Assessing spatial uncertainty in reservoir characterization for carbon sequestration planning using public well-log data: A case study

Erik R. Venteris and Kristin M. Carter

ABSTRACT

Mapping and characterization of potential geologic reservoirs are key components in planning carbon dioxide (CO_2) injection projects. The geometry of target and confining layers is vital to ensure that the injected CO_2 remains in a supercritical state and is confined to the target layer. Also, maps of injection volume (porosity) are necessary to estimate sequestration capacity at undrilled locations. Our study uses publicly filed geophysical logs and geostatistical modeling methods to investigate the reliability of spatial prediction for oil and gas plays in the Medina Group (sandstone and shale facies) in northwestern Pennsylvania. Specifically, the modeling focused on two targets: the Grimsby Formation and Whirlpool Sandstone. For each layer, thousands of data points were available to model structure and thickness but only hundreds were available to support volumetric modeling because of the rarity of density-porosity logs in the public records. Geostatistical analysis based on this data resulted in accurate structure models, less accurate isopach models, and inconsistent models of pore volume. Of the two layers studied, only the Whirlpool Sandstone data provided for a useful spatial model of pore volume. Where reliable models for spatial prediction are absent, the best predictor available for unsampled locations is the mean value of the data, and potential sequestration sites should be planned as close as possible to existing wells with volumetric data.

INTRODUCTION

Geologic sequestration of carbon dioxide (CO_2) is a promising approach for reducing atmospheric greenhouse gas levels. Sequestration of CO_2 in geologic units may be accomplished using a variety of

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different storage mechanisms. The commonly discussed storage types include volumetric, solution, adsorption, and mineral. Volumetric storage refers to the amount of CO_2 that is retained in the pore space of a geologic unit, generally as a supercritical phase retained by structural or stratigraphic traps or by overlying cap rock (Wickstrom et al., 2005). Mapping the location and estimating the total capacity of this storage type for several geologic units in the north central Appalachian Basin have been the focus of our research.

As in oil-and-gas exploration, reservoir characterization is a key task in planning CO_2 injection projects. Spatial models and maps are needed to ensure (1) sufficient overburden to maintain CO_2 in a supercritical state (approximate depth of 2500 ft [762 m]), (2) large enough porosity and permeability to support a practical injection rate, and (3) sufficient total CO_2 capacity to ensure the economic viability of the project. In addition, selection and evaluation of potential injection sites require a detailed understanding of the overlying and underlying formation(s) that would serve as seals (a topic beyond the scope of this contribution). Accordingly, rock characteristics critical to characterizing a potential sequestration reservoir include depth, thickness, porosity, water saturation, permeability, and the lateral and vertical heterogeneity of these parameters. Petrophysical analyses of geophysical well logs and core samples are used to determine these properties at individual boreholes, and the spatial models are used to estimate values for these throughout the area of interest.

The selection of sites for carbon sequestration projects includes a wide range of geologic and nongeologic factors (Wickstrom et al., 2005; Venteris et al., 2008). Because of the complexity of site selection and planning, predicting the sequestration capacity at unsampled locations is advantageous. Maps and other spatial models of reservoir characteristics are the most convenient methods available to provide such information. Geostatistical reservoir characterization methods (Deutsch, 2002) provide an objective, optimized, and scientifically defensible method for estimating reservoir characteristics at unsampled locations, providing measures of the accuracy of such estimates and facilitating the generation of continuous models (rasters) for use in regional capacity calculations (Venteris et al., 2008).

As part of our early research efforts, we used kriging to map structure elevation data and thickness for the Medina Group/"Clinton" Sandstone in Pennsylvania, West Virginia, and Ohio. The Medina was chosen for more detailed study because a large number of borings are available in northwestern Pennsylvania, and our previous mapping effort showed relatively high accuracy in structure and isopach mapping relative to other potential reservoirs (Carter and Venteris, 2005; Wickstrom et al., 2005). The lack of prominent faulting in the formation also simplified the application of geostatistical methods. In this study, conducted at a higher resolution with more data than the previous works, we seek more fully to characterize the reservoir through refinement of the structure and isopach models and through the addition of spatial models of the available pore space.

Our case study uses geostatistical methods (kriging and stochastic simulation) to quantify the strength of spatial prediction for a range of reservoir parameters based on a typical public oil-and-gas data set for the Appalachian Basin. A major goal of this study was to investigate the usefulness of the available public data for each of the various reservoir parameters to identify knowledge gaps and design future data collection efforts. This contribution illustrates the dangers of mapping with black box approaches typical of some reservoir characterization software that do not encourage or allow the modeler to explore the data for outliers, investigate and quantify the spatial structure of the data for use in prediction, and evaluate the error of the predictions. A map, whether drawn by computer algorithm or hand contouring, implies that the person creating the maps can predict values at unsampled locations. The quality of that prediction must be evaluated. For accurate spatial prediction, (1) the error in the measurements must be small compared to the magnitude of spatial variability, (2) that spatial variability must be at least partially ordered in space (not random), and (3) the distance between the samples (wells) must be less than the range of the spatial structure. If these conditions are not met, predicted values beyond the data points are highly suspect and the map is of little value. This work seeks to illustrate these spatial modeling issues using various reservoir parameters of the Medina Group.

