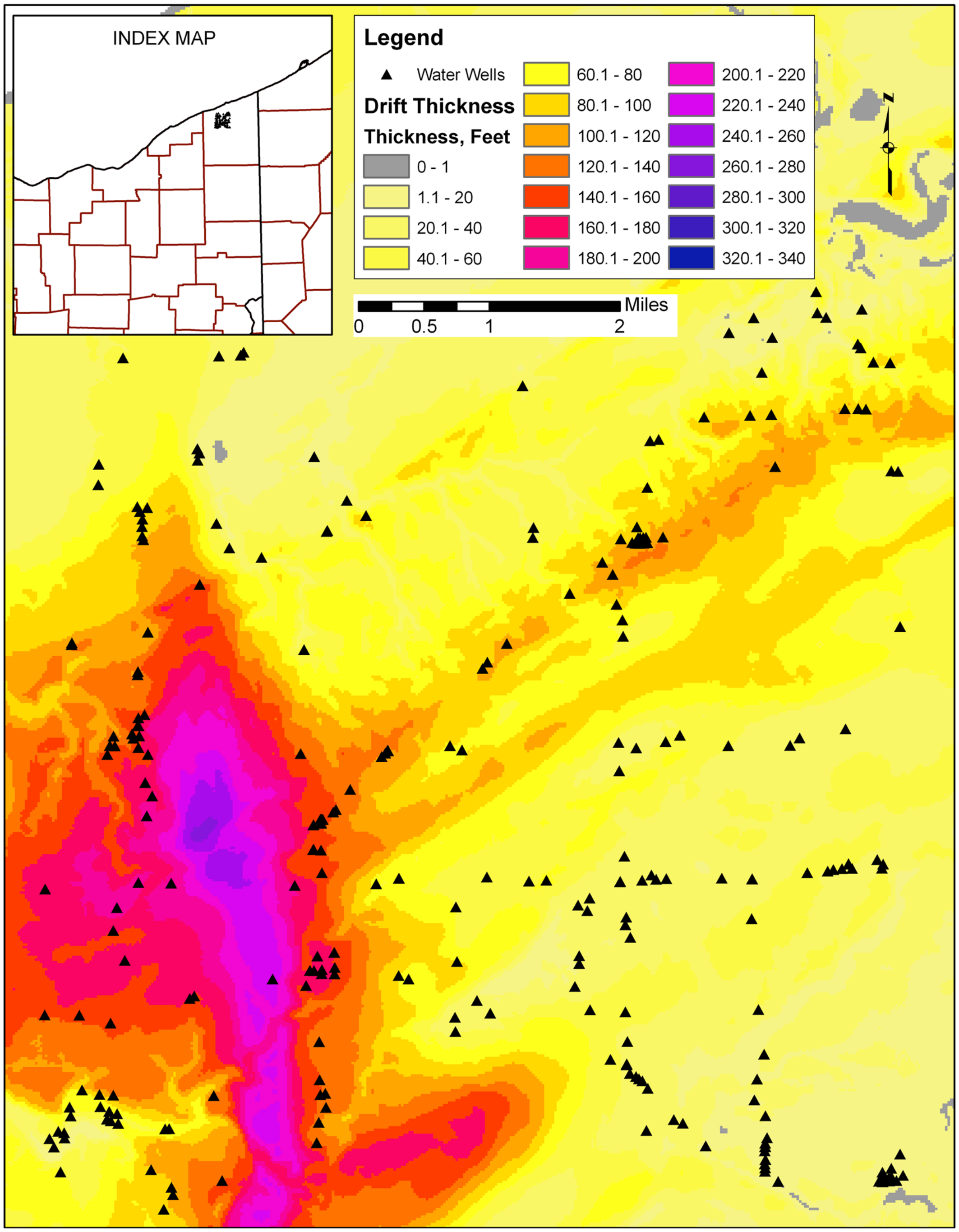


Figure 1. Map of drift thickness for part of the Ashtabula South 1:24,000-scale quadrangle, Ohio.

part of the current project. External validation was conducted for BT based on new bridge borings that were not used to create the map. Bedrock elevations from bridge borings were compared with interpolated elevations based on a TOPOGRID model of BT contours. RMSE error was found to be 22 feet. Assuming zero covariance between the error in the DEM and BT, the total error DT is

$$E^2_{DT} = \sigma^2_{DEM} + \sigma^2_{BT} \quad (1)$$

where σ^2_{DEM} is the error (expressed as a variance) in the DEM and σ^2_{BT} is the error in the BT. Assuming an error of 7 ft RMSE for the DEM, the total RMSE error in DT for this area is 23 feet. Hence, the error in DT is dominated by the error in the BT. Because of this uncertainty, drift thickness less than this value may in reality be areas of bedrock outcrop. For the current mapping project, areas of negative drift thickness are corrected to a DT value of zero feet. Areas of thin drift (less than 5 feet) are usu-

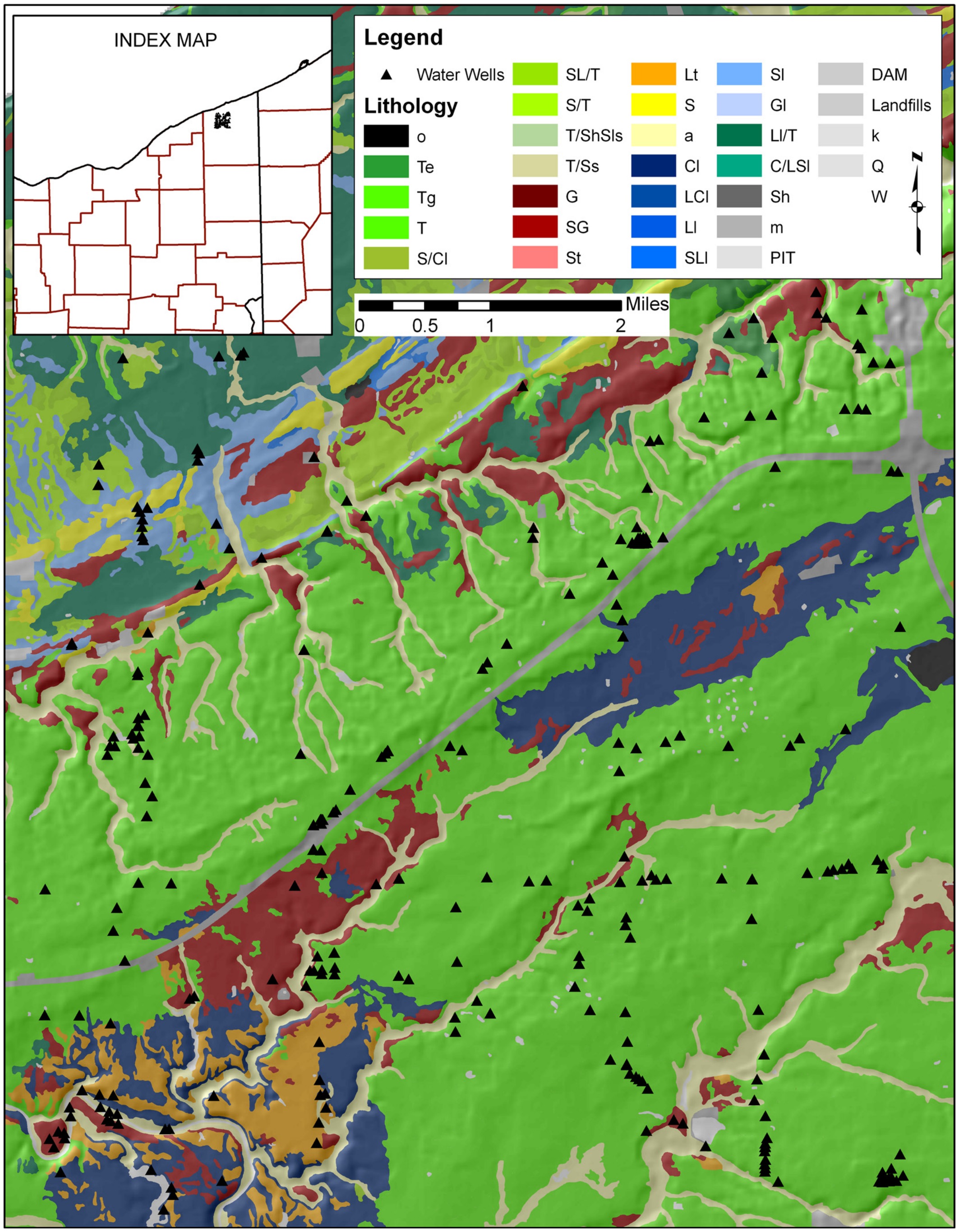


Figure 2. Parent material map based on SSURGO.

ally also identified in the parent-material (soil survey) maps, providing another means to confirm the presence of outcrop. Surficial materials at such locations are marked with parentheses on the “stack” maps to indicate that drift coverage is discontinuous in the area.

Other Base Maps

Legacy geologic maps are also used in mapping. Digital versions of the bedrock geology map (Ohio Division of Geological Survey, 2003) are used to map the bedrock base of each stack unit (the entire area of interest in the present mapping is underlain by shales of Devonian age). Existing maps of surface glacial deposits are compared to the parent material maps (from the soil survey) to aid in the assignment of surface units, especially in interpreting depositional environment. Often, lithology information is obtained from the well data and the soils maps without a