STUDY AREA

The current study area encompasses two major oil-and-gas fields in northwestern Pennsylvania and incorporates publicly available geologic data from more than 5600 deep wells that penetrate the Early Silurian–age Medina Group throughout Erie, Crawford, Mercer, and Venango counties (Figure 1). In general, oil and gas fields are of interest in sequestration projects because

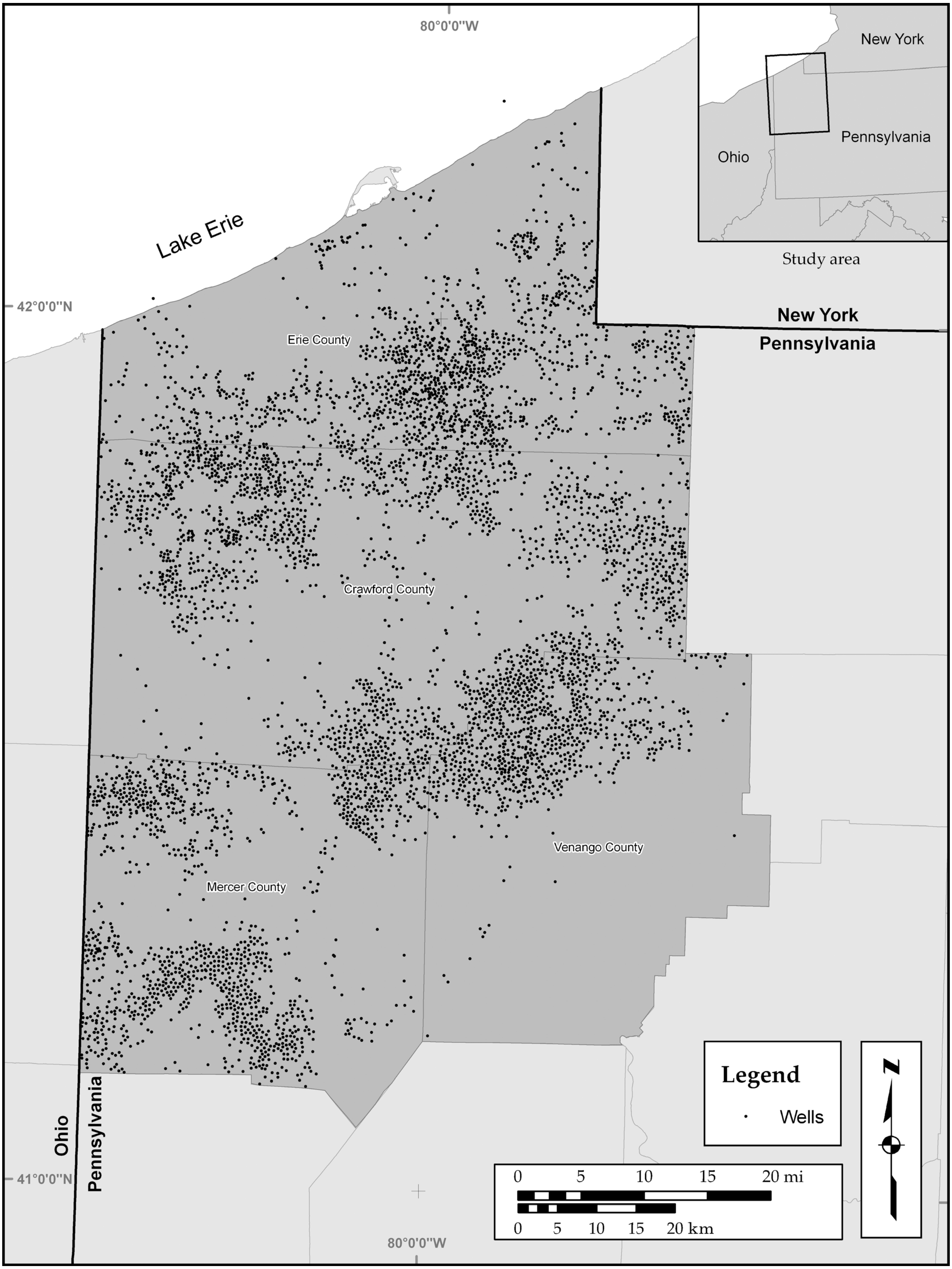


Figure 1. Map of northwestern Pennsylvania, showing the well locations used in this study.

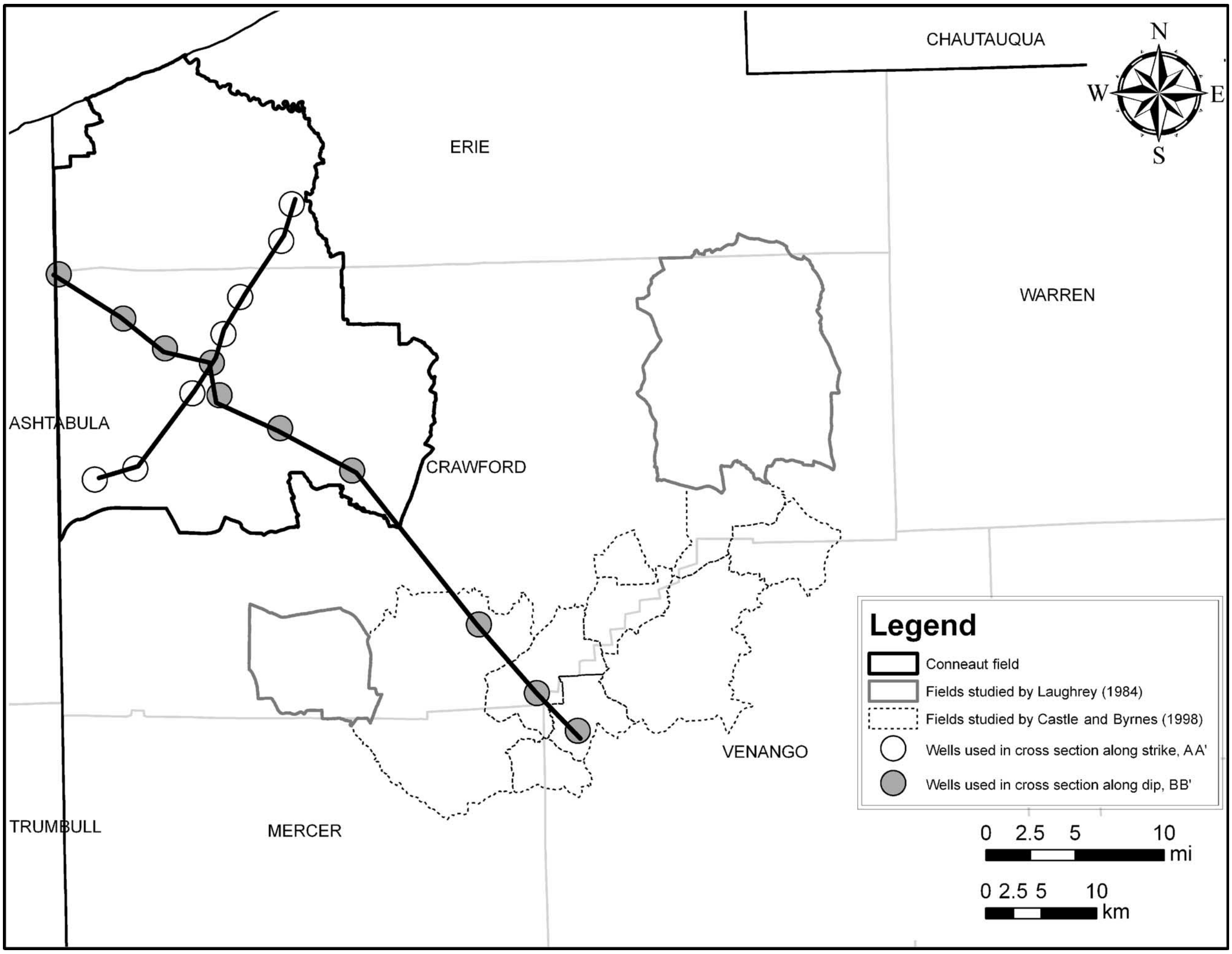


Figure 2. Map of northwestern Pennsylvania, showing the locations of the Athens and Conneaut fields and the locations of the cross sections in Figures 4 and 5.

of demonstrated fluid and gas storage capacity and the potential at some locations for CO_2-enhanced oil recovery. The Medina Group has been extensively explored throughout these and surrounding areas, but perhaps the most notable Medina producing areas are the Athens and Conneaut fields, which are discussed in further detail below as examples of the productivity of this play in northwestern Pennsylvania.

Oil and Gas Fields

The Conneaut field in western Crawford and Erie counties encompasses 128,050 ac ($5.2E^8$ m^2) (McCormac et al., 1996) (Figure 2). The field was discovered in 1957 and produces oil and gas primarily from the Grimsby Formation and Whirlpool Sandstone (Lytle et al., 1961). A part of the field features a thin sandstone lens within the upper part of the Cabot Head Shale that thickens considerably and provides additional production. Operators call this the Tracy sand. Where the Tracy sand is well developed, the Pennsylvania Geological Survey typically includes it within the Grimsby Formation. The average producing depth of Medina units is approximately 3600 ft (1097 m), and pay thicknesses average 12 ft (4 m). Reservoir porosity ranges from 3 to 18%, averaging 10%. Reservoir temperature and initial pressure were reported at 104°F (40°C) and 1100 psi (7584 kPa), respectively (McCormac et al., 1996). The total cumulative gas production is 98.1 bcf ($2.7E^{12}$ L) through 2006, and the total estimated cumulative oil production for the past 22 yr is roughly 1.6 million bbl ($2.5E^8$ L) (WIS, 2009).