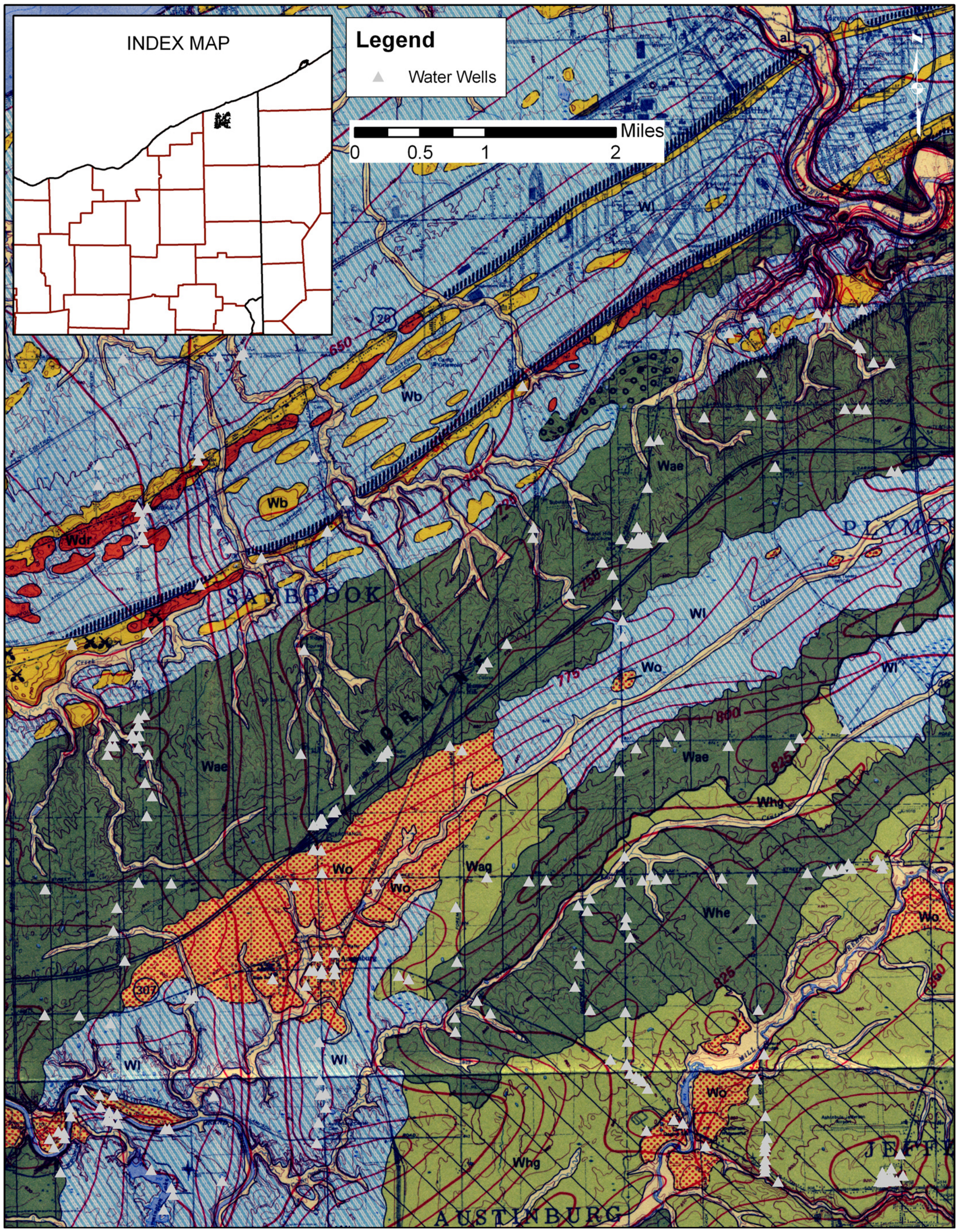


Figure 3. Glacial-geologic map of the study area taken from White and Totten (1979).

geomorphic interpretation. However, such interpretations are critical to the use of this data for its intended applications. For example, identification of sand and gravel (a lithology) as either an outwash or ice contact deposit (a geomorphic interpretation) is key to groundwater modeling, as there will be marked differences in facies hydraulic structure and conductivity between the materials.

County-scale glacial-geology maps (Figure 3) were available for the three counties of the 2006 STATEMAP project area (White, 1971; White and Totten, 1979; Totten and White, 1987). These maps were scanned and rectified (not digitized in a vector format) and used in the GIS as an additional layer to aid in the mapping of surface units (assignment of lithology, etc).

Water-Well and Other Boring Data

Mapping in the subsurface is based on lithology and other information available from borings drilled for water wells and engineering studies. The most spatially dense data set are water well records from Ohio Division of Water (ODOW). It is a legal requirement that the records (logs) from the drilling of water wells be filed with the state. The lithology (texture), thickness, and occasionally color of layers encountered while drilling the well are contained in the records. The records are obtained as Excel spreadsheets (ODOW, 2005) and converted to a geodatabase for use in ArcGIS. An ArcGIS Visual Basic application was built to display the well location and lithology on paper base maps (Figure 4). The water well data provide critical information on lithologic sequences with depth, but the unit "clay" requires careful interpretation. It is likely that the "clay" unit of the water-well records contains lithologies that range from clay to silt. The identification of silt units is strongly underrepresented compared to the proportion indicated in more detailed and reliable texture data (textures based on laboratory work) such as those from bridge borings (Table 1). The lithology "clay," therefore, is reinterpreted in this modeling to mean clay and silt.

More accurate and detailed depth information is available from the Ohio Department of Transportation in the form of detailed records from geotechnical borings drilled to support bridge construction. These data are available as paper records from ODOT (Figure 5). A digital relational database (Figure 6) is in development

Table 1. Comparison between sediment textures in water-well and bridge-borings in Ashtabula County. The comparison contains many sources of serious bias, as the water-well data generally extends to greater depths than the ODOT bridge boring data, and the spatial distribution of bridge borings is seriously biased. However, it is clear the silt is grossly underrepresented in water wells. The column "Bridge Boring" gives the textural percentage used to define each lithlogic class in the bridge borings.

Texture Class	Water Well	Bridge Boring	Cutoff for Bridge Boring
Clay	0.6	0.37	>40%
Silt	0.004	0.26	>40%
Sand	0.18	0.07	>40%
Gravel	0.21	0.07	>30% sand, >10% gravel

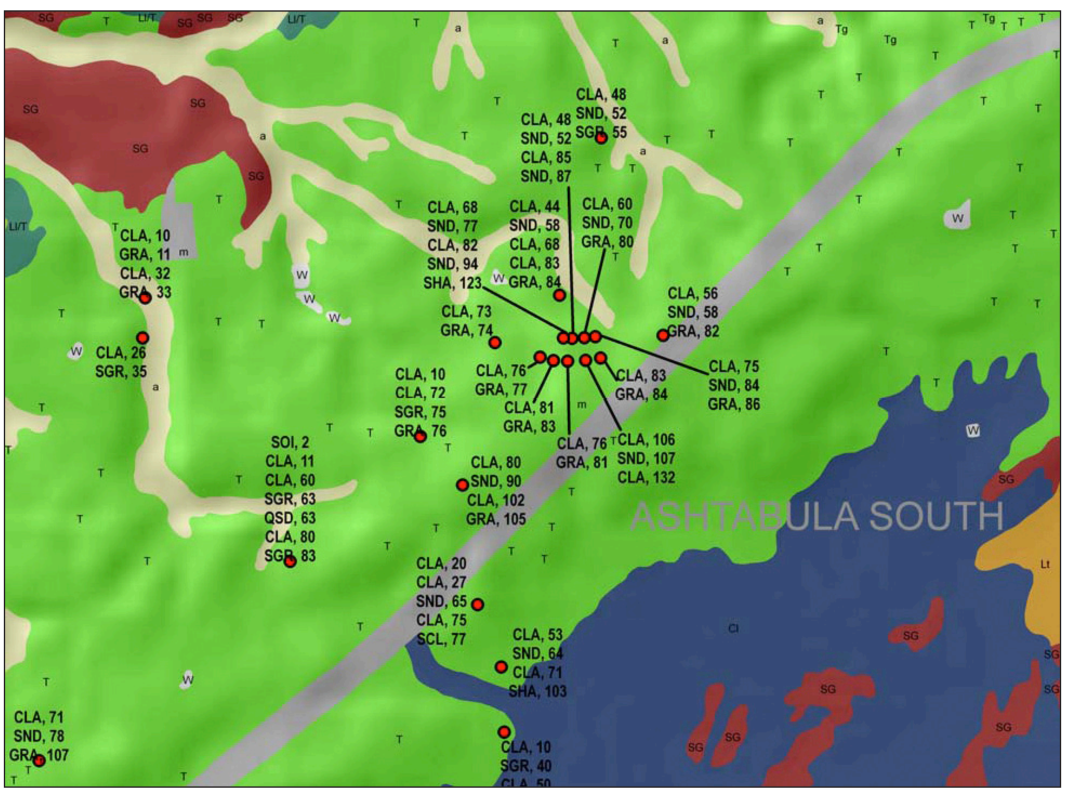
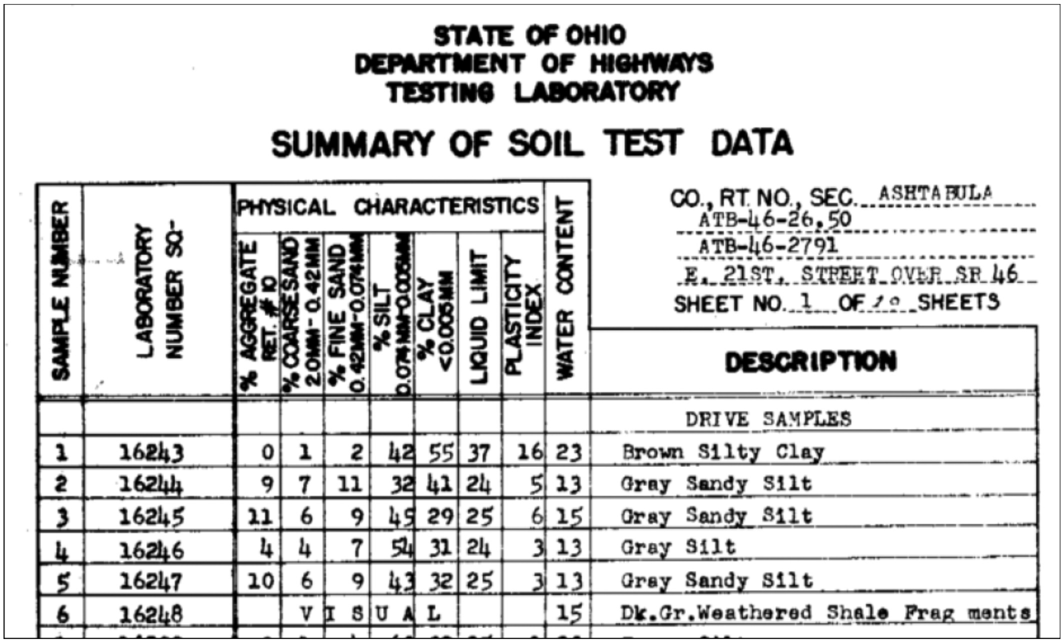


Figure 4. Close-up example of water-well postings.



STATE OF OHIO
DEPARTMENT OF HIGHWAYS
TESTING LABORATORY

SUMMARY OF SOIL TEST DATA

CO., RT. NO., SEC. ASHTABULA
ATB-46-26.50
ATB-46-2791
E. 21ST. STREET OVER SR 46
SHEET NO. 1 OF 10 SHEETS

SAMPLE NUMBER	LABORATORY NUMBER SO-	PHYSICAL CHARACTERISTICS % AGGREGATE RET. # 10	% COARSE SAND 2.0MM - 0.42MM	% FINE SAND 0.42MM-0.074MM	% SILT 0.074MM-0.005MM	% CLAY <0.005MM	LIQUID LIMIT	PLASTICITY INDEX	WATER CONTENT	DESCRIPTION
										DRIVE SAMPLES
1	16243	0	1	2	42	55	37	16	23	Brown Silty Clay
2	16244	9	7	11	32	41	24	5	13	Gray Sandy Silt
3	16245	11	6	9	45	29	25	6	15	Gray Sandy Silt
4	16246	4	4	7	54	31	24	3	13	Gray Silt
5	16247	10	6	9	43	32	25	3	13	Gray Sandy Silt
6	16248		V	I S	U	A L			15	Dk.Gr.Weathered Shale Frag ments

Figure 5. Scan of a portion of an ODOT bridge boring record.