The Athens field is located in eastern Crawford County and includes 23,456 ac ($9.5E^7$ m^2) (McCormac et al., 1996) (Figure 2). The field was discovered in 1974 and produces gas from both the Grimsby Formation and Whirlpool Sandstone (Laughrey, 1984). The average producing depth of these reservoir rocks is

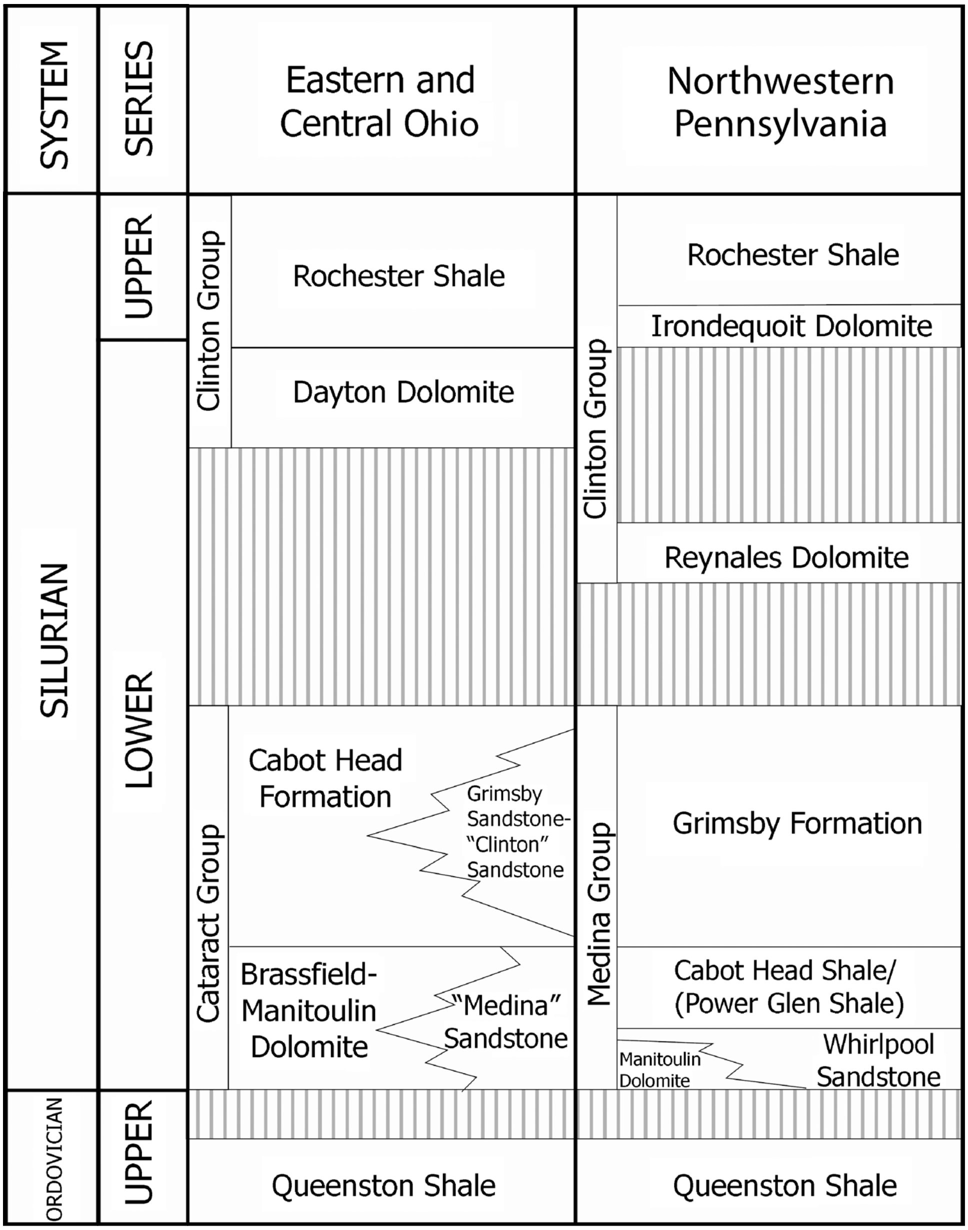


Figure 3. Stratigraphic column showing the rocks of the Medina Group in northwestern Pennsylvania and equivalent rocks in Ohio.

approximately 4800 ft (1463 m) and pay thicknesses average 42 ft (13 m). Porosity ranges from 2 to 9%, averaging 5.6%. Reservoir temperature and initial pressure were reported at 106°F (41°C) and 1220 psi (8412 kPa), respectively (McCormac et al., 1996). The total cumulative gas production through 2006 for the Athens field is 30.5 bcf ($8.6E^{11}$ L), and the total estimated cumulative oil production through 2002, the last year oil production was reported, is less than 1000 bbl (WIS, 2009).

Lithostratigraphy of the Medina Group

The Medina Group of northwestern Pennsylvania consists of three major lithostratigraphic units, in ascending order: the Whirlpool Sandstone, the Cabot Head Shale (sometimes called the Power Glen Shale), and the Grimsby Formation (Figure 3). The Whirlpool Sandstone forms the basal unit of this lithostratigraphic interval and, throughout much of the basin, is composed of a white to light-gray to red, fine- to very fine-grained, moderately well-sorted quartzose sandstone with subangular to subrounded grains (Piotrowski, 1981; Brett et al., 1995; McCormac et al., 1996). The Cabot Head Shale is a dark-green to black marine shale with thin quartzose siltstone and sandstone laminations that increase in number and, in places, thicken upward in the unit (Piotrowski, 1981; Laughrey, 1984). The sandstones of the Grimsby Formation are very fine- to medium-grained monocrystalline quartzose rocks, with subangular to subrounded grains, variable sorting, and thin, discontinuous, silty shale interbeds. Cementing materials include secondary silica, evaporites, hematite, and carbonate minerals (Piotrowski, 1981; McCormac et al., 1996).

We prepared lithostratigraphic cross sections (Figures 4, 5) parallel and perpendicular to strike within the Conneaut field area to further illustrate Medina geology, thickness, and geophysical log responses. These structural cross sections are hung on the top of the Rochester Shale. Gross thicknesses of the Grimsby Formation and Whirlpool Sandstone range from 85 to 170 ft (26 to 52 m) and 10 to 30 ft (3 to 9 m), respectively. Gamma-ray logs are included for all wells (Track 1) and where available, density and neutron porosity logs (Track 2) are provided.

The depth to the top of the Medina Group ranges from approximately 2000 to 6400 ft (610 to 1951 m) throughout the study area. The structure on top of the Medina Group strikes northeast–southwest and dips southeastward at a rate of 30 to 50 ft/mi (6 to 9 m/km, Figure 6). Figures 7 and 8 illustrate the thickness of the Grimsby Formation and Whirlpool Sandstone across the study area, respectively; the gross thicknesses of the entire Medina Group ranges from just less than 80 ft (24 m) to about 400 ft (122 m). Early studies of the Medina and equivalent units were performed in the 1960s through early 1980s (Yeakel, 1962; Knight, 1969; Martini, 1971; Piotrowski, 1981; Cotter, 1982, 1983; Laughrey, 1984). A summary of these and related works is provided by McCormac et al. (1996).

The depositional history of the Medina Group/"Clinton" Sandstone began near the end of the Taconic orogeny in the Early Silurian. During this period, clastic material was being eroded from both foreland fold-belt highlands adjacent to the eastern edge of the Appalachian Basin and the plutonic igneous rocks of the island arc orogen (Laughrey, 1984; Laughrey and Harper, 1986; McCormac et al., 1996). The directions of sediment transport from these highlands were both parallel (i.e., northeast–southwest trending) and perpendicular (northwestward) to the shoreline (Figure 9) (Laughrey and Harper, 1986), which ran from what is now northern Beaver County to central Warren County in Pennsylvania (Piotrowski, 1981). Martini (1971) interpreted the Medina depositional system as a shelf, longshore-bar, tidal-flat, and delta complex based on outcrop studies conducted in western New York and southern Ontario. The Whirlpool Sandstone is the basal transgressive unit of this system and is overlain by shelf muds, transitional silty sands, and lower shoreface sands of the Cabot Head Shale. These sediments were in turn overlain by shoreface and nearshore sands of the lower Grimsby Formation and later, argillaceous sands at the top of this unit (Laughrey, 1984; Laughrey and Harper, 1986; McCormac et al., 1996). Laughrey (1984) divided the Medina Group's depositional system into five facies: (1) tidal-flat, tidal-creek, and lagoonal sediments; (2) braided fluvial-channel sediments; (3) littoral deposits; (4) offshore bars; and (5) sublittoral sheet sands. Facies 1, 2, and 3 sediments comprise the Grimsby Formation, which was deposited in a complex deltaic to shallow-marine environment. The deeper offshore-mud and sand-bar deposits of Facies 4 were reworked by both storm and tidal currents to become transitional sandstones of the Cabot Head Shale. The Whirlpool Sandstone is included in facies 5, which formed in nearshore marine and fluvial, braided-river environments that existed at the beginning of a marine transgression (Piotrowski, 1981; Laughrey, 1984; McCormac et al., 1996). With the advent of sequence stratigraphy as an important reservoir rock interpretation tool in the 1990s, several studies reevaluated Early Silurian–age rocks in the northern Appalachian Basin, including those of Castle (1998, 2001), Hettinger (2001), and Ryder (2004). Research performed by Castle (1998, 2001) on Medina and equivalent cores and outcrops throughout the basin identified six different depositional facies for this rock sequence, including fluvial, estuarine, upper shoreface, lower shoreface, tidal channel, and tidal flat. Furthermore, Castle identified three types of sequences in these rocks: (1) a fining-upward sequence, which includes upper and lower shoreface facies associated with incised valley-fill deposits; (2) a coarsening-upward sequence (type A) that comprises several tidal facies and is representative of a progradational shoreline; and (3) a coarsening-upward sequence (type B), which comprises fluvial and estuarine facies that are interpreted as aggradational. Of these three, the coarsening-upward sequence (type B) prevails in oil and gas wells of the study area (Castle, 1998, 2001).