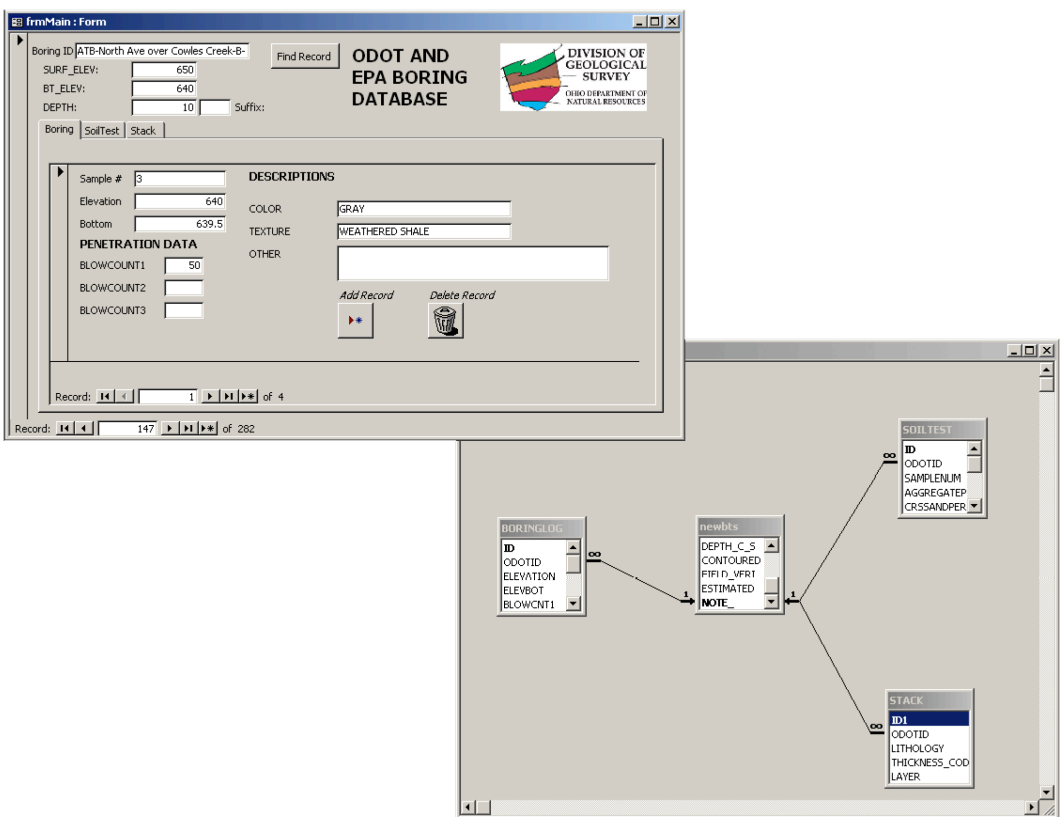


Figure 6. Schematic showing fields, tables and database relationships for the bridge boring/ OEPA database, built by the Ohio Division of Geological Survey.

by ODGS to facilitate computer-based analysis of these data. ODOT records provide detailed engineering data on texture, mechanical strength (blow counts, plasticity indexes, liquid limit, wetness), and lithology (color, texture, texture class). ODOT bridge borings provide excellent site information, but have limited spatial density and a strong locational bias. The borings are mainly collected where roads intersect major streams and the depth is usually limited to approximately 50 ft, which is insufficient in typical buried valleys where drift thickness can exceed 300 feet.

Further depth information is available from OEPA in the form of detailed site studies. Engineering firms with projects such as sanitary landfills and industrial facilities file with OEPA their detailed studies of the subsurface. These reports typically contain several well borings (typically 10 to 30 wells) with a wide range of engineering data. The types of information are usually similar to ODOT records, but with inconsistent coverage (one well may contain good textural information, but lack blow counts, etc.). Digital capture of all wells in these sites is beyond the mapping goals (site studies vs. regional mapping) and resources (time/ labor constraints) of the ODGS. Typically, the best well of the group (with represtative geology and data compatible with the ODOT database) is chosen from each site and entered into the same database as the bridge borings.

Qualitative Mapping—Ashtabula South Quadrangle Case Study

The idea for mapping in three dimensions using stack sequences and 2D polygons is based on previous surficial mapping approaches (Kempton, 1981), with refinements unique to ODGS (Brockman et al., 2004). The emphasis in ODGS work is on lithologic characterization, so stack sequences describe both layer lithology and thickness (estimated to within 50%) from the surface to bedrock. Little attempt is made in this mapping work to assign time units to the layers, except where distinctions between the Wisconsinan and prior glaciations are well known or obvious. Tills are not mapped by traditional stratigraphic units (for example, the Hiram and Waverly tills of White and Totten, 1979) but are divided where there are significant changes in texture or chemistry (carbonate content).

Base data are compiled into a stack model using traditional geologic mapping methods (drafting) followed by GIS digitization. Experience has shown that accurate and efficient generalization and interpretation require the geologist to utilize much information in a spatial context. Large scale (1:24:000) mapping conducted using transparent Mylar and paper base maps can display much more information at a legible scale at one time than any practical (inexpensive) computer screen. After compilation, hand-drawn maps are digitized and attributed to make GIS coverages using standard GIS techniques.

The first step in mapping is to delineate the major lithologic and geomorphic units present at the surface. Polygons of surface features are drawn initially by generalizing (as appropriate for a 1:100,000-scale map) the parent material polygons from the interpreted soil-survey map. Elevation contours and DEMs are often used as an additional guide to generalization (breaks in slope, or stream and erosion patterns). The surface model is further refined by adding geomorphic interpretations based on the mapper's own knowledge, aided by legacy geologic maps such as the glacial-geology series. The surface model (Figure 7) is also checked and verified using information from the various water-well logs and other boring data.

The difficulty and need for geologic interpretation increases greatly when mapping in the subsurface. Subsurface transitions are delineated on the maps using a contrasting line color, which is expressed as a different line style on the final map (solid lines for changes in surface materials and dashed lines for subsurface transitions (Brockman et al., 2004; Swinford et al., this volume)). Subsurface polygons denote large changes in thickness and lithologic sequence. The first step in subsurface mapping is inspection of the drift thickness map. The geologist looks for major geomorphic features, which provide a rough idea of where the major transitions will be drawn. In general, breaks in thickness that delineate buried valleys and end moraines are the most common and critical to communicating the geology of the area. Once major thickness transitions are denoted, a stratigraphic model is developed to assign stack sequences to each mapping polygon. This model is based on inspection and analysis of the well data in the area. In general, detailed information (mainly texture, but penetration and plasticity tests are also useful) from bridge borings and environmental study sites are used to develop an initial conceptual model. The model is then verified and extended spatially using the more general water well data (which are usually posted to the parent material and drift thickness base maps) and an understanding of the expected configuration of sediments for the given geomorphologic environment.

An illustrative example of mapping at depth is provided for the SW corner of the Ashtabula South Quadrangle. This area is unusually complex, as it contains the Painesville end moraine superimposed on the buried valley associated with the Grand River. The area surrounding these features contains end moraines, beach ridges, and lacustrine sediments. The main subsurface feature, a major north-south bedrock valley, was dammed (to the north) when glacial ice occupied the Lake Erie basin. The feature is approximately four miles wide and contains drift with a thickness up to 300 feet (Figure 1). When mapping this buried valley, we have to make two major decisions:

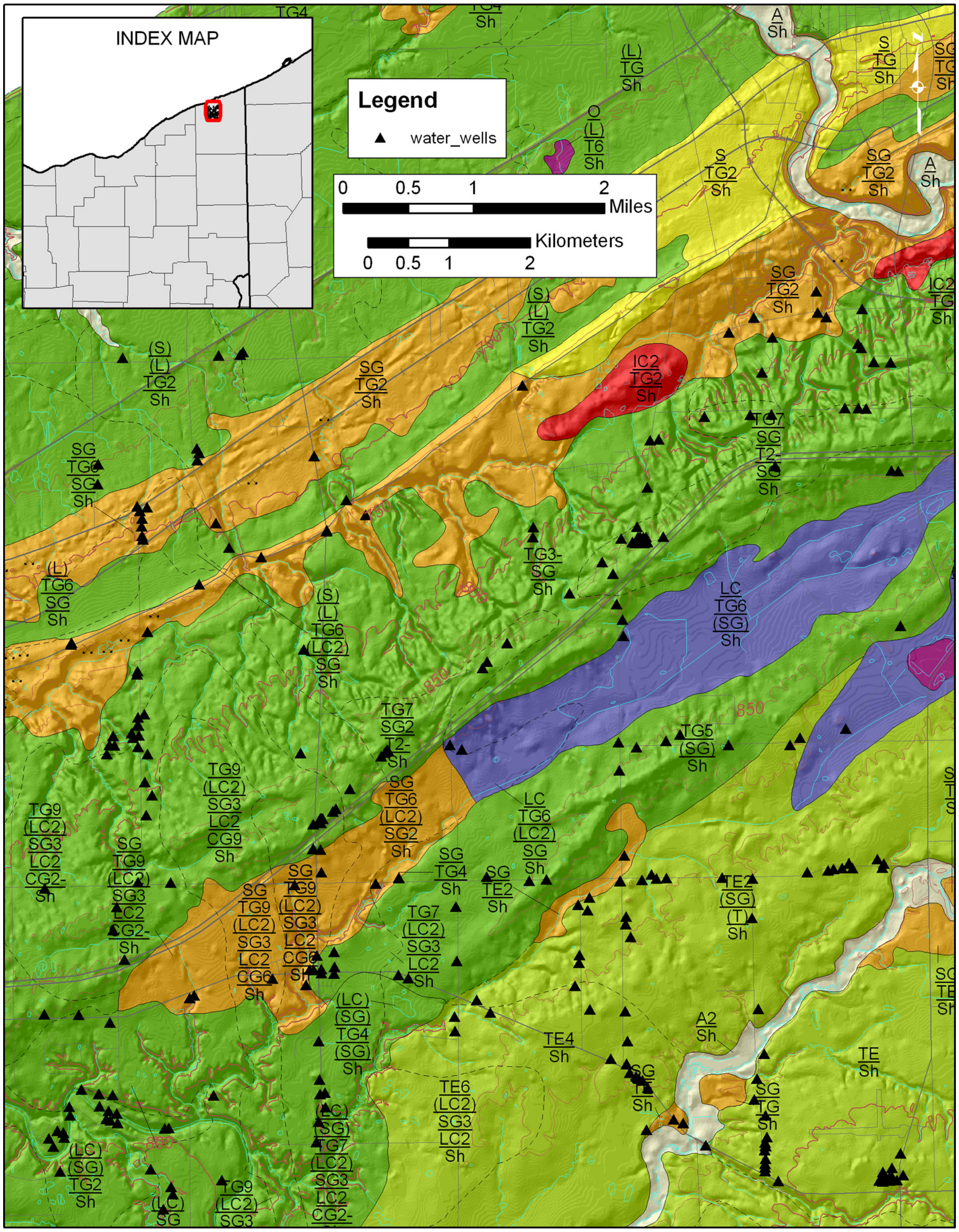


Figure 7. Preliminary model of the subsurface geology at head of the Grand River. This is a portion of the "stack" map for the 1:100,000 scale Ashtabula Quadrangle. The map is currently under review. Some key abbreviations: TG = Wisconsinan till unit high in silt content, TE = Wisconsinan till unit high in clay, SG = sand and gravel, LC = silt and clay (generally lacustrine), Sh = shale bedrock, S = Sand, CG = buried-valley deposit with undifferentiated lithology.