METHODOLOGY

Geophysical Log Interpretation

We evaluated two types of geophysical logs for the current study: gamma ray and density-porosity logs. Each of these provides information critical to performing volumetric calculations of potential CO_2 sequestration

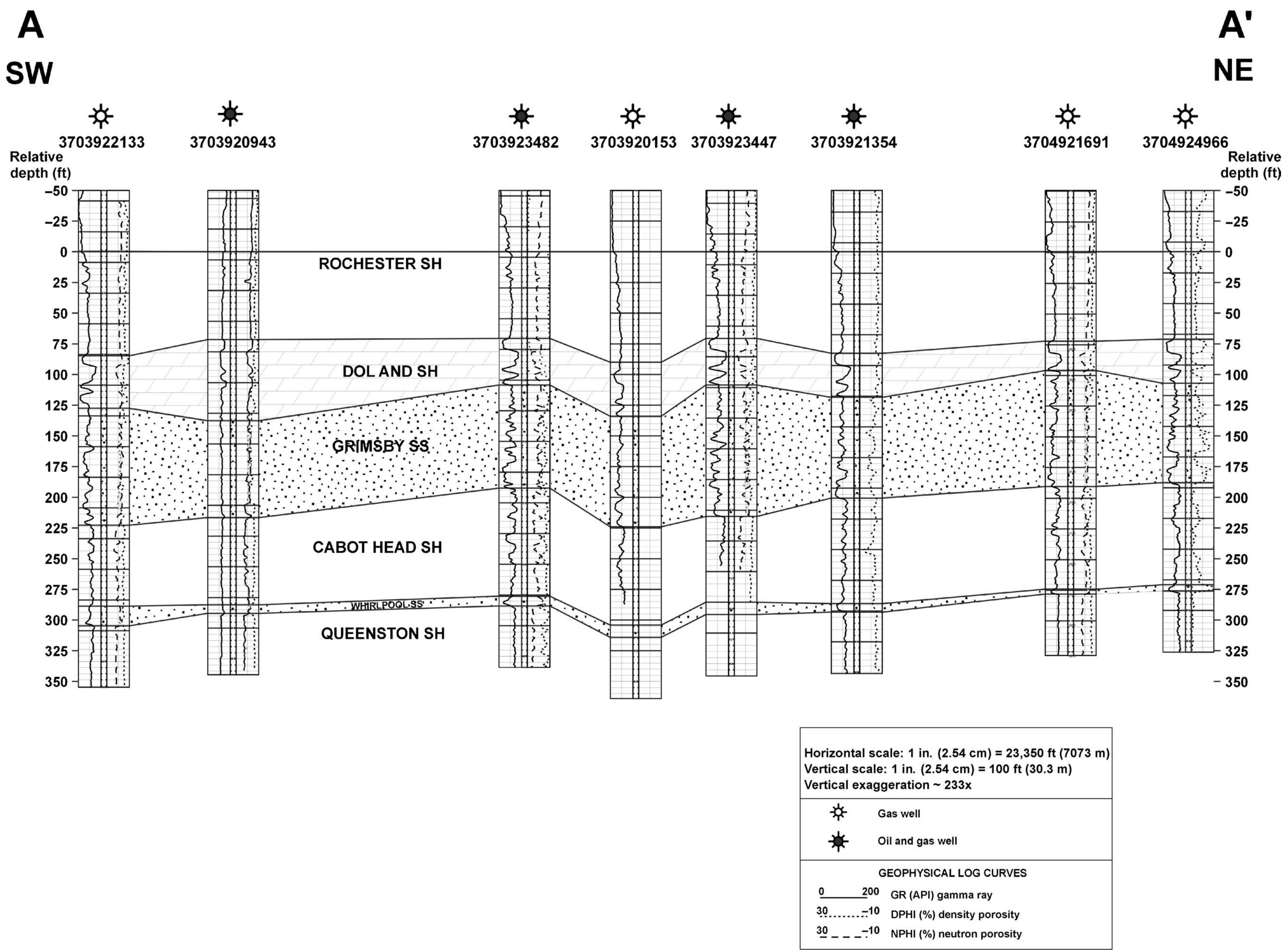


Figure 4. Cross section A along strike, showing geophysical logs and picks for the major rock layers from the Rochester Shale to the Queenston Shale.