1. What is the best way to draw polygons to communicate the important transitions in thickness and lithology?
2. How do we best generalize available well data into a stratigraphic model to assign stack sequences to these polygons?

Maps of drift thickness are used to provide an initial impression of the subsurface configuration. The DT map (Figure 1) shows the superposition of the north-trending Grand River buried valley and the SW-NE trending Painesville moraine. Some "fingers" of increasing drift thickness off the main valley are due to the Painesville moraine, whereas others are due to the presence of buried side valleys. The bedrock-topography map must be used in conjunction with the drift thickness map for proper interpretation. These maps were used to develop basic ideas on mapping the subsurface, such as the locations and extents of major subsurface polygons, total depth needed for stack sequences, boundaries of major subsurface morphologic units (in this case delineating a reasonable extent of lake sediments when the buried valley was flooded), and cartographic concerns such as minimizing small and sliver polygons caused by the interaction of surface features and subsurface polygons.

Borehole information is used to develop a generalized stratigraphic sequence or "stack" for each polygon. Each stack contains the lithology (and geomorphology, where applicable) and thickness estimate (within ±50%). The goal is to generalize information from many wells into vertical sequences and identify horizontal transitions and breaks in the sequences (overall depth or lithology) that warrant drawing additional polygon boundaries.

Stack sequences for the study area were mainly based on water-well lithology logs. Detailed (bridge) boring data were not available for this geomorphic feature within the quadrangle boundary. Only one detailed site with limited depth (~100 ft) existed to the southwest (in the Jeffersonville 1:24,000-scale quadrangle), so stratigraphic models were developed mainly from the water-well database. The first attempt at a stratigraphic model was based on interpretation of common patterns in lithology. An attempt to correlate first clays, first gravels, second clays, second gravels and so on was done. Some patterns emerged, but it was clear there was much variability between the data. Differences in vertical resolution and quality between loggers, complex spatial variations in geology, and blunders all made it difficult to create a generalized stack. The preliminary subsurface model and stratigraphic sequence (Figure 7) was subject to a more rigorous review, aided by results of geostatistical and statistical analysis.

Quantitative Mapping—Geostatistical Modeling (Sequential Indicator Simulation)

Geostatistical simulation techniques exist to model and simulate categorical variables such as lithology. Such methods are common in oil and gas exploration (Deutsch, 2000) and have been used to characterize surficial deposits for ground-water modeling (Carle and Fogg, 1996; Ritzi et al., 2000). The various forms of geostatistical simulation are generally preferred over indicator kriging for modeling of surficial deposits because buried-valley and other surficial deposits have high spatial complexity. In addition, the sample spacings of typical well data sets contain gaps or average spacings that greatly exceed the scale of autocorrelation. In this context, the rigorous techniques of uncertainty analysis and superior ability to extrapolate results beyond the well data (due to sequential approach used in simulation algorithms) of simulation techniques are valuable. While model results in sparsely sampled regions are not reliable for predicting the position of lithologies (say for drill planning), such extrapolation is useful for groundwater simulation, provided many realizations are used to understand the range of possible results in poorly constrained areas. There are also many theoretical reasons (missing variance and inherent smoothing of kriging, etc.) to choose simulation techniques over kriging (Deutsch, 2000).

The goals and output results of geostatisical simulation are different than those of indicator kriging. Kriging provides the best estimate of values at unsampled locations. The goals of simulation are to use kriging in conjunction with Monte Carlo techniques to produce many different realizations faithful to the data locations and reproduce global statistics (histogram) and local spatial structure (variogram). Each realization represents a statistically valid, potential configuration of the subsurface. However, interpolated values in each model are not optimal estimates and can vary widely between realizations. The variation between realizations is the strength of the method, as it is the basis for evaluating the uncertainty of the model. The more tightly constrained the model (large amount of well control, predictable spatial structure with strong (repeated) patterns), the less variability between runs. Summary statistics that characterize the differences between realizations provide a rigorous and convenient way to assess model uncertainty.

A full development of sequential indicator simulation (SISIM) (Journel, 1983) is not presented here. However, the basics of the algorithm are described to provide the reader with insight as to how the technique works and the configuration of the data and spatial autocorrelation will affect results. First, a regular three-dimensional grid is specified for the volume of interest (for efficiency) and a random interpolation order is chosen for the cells. This is important, as simulated values are treated as data points and used to calculate kriging weights for subsequent cells. SISIM is based on the calculation of a conditional distribution for each cell, which is randomly drawn from to assign a lithology. The conditional distribution is based on the kriging estimate (local information) and the global probability. For each lithological type (***k***) at location (**u**), the conditional probability is

$$p_k^*(\mathbf{u}) = \sum_{\alpha=1}^{n} \lambda_\alpha i(\mathbf{u}_\alpha ; k) + \left(1 - \sum_{\alpha=1}^{n} \lambda_\alpha\right) p_k(\mathbf{u}) \qquad (2)$$

where λ_α is the simple-kriging weight, i is the indicator code (a binary variable for each lithology, i.e., sand (1) or not sand (0)) for a neighboring data point (either a "real" data point, or a simulated cell) and $p_k(\mathbf{u})$ is the global probability for the respective lithology. Hence, the conditional probability is a function of the values of neighboring cells (whose influence with distance is defined by the variogram and kriging) and a global probability. Next, p^*_k results for each lithology are combined to define the cumulative conditional distribution function (ccdf). A random number between 0 and 1 is drawn, and the ccdf is used to assign a lithology for that cell.

Some key aspects of the algorithm should be considered when evaluating an individual realization:

1. Global probabilities have decreasing influence with increasing density of neighboring data (due to the presence of well control or cells that are filled in later in the grid order). In data-rich regions, results are mainly influenced by the data values and the variogram (the distance of influence increases with range; the nugget effect (if used) decreases the kriging weights and increases the influence of global proportions). In sparsely sampled areas, initial cells are controlled by the global probabilities.
2. Randomness and subsequent differences between realizations arises from two sources: the random path for assigning cell values and the random draw to assign a lithology from the conditional distribution function. Once a lithology is assigned to an empty cell, it becomes a data point and influences the neighboring results. This is generally a good feature of sequential simulation, as it tends to produce geologic bodies even in areas poorly constrained by wells (for example, once sand is assigned to a cell, it is more likely that neighboring cells also will be assigned as sand, creating a sand layer). The end result is that, even in areas of little or no data, global statistics and spatial structure are preserved.

The sequential indicator simulation algorithm in GSLIB (Deutsch and Journel, 1998) was used to model lithology (clay, silt, sand, or gravel) for the southwest portion of the Ashtabula South Quadrangle described above.

Workflow

The work presented here was a preliminary exploration, mainly intended to create 3D models for comparison with the stack maps. A far more rigorous modeling of the area (conducted in elevation space, using simulations nested by stratigraphic units, and models of spatial structure based on well statistics (Ritzi et. al, 2000)) is presented in Venteris, 2007. The preliminary investigations presented here were conducted to test whether lithologic information from the water wells could be extended (interpolated) into continuous models using geostatistical simulation techniques. The amount of similarity between models created by the two techniques could provide insight into the geology of the study area and the quality of information contained in water wells.

The first step in modeling was to define the spatial domain of the model. The area for study was chosen for geological interest and the presence of sufficient water-well data to support simulation. The lack of detailed ODOT borings was a significant disadvantage to this study area. The models were created in depth-space rather than using real world elevations. Such an approach was advantageous for preserving lateral continuity for layers that follow topography such as till sheets and for comparison with the stack model, which were also modeled as depth and thickness. A three dimensional grid with cell dimensions [x=200 ft, y=200 ft, z=2 ft] (data continuity is much higher in the z direction) was defined for modeling. This domain contained both unconsolidated sediments and bedrock, the boundary between the two defined by the DT grid. A FORTRAN program was written to convert the 2D ASCII format DT grid into a 3D GSLIB format voxel, which was then used to clip the model results. Geostatistical simulation was only conducted for the portion of the data containing unconsolidated sediments. Bedrock and unconsolidated sediments were not modeled together because the probability of either lithology group is not spatially constant over the domain (stationarity).

Well data were converted to a data format appropriate for geostatistical modeling. Water well data from ODOW were converted to a simple set of indicator codes. The conversion required some interpretation and generalization. For example, a water well record described as C/R or "Clay and Rock" was coded as clay, assuming that the driller was describing a till with rock fragments. There were many lithologies that require interpretation in the water-well database, but their overall proportion in the dataset was small. Most descriptions were of common and easily classified lithologies. Unconsolidated lithology classes from the water wells were reclassified into four indicator variables [clay=1, silt=2, sand=3, gravel=4]. In addition, the wells were discretized in the vertical direction. Lithologies for wells in the ODOW database were given a range of depth (upper and lower values). The water wells were discretized at one-foot increments to provide sufficient continuity of lithology values for the intended vertical resolution of the voxel model.

SISIM required the assignment of global probabilities for each lithology. For this data set, clay was the dominant lithology (Table 2). Silt is grossly under represented in the water-well dataset as discussed above, and so cells modeled as clay include both clay and silt. The data were checked for clustering bias using the DECLUS routine in GSLIB. Bias due to clustering is less than 5% for this dataset and is not considered a significant source of error.

The next step was to define the spatial structure (variogram) for use in assigning kriging weights. First, experimental variograms were calculated from the data. Experimental variograms were used to create model variograms for input into the simulation (kriging) procedure. Model variograms can be created by visual estimation, trial and error modeling, and automatic fitting routines. Key information to obtain from the experimental variograms was the overall shape (expressed as a function, usually spherical), the range of autocorrelation (where the variogram intercepts the sill), and the magnitude of the nugget effect (non-zero intercept, caused by small-scale variability below the distance of the lag spacing and measurement error).

Experimental variograms were calculated (using GAMV routine in GSLIB) for each lithology (except silt, for which there are insufficient data points) in the vertical and horizontal directions. A range of experimental variograms were calculated to explore many possible scales of spatial structure (by adjusting lag spacings and the number of lags) and to check for anisotropy. There was some indication of anisotropy (semi-variance values exceeding sill), but the noise in the data set precluded an accurate estimate of directionality. Indicator variograms in the vertical direction (Figure 8) were generally smooth,

Table 2. Proportions of each lithologic unit for the simulated area.

Texture Class	Water Well
Clay	0.816
Silt	0.002
Sand	0.137
Gravel	0.045

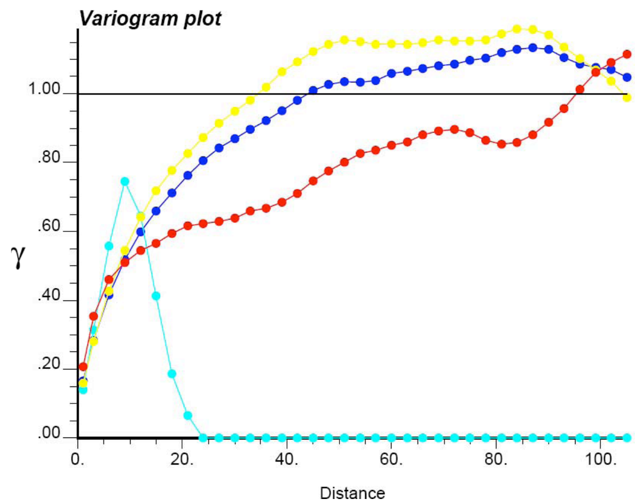


Figure 8. Indicator variograms in the vertical direction. Dark blue is clay, light blue is silt, yellow is sand, and red is gravel.

had a small nugget effect, and were fit with a basic spherical model (Table 3). Experimental variograms were much less stable in the horizontal direction. Smooth variograms were possible using large lag spacings (Figure 9) but a more revealing picture was obtained by using small lag spacings (Figure 10). The smooth experimental variograms suggested a very large nugget effect and a range of around 3,000 feet. The gravel lithology never fully approached the sill, which suggested an anisotropic structure. Experimental variograms using a smaller lag spacing showed a more complex picture. For small lag spacings the nugget was much reduced, but the semi-variance oscillated widely, making range selection ambiguous. This "hole effect" could have been due to the natural spatial structure of the glacial sediments or a result of incomplete and noisy sample data. Determining the range (point of intercept with the sill) was essential for kriging and simulation. The variograms showed an initial structure (local maxima) at about 1,500 feet. All variograms intercepted the sill several times over the range of 1,500 to 5,000 feet.

Several variograms were used in the simulations, as the experimental variography did not provide clear guidance for the horizontal variogram model (a different, more rigorous approach to characterizing spatial structure for SISIM modeling is presented in Venteris, 2007). Three example variogram models were used to demonstrate a reasonable range of results. No attempt was made to choose the best model from the range of possibilities. Rather, multiple scenarios were run to illustrate the effect of variogram parameters on results. Model variograms for simulation were loosely based on the experimental horizontal variograms (vertical models are held constant (Table 3)). For the first experiment, the horizontal range for all lithologies was set to 2,000 feet (a compromise

Table 3. Model variogram parameters used in the three indicator simulation runs. The nugget effect is zero for the short range and long range models. The nugget is 0.5 for the short-range with nugget model.

Indicator	Horiz. Range (Anisotropic)	Vertical Range	Contribution
Nugget			
1	2000	50	0.5
2	2000	15	0.5
3	2000	40	0.5
4	2000	80	0.5
Short Range			
1	2000	50	1
2	2000	15	1
3	2000	40	1
4	2000	80	1
Long Range			
1	5000	50	1
2	5000	15	1
3	5000	40	1
4	5000	80	1

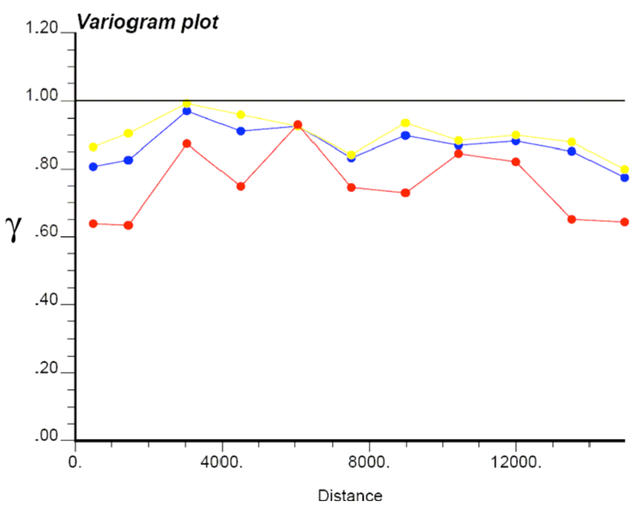


Figure 9. Indicator variograms in the horizontal direction (isotropic) using a lag separation of 1500 feet and a lag tolerance of 800 feet. Colors and lithologies are the same as in Figure 8.

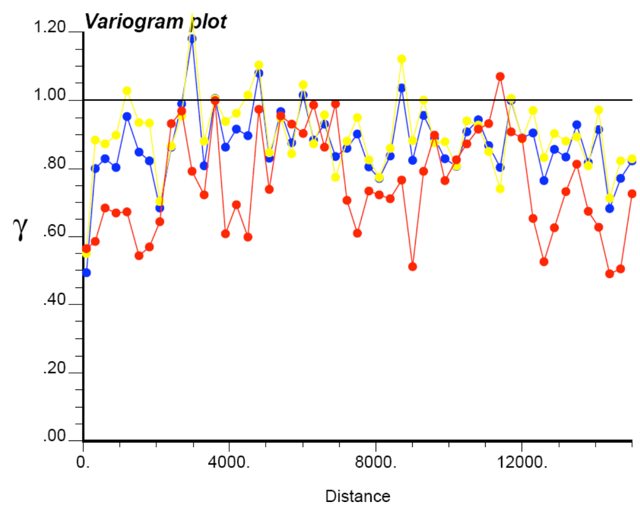


Figure 10. Indicator variograms in the horizontal direction (isotropic) using a lag separation of 300 feet and a lag tolerance of 150 feet. Colors and lithologies are the same as in Figure 8.

between the ranges of clay and sand (intercept at 1,500 feet) and gravel (around 2,500 feet)) with a large nugget contribution (0.5, or 50% of the variance due to measurement error and spatial variation below the scale of the lag distance). For the second model, the range was held to 2,000 feet, but the nugget effect was set to zero (assuming nugget due to inadequate sampling rather than geologic variability). For the final model, it was assumed that both early oscillations and large nugget effects were spurious. The variograms were modeled with a range of 5,000 feet and a nugget effect of zero. This model represented the maximum amount of spatial continuity that could reasonably be interpreted from the experimental variogram results.

Lithologies were simulated using the SISIM algorithm as implemented in GSLIB. 16 individual realizations were produced for each variogram model. As a rule of thumb, the number of realizations should be around

100. Running this model in GSLIB resulted in a stack overflow and program discontinuation after 16 runs. The solution was to run multiple batches and then write software to recombine them for final products. Modified software to process 100 runs was not complete at the writing of this contribution. The goals of this study are mainly exploratory and illustrative, so the limitation to 16 realizations had little meaningful impact.

To find the most common value and assess the variability of the realizations for each cell, the realizations were post-processed. Firstly, the portion of the model at or below bedrock was removed (clipped). FORTRAN programs were written to post-process the SISIM runs. The mode value was used as the most common value between runs. The algorithm did not break ties between lithologies (a very rare occurrence), and cells with an ambiguous mode were written to "no value." Cells that did not contain a well data point could take any value from realization to realization. The variety of lithologies written to each cell was of interest. Variation between runs for each voxel cell was evaluated using Shannon's (1948) entropy where p_i was the proportion of each lithology within the

$$H = -\sum_{i=1}^{n} p_i \ln p_i \tag{3}$$

set of realizations. Values close to zero indicated consistent values between runs, and values near 1 represented high variation between runs.

RESULTS

Qualitative Mapping

A wide range of surface features of mappable size exist in the study area. The preliminary stack map is presented in Figure 7. The major surface geomorphic feature is the Painesville end moraine, which trends from the southeast to the northwest. On the lake ward side (to the northwest), sand and gravel beach ridges are superimposed. Most alluvial deposits are too small to be mapped at 1:100,000 scale. Behind the end moraine is a small southeast/ northwest trending lacustrine deposit. In the far southwest corner is a large sand and gravel deposit, which was previously interpreted as outwash (White and Totten, 1979). The far southeast corner is occupied by till in the form of small end moraines and ground moraine. There is also a major alluvial valley deposit in this part of the study area. For the stack maps, tills are not differentiated into end and ground moraines, as on a traditional glacial-geology map. Instead, tills are divided on the basis of broad textural class where the unit "TG" represents a silt-rich unit found lake ward and "TE" indicates a clay-rich till found inland.

The major subsurface feature in the study area was the north-south trending buried valley, and it was the major challenge to mapping in the study area. A generalized stratigraphic model was developed from a wide variety of information, little of which could provide definitive guidance or insight. The first task toward modeling the stratigraphy was to use previous studies (White and Totten, 1979), wells, and base maps to develop a general reconnaissance model of the subsurface. This initial survey gave a basic sense of the sediments that might be encountered in the subsurface and, in particular, indicated that lacustrine sediments were an important component of this buried valley.

The surface was dominated by tills of Wisconsinan age that ranged in thickness from nearly 0 to 100 feet in the study area (Figure 11). A rough estimate of the thickness of this unit was estimated from the wells using the first gravel or sand as the boundary between the Wisconsinan tills and underlying sediments. However, the marker was very thin, absent, or ambiguous in many of the wells. The map was useful for estimating thickness within ±50% for defining stack sequences, but was interpreted with caution.