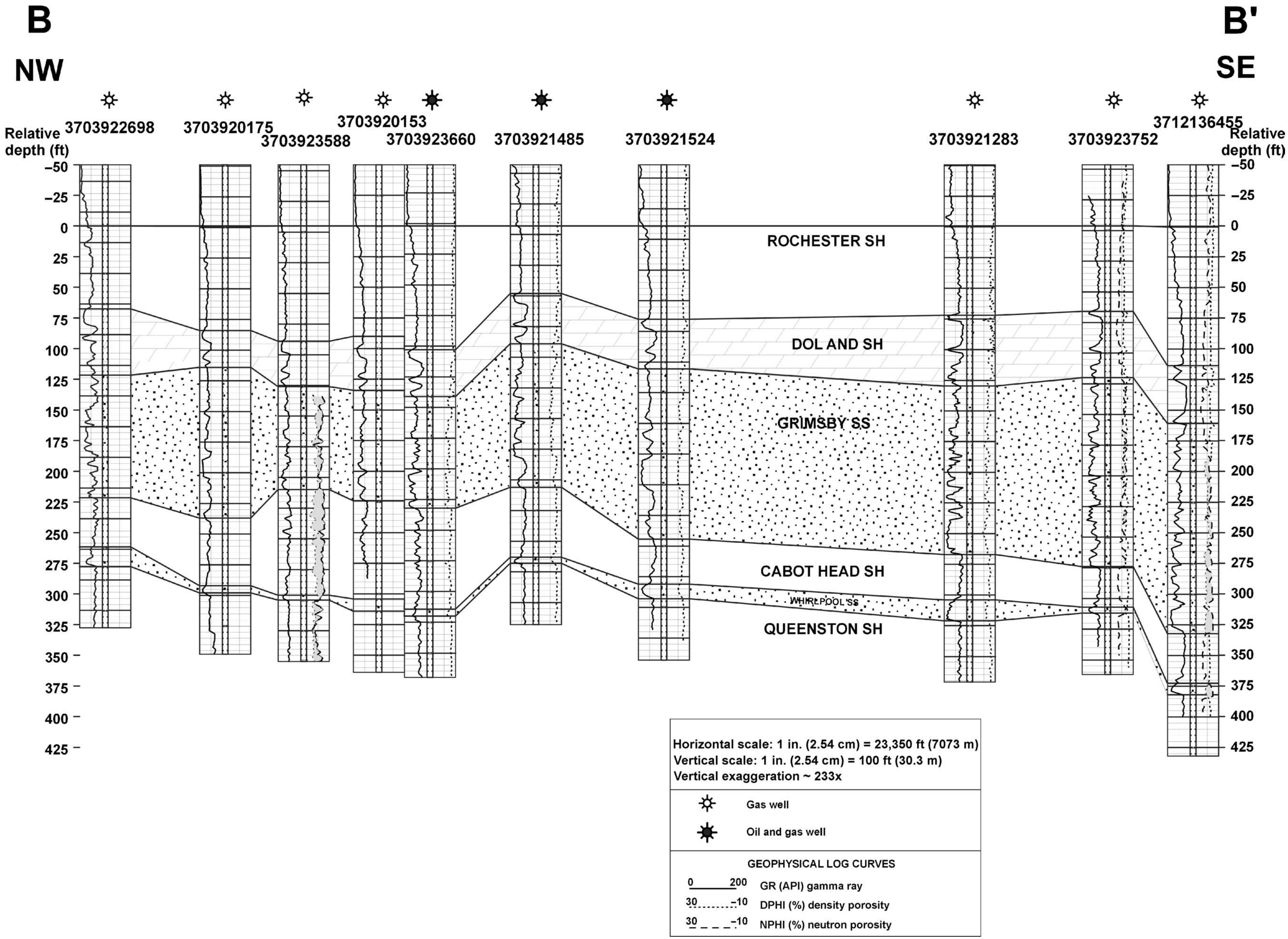


Figure 5. Cross section B along dip, showing geophysical logs and picks for the major rock layers from the Rochester Shale to the Queenston Shale.