The next issue was determining a generalized stratigraphy below the major till unit. The task was highly interpretive. Water well records only provided basic lithology (clay, silt, sand, etc.) and gave no information on the geomorphic environment. Hence, a lithology of "clay" could have referred to till or lacustrine deposits (perhaps ice contact as well). The buried valley likely contained till, lacustrine, sand, and gravel deposits. However, the only direct evidence for the existence of lacustrine deposits was from an ODOT bridge boring south of the study area (Figure 12). This well showed a 25-foot thick layer that contained 0% aggregates at a depth of 40 feet, which is likely a lacustrine deposit. Even with this high resolution and quality evidence, a low aggregate till could not be completely ruled out for this layer, however.

Further information to aid interpretation was provided by a plot of the proportion of sand and gravel with depth for all the wells of the study area (Figure 13). Sand and gravel did not commonly occur in the upper 50 feet of the surficial deposits (where Wisconsinan till predominated). Below 50 feet, the likelihood of encountering sand and gravel deposits increased up to a maximum of 40% at a depth of 105 feet. Then the proportion of sand and gravel dropped off again, to around 0.25 from 120 to 145 feet. Finally, the proportion increased again, but was interpreted with caution, as a limited number of wells penetrated to this depth. (The trends in the proportion of sand and gravel had implications for geostatistical simulation and are discussed later). This plot was used to guide the placement of sand and gravel layers within the stack sequences.

This variety of information was interpreted, combined and simplified to create the "stack" for each of the polygons. A base stack was developed for the center (thickest part) of the end moraine and buried valley, which

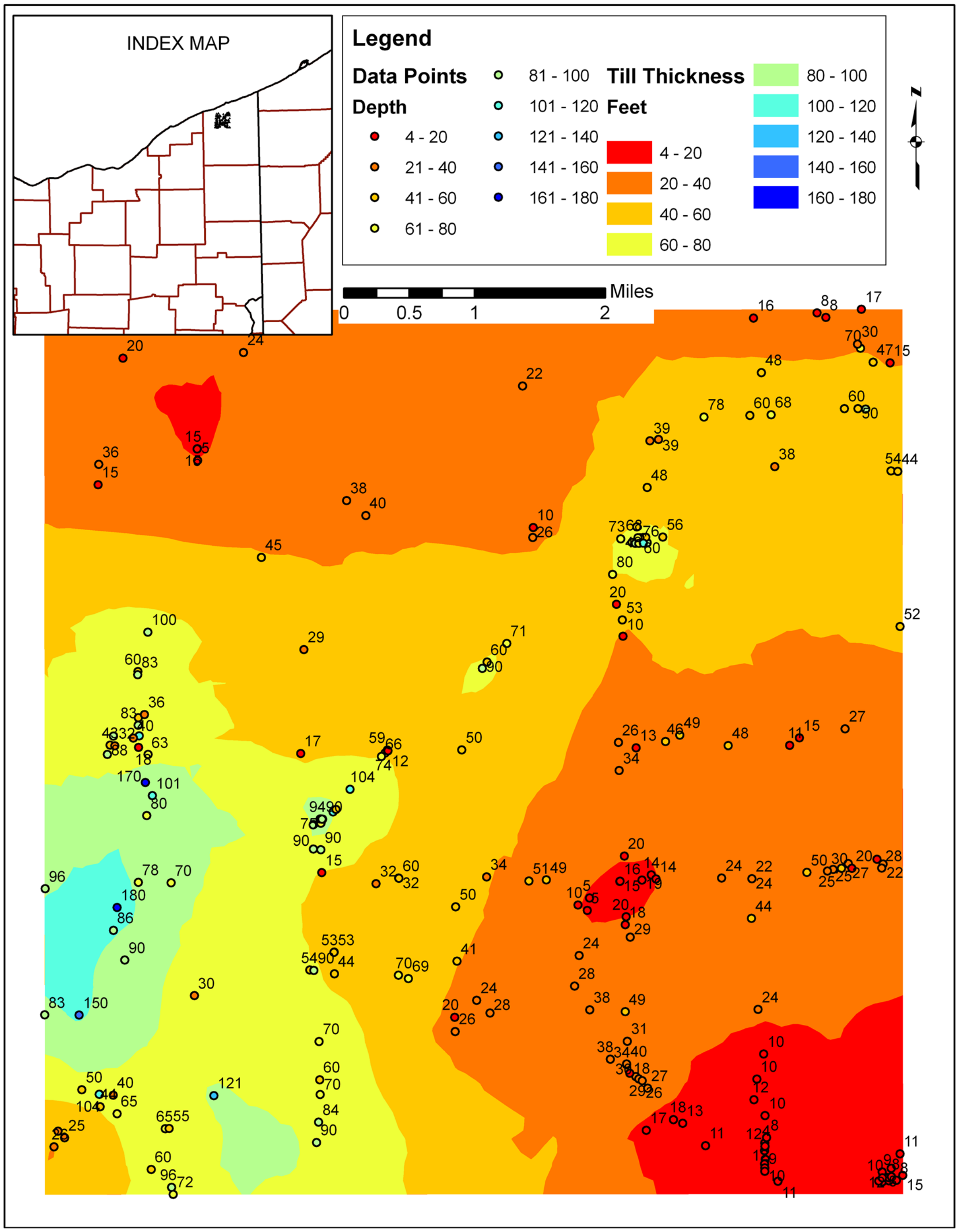


Figure 11. Estimated thickness of Wisconsinan till from kriging of water-well data.

was correlated outwards, eliminating lower units as the bedrock elevation increased. The data could have been interpreted and generalized in many ways, so several stack models were possible (Table 4). A range of models was given with varying degrees of complexity and interpretation. The layer of Wisconsinan tills (TG) was the most certain of the units and was used in all models. Model 1 was the most detailed and heavily interpreted version. The sand and gravel unit noted at the base of the tills was included in the second layer as (SG). Lacustrine deposits identified in the detailed bridge boring occurred below this unit. This was followed by a sequence of sand and gravel units estimated to be between 15 and 45 feet thick (SG3). This unit was based on information from Figure 13 (sections where the proportion of sand and gravel exceeds 30%). This was followed by another lacustrine unit, inter-

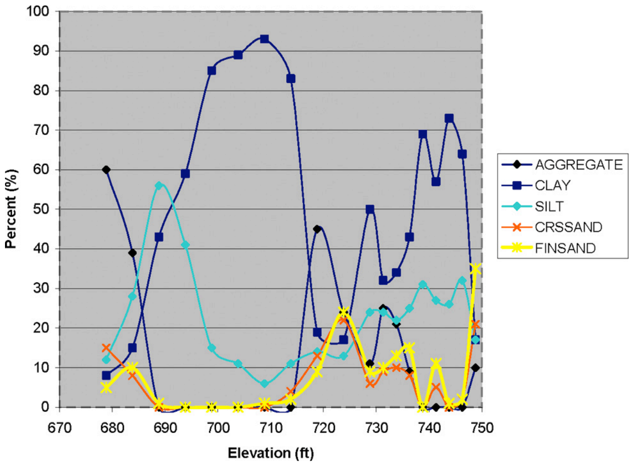


Figure 12. Texture analysis from an ODOT bridge boring close to the study area.

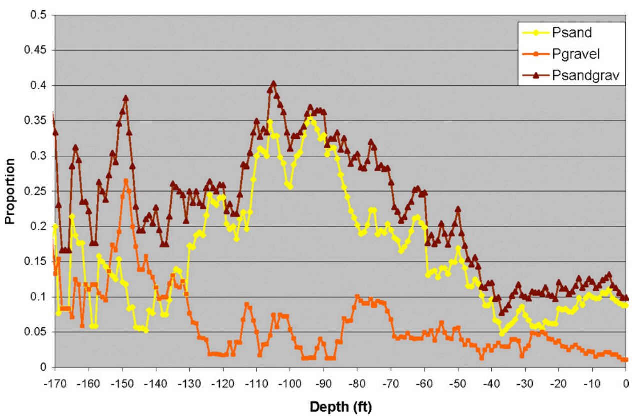


Figure 13. Proportion of sand, gravel and sand, and gravel with depth for all the wells in the study area.

Table 4. Potential stack models for the part of the study area with the thickest drift (an end moraine superimposed on a buried valley). The complex models (e.g., #1) might provide more information, while the simpler ones (e.g., #4) may provide a more reasonable picture of what is known about the geology in the area. The numbers represent thickness divided by 10, and are considered accurate to within 50%. Parentheses indicate that the presence of a layer is discontinuous between wells. Abbreviations are as follows, TG- Wisconsinan till with high silt content, SG- sand and gravel deposits, LC- silt and clay (generally lacustrine) deposits, CG- undifferentiated buried valley deposits with insufficient well control or extreme complexity that prevents differentiation of lithology.

	Model 1	**Model 2**	**Model 3**	**Model 4**
Layer 1	TG9	TG9	TG9	TG9
Layer 2	(SG)	(LC2)	SG4	CG16
Layer 3	LC2	SG3	CG11	
Layer 4	SG3	LC2		
Layer 5	LC2	CG9		
Layer 6	(SG)			
Layer 7	CG7			

preted from the drop in the proportion of sand and gravel. A buried till could was a possible alternate interpretation for layer 5. The water wells indicated a dominance of clay for this depth, but there is no information on aggregate content, etc., to show how this clay was deposited. Layer 6 in this model represented deep sand and gravels, which were mainly identified from detailed EPA site studies and descriptions in previous publications (White and Totten, 1979). This was a unit of pre-Wisconsinan till or sand and gravel that was oxidized and probably occurs near the bedrock interface. The rest of the sequence (on average, 70 feet of material) was essentially unknown because there were few borings that penetrated to this depth that contained material descriptions. This unit was designated as CG, which denoted buried-valley lithologies that range from clay to gravel. Model 2 was simplified by eliminating two units. The first sand and gravel (layer 2) of Model 1 was eliminated because it was often nonexistent or too thin to map. Also, the bottom-most sand and gravel of Model 1 was eliminated because evidence for its existence is questionable. Model 3 further simplified the model by removing the upper LC unit because it was confirmed at only one location. Likewise, the lower LC unit was eliminated, as it was purely an interpreted unit. There was little evidence to differentiate this interval between till or lacustrine deposits, so inclusion of this interval with the CG unit was justified. Model 4 represented the most conservative model. Here, everything below the Wisconsinan till unit was considered unknown. The justification for this approach was that the depth of occurrence and lithology of the buried-valley deposits below the till was essentially unknown and unmappable.

The choice of final stack model for the map was arbitrary. Decisions must be based on the judgment of the geologist, using a compromise between the limited available information (what can be justified on the data or evidence) and the need to communicate what likely would be encountered below the surface (based on geologic knowledge and interpretation). Model 4 was considered too simplistic. From Figure 13, it was clear that there was a nearly even chance of encountering a sand and gravel layer at depths ranging from 70 to 110 feet. The increased likelihood of sand and gravel layers over this depth range was not communicated in Model 4. Model 3 was also probably too simplistic. Here, the presence of sand and gravel was communicated, but no lacustrine deposits were designated. Model 2 contains all the major components that we expected to find in this buried valley. Two lacustrine deposits were designated, which bracketed the most probable stratigraphic position and thickness of sand and gravel. The stack model communicated the main idea of the deposit: tills underlain by buried-valley deposits that have more fine-grained materials than was typical for Ohio (due to the ice damming to the north). However, model 1 was too detailed and seems over-interpreted compared to the quality of the data. The bottom SG unit was only identified in a few wells and did not provide the user with particularly useful new information. The SG unit of Layer 2 was much more common in the well data, but thickness and depths are inconsistent.

In summary, it was difficult to correlate lithologies between wells with confidence. This was consistent with the results of variogram modeling, which indicated that spatial patterns were noisy at best (large nugget effect). Finding meaningful and reliable patterns between data points was a serious issue for both qualitative and quantitative mapping approaches.

Geostatistical Simulation

Example realizations, mode, and entropy are presented for each of the three variogram models to compare results. The results demonstrate the range of possible configurations (individual realizations) and the amount of spatial continuity using long and short autocorrelation ranges and the nugget effect. The results are presented as fence diagrams for an overview, and cross sections are provided for close inspection. An overview of the model domain, well data, and bedrock surface is found in Figure 14.

Individual realizations are presented in Figure 15, with two example realizations (of the 16 calculated) provided for each variogram model. Each obeys the data values, spatial structure, and histogram of the original data. Each realization is one possible configuration of the subsurface from a range of possibilities. There are clear differences between results. The 2000-foot range, large nugget effect model (Figure 15-A) produces realizations with a high amount of randomness. For example, simulated sand and gravel bodies contain many cells of clay, and regions of clay are “speckled” with sand and gravel

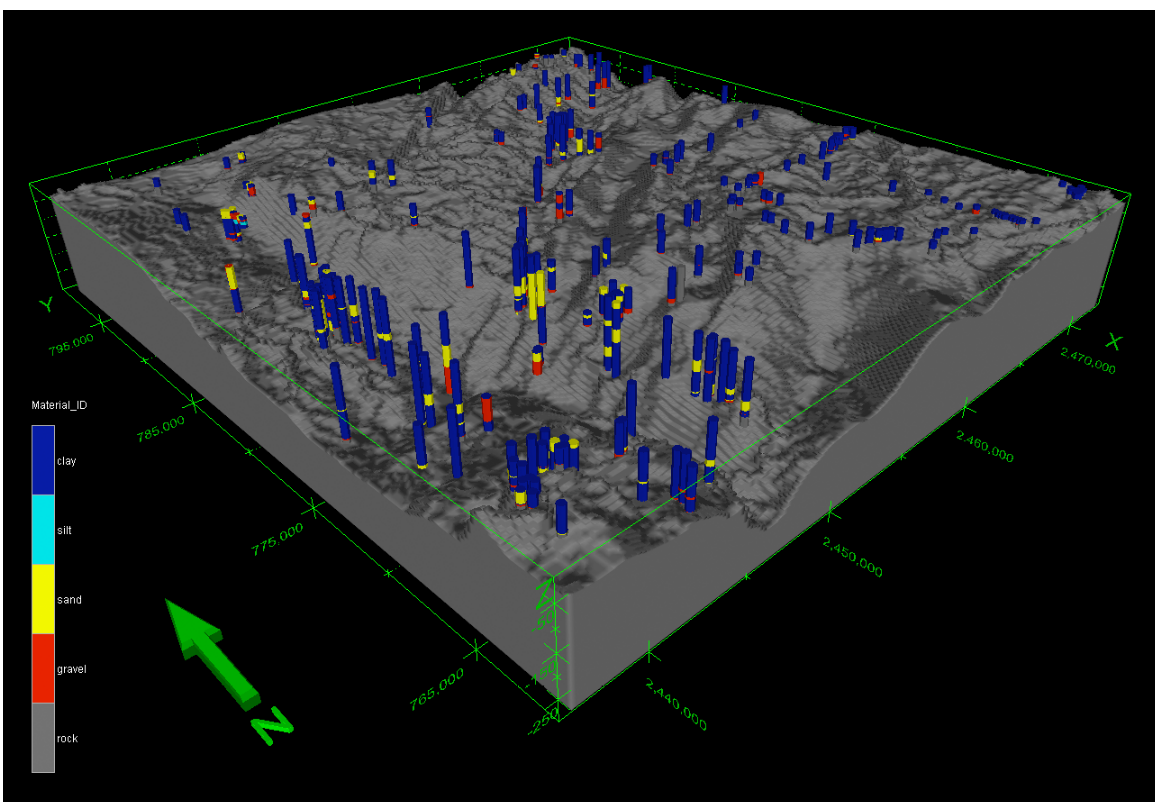


Figure 14. Overview three-dimensional model showing wells, their lithology, and the bedrock surface (in units of depth, not elevation).

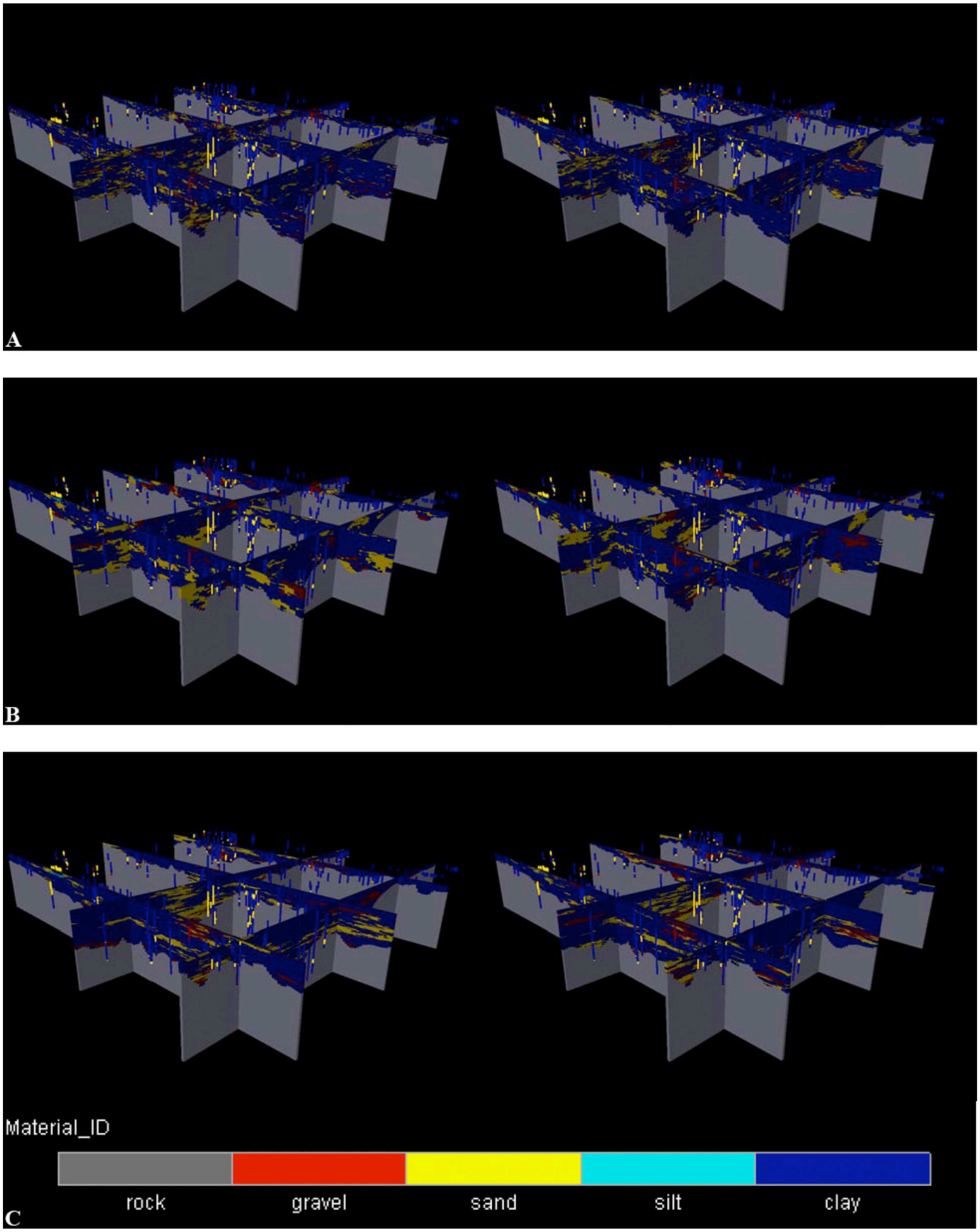


Figure 15. Example realizations for models. A, short-range variogram and high nugget effect; B, short range variogram with no nugget effect; C, long-range variogram with zero nugget effect. The spatial orientation is the same as for Figure 14 (north to the upper left corner).

cells. Such a model would have low flow continuity when modeling groundwater flow. Retaining the range (2000 ft) but removing the nugget effect produces a lithologic model with more continuous bodies (Figure 15-B). There is much more spatial continuity, and "speckling" is minimized. Extending the range to 5000 feet (Figure 15-C) produces elongate horizons of sand and gravel. Such results are visually pleasing, as they produce a layered look to the geology, which is compatible with stratigraphic concepts. However, this model is the least faithful of the three to the results of experimental variography. It represents the maximum extent of spatial continuity of sand and gravel bodies that could be reasonably interpreted from the data.

Inter-run variability between the short-range/high nugget and long-range models was investigated more closely by looking at an individual slice through the models. A cross-section (Figures 16, 17, 18 and 19) was chosen that has wells proximal to guide interpolation, but not within the displayed cells. This location was chosen in order to investigate the variation in simulation results where there was some well guidance, but also significant gaps. There, little commonality was found between single realizations of the short-range model and those of the long-range model (Figures 16-A and 18-A). As noted above, the short-range model had more interspersion between lithologies, and less contiguous sand and gravel bodies (increased influence of marginal probabilities over kriging weights). For the short range and nugget model, the data had limited influence on the results. For example, silt lithologies were found throughout the model, even though they were not present in any nearby wells.

The mode of the 16 runs (Figures 16-B and 18-B) also showed the increased randomness of the short-range model. The mode for the short-range model showed only one stable sand body, the result of nearby wells constraining the results. The lithology "clay" was the mode for most of the area. For the short-range model, the global proportions heavily influenced the results. The mode for the long-range model showed more sand and gravel in laterally extensive bodies. These sand and gravel bodies existed from simulation to simulation because surrounding wells contributed to the ccdf, so that each random-draw was constrained by data (the left terms of equation 2 had more influence than the global proportions).

The entropy results (Figures 17 and 19) further illustrated the differences between the models. For the short-range model, entropy results were mainly "granular" with little pattern, save for an area of low entropy in the upper right, where there was influence from a well. There were clear patterns in entropy results for the long-range model. The upper 60 feet or so generally had low entropy. The wells in the area were consistently clay, except toward the center, where there was less well control (allowing for more variation between realizations). The area of high entropy in the deep, central portion was produced

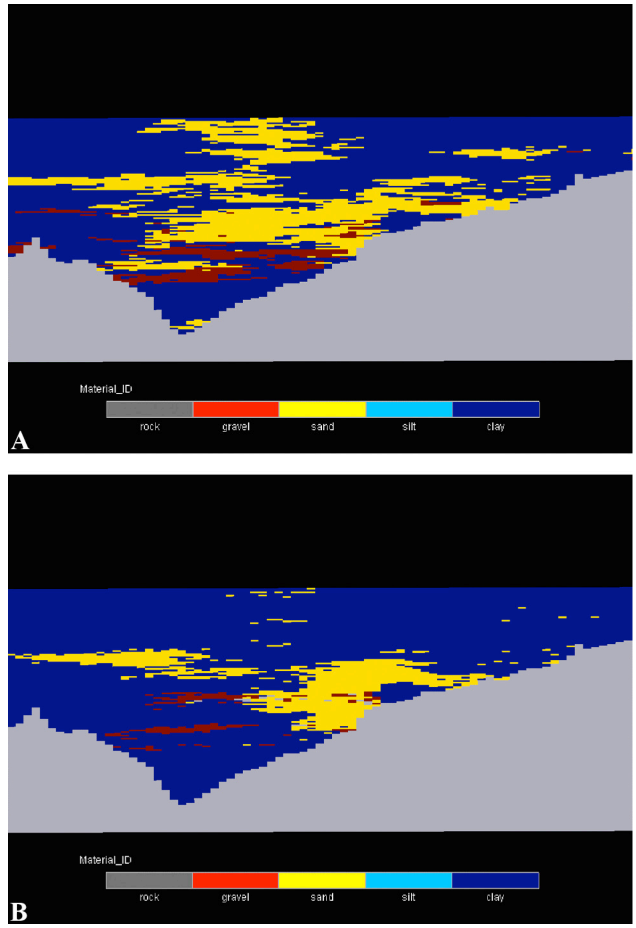


Figure 16. East and west-oriented cross section. Cross section is about 14,500 feet across and contains depths ranging from 0 (top) to 300 feet. Cross section results for long-range variogram with zero nugget effect. A, single realization; B, mode.

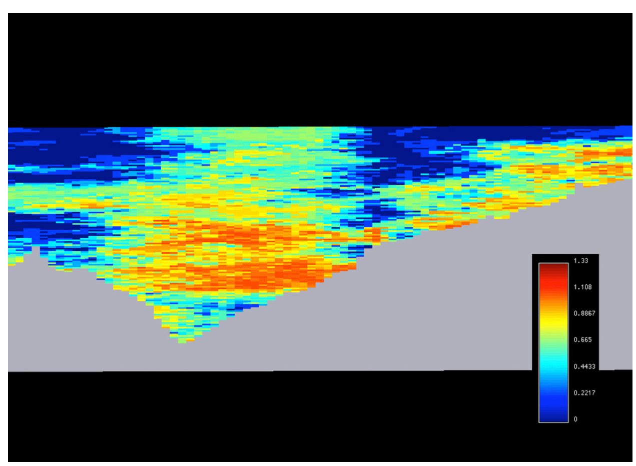


Figure 17. Cross section showing entropy results for long-range variogram. Orientation and dimensions are the same as Figure 16.

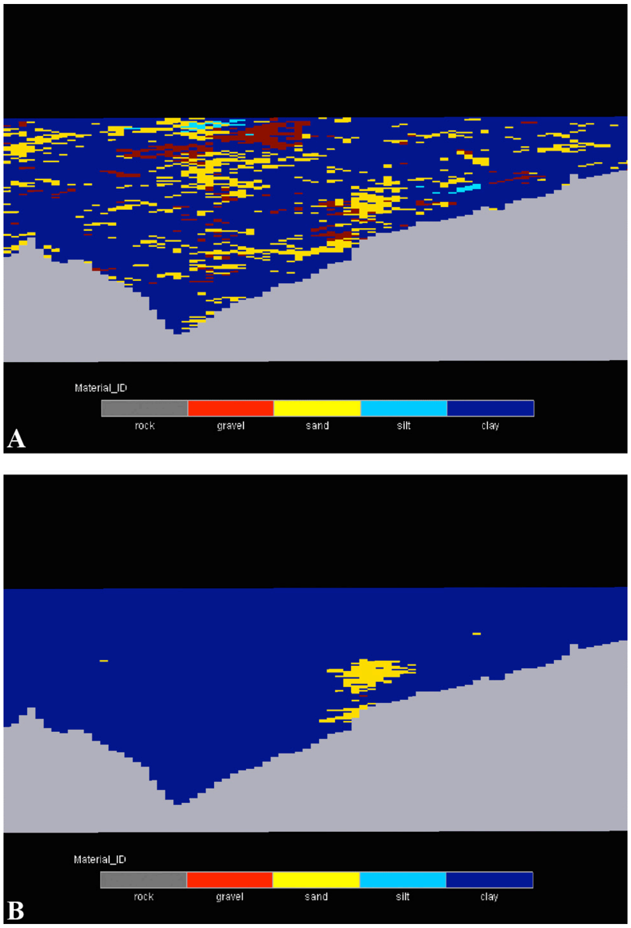


Figure 18. Cross section results for short-range variogram with nugget effect. A. single realization, B. mode. Orientation and dimensions are the same as Figure 16.

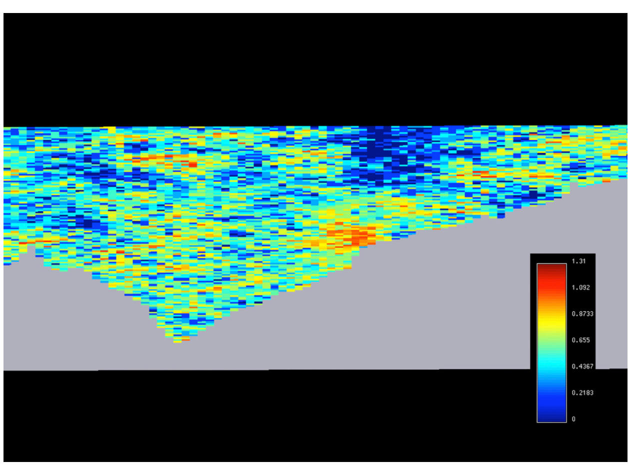


Figure 19. Cross section showing entropy results for short-range variogram with nugget effect. Orientation and dimensions are the same as Figure 16.

by alternation of sand and gravel between runs. True distinction between sand and gravel was questionable; an alternate modeling approach using hydrofacies (Ritzi et al., 2000) where the domain is divided into high and low conductivity units, which are modeled within stratigraphic units, is a better approach (Venteris, 2007).

CONCLUSIONS

The results raise important questions about the mapping of lithologies in buried valleys, particularly the feasibility of mapping and spatial modeling at 1:24,000 and more detailed scales. Most issues can be corrected with adequate well control coupled with geophysical studies, but this is not practical for the scales of interest due to the resources involved. Are the data good enough and is the geology predicable enough at this scale of interest to support county and regional-scale mapping of buried-valley deposits?

Of primary concern is the low horizontal continuity (lateral consistency) of lithologies between water wells for the current data set. This creates difficulties for both stack mapping and geostatistical simulation. Assigning a stack to a polygon implies that there is a predictable stratigraphy at that location. At simple locales (such as till over bedrock), the meaning of the stack is clear, and it is likely a reasonable prediction of the geology at that location. Tills can be correlated over large distances (Ehlers, 1996, chapter 9). Much of the surficial mapping work in Ohio is based on the correlation of tills. For this study (Figure 11), the scale of autocorrelation for predicting thickness of Wisconsinan till was on the order of 35,000 feet. The picture is less clear for mapping the lithologies of buried valleys. As seen in the water wells and simulation results, the depth of occurrence and thickness of sand and gravel bodies is highly variable. Some of this variability is due to the fact that lithologic layers encountered include both those that extend for long distances (stratigraphic units) and short distances (facies units). There are depth horizons where the occurrence of gravel is more probable, but these cannot be reliably traced from well to well. Such cases require careful consideration of what the stack sequence is predicting and communicating about the geology. In well-constrained situations, the stack can give accurate stratigraphic information, i.e., it represents a typical configuration of sediments for that polygon. When the driller puts in a new hole, he could expect a configuration and thickness of sediments similar to the stack sequence on the map. For more variable systems, an alternative, more probabilistic interpretation of the stack is warranted. In this case, the stack is an "average" sequence, which identifies the types of expected lithologies and their most likely vertical positions. For any location, however, portions of the stack may be absent and extra layers may be present. Wide ranges in thickness are possible as well. Comparison of the chosen stack model with the variability demonstrated in the geostatistical simulation results shows the difficulty in applying a stack sequence to complex buried-valley sediments.

Another important issue is the reason behind the poor horizontal correlation between wells. Several possible interpretations exist, the end members being:

1. The geology of this buried valley is predictable at this scale (well spacing), but the water well data are noisy and provide inconsistent information on stratigraphic and facies units. These complications mask the prediction of stratigraphy.
2. The water-well data are accurate, but geological variability occurs at scales well below the sample spacing (perhaps on 100m scales). The sample density is insufficient.

There is reason to believe that both case 1 and 2 are true. The water-well dataset is known to be noisy. Drilling crews with a wide range of geological training and experience produce these records as a legal requirement with the State of Ohio. Some water wells provide a very good approximation of local geology, while others contain serious errors in interpretation. Some of these errors were detected and fixed through the processing of the water wells into indicator variables, but certainly misidentifications and other blunders remain in the dataset. Past studies have suggested that case 2 may also be a contributing factor. Ritzi et al (2000) found that the range of autocorrelation for buried valley sediments is less than 1,000 feet. Therefore, very dense sampling is required (such as is conducted for site remediation studies) to make accurate three-dimensional models from experimental variography. An alternative is to use sources of more detailed information (geophysical profiles, outcrops) to develop models of spatial structure for geostatistical simulation.

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