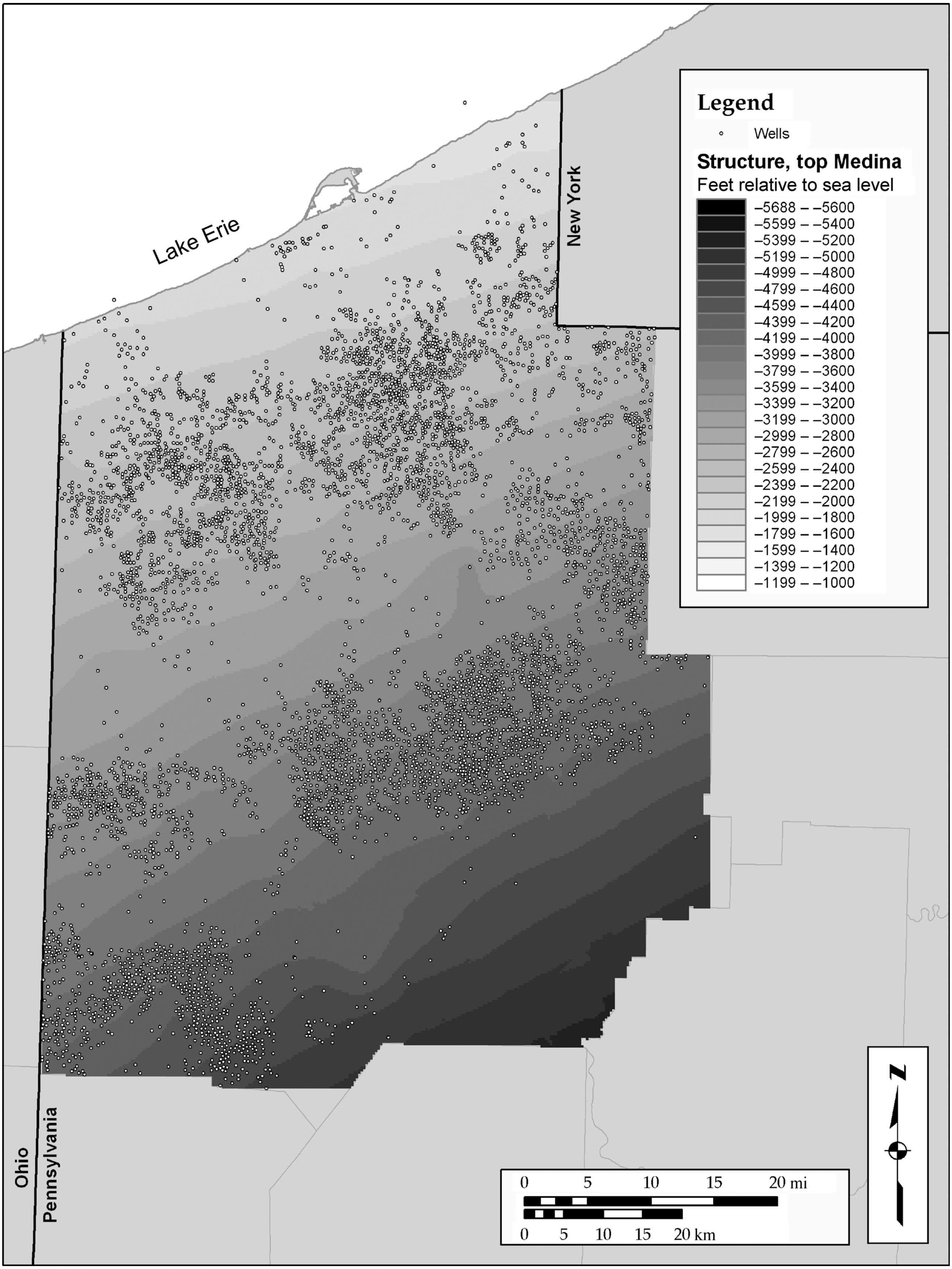


Figure 6. Structure map (interpolated using ordinary kriging) drawn on the top of the Medina Group in northwestern Pennsylvania.

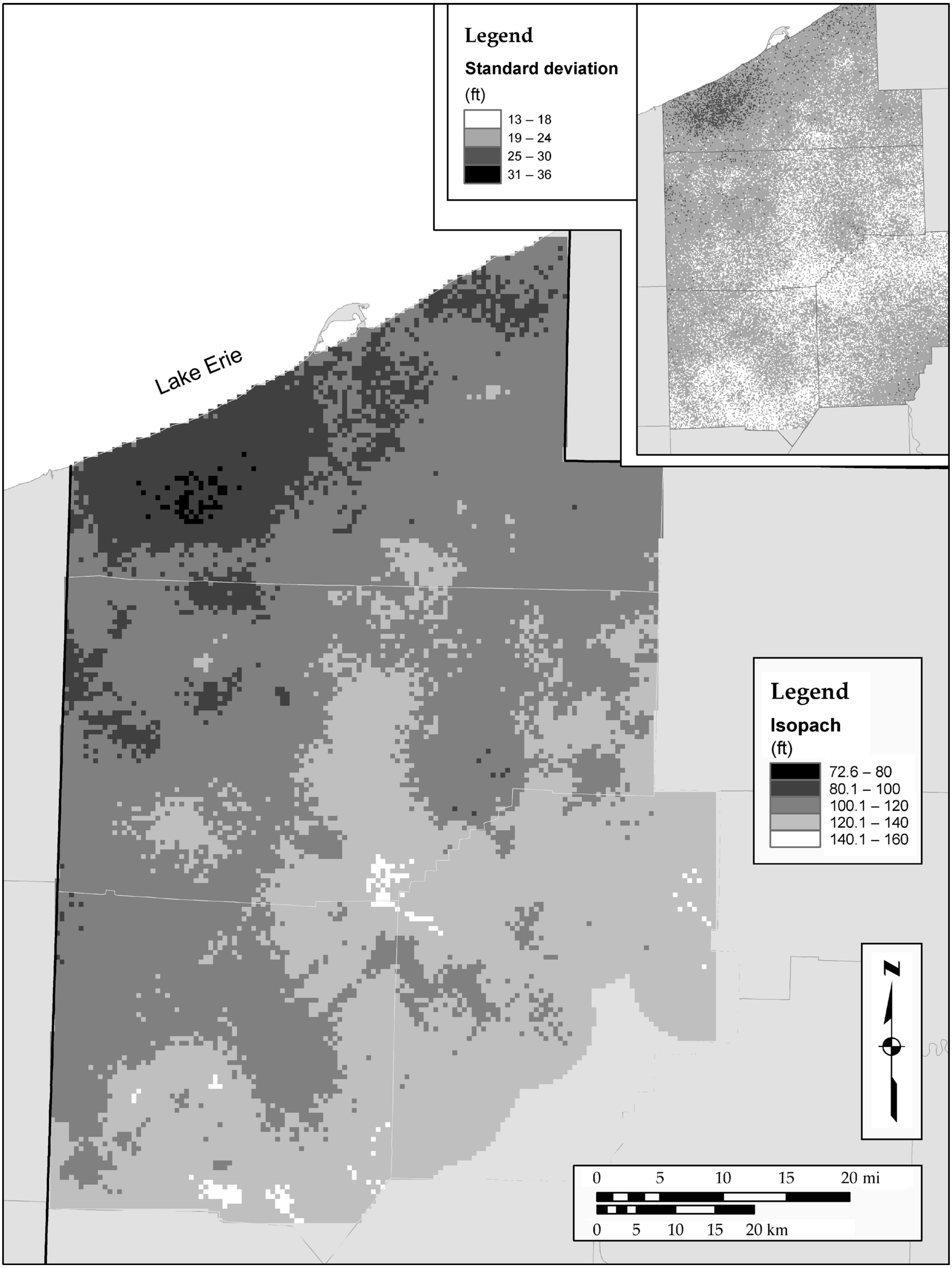


Figure 7. Results from 100 SGSIM runs showing the average thickness and standard deviation (inset) of the Grimsby Formation.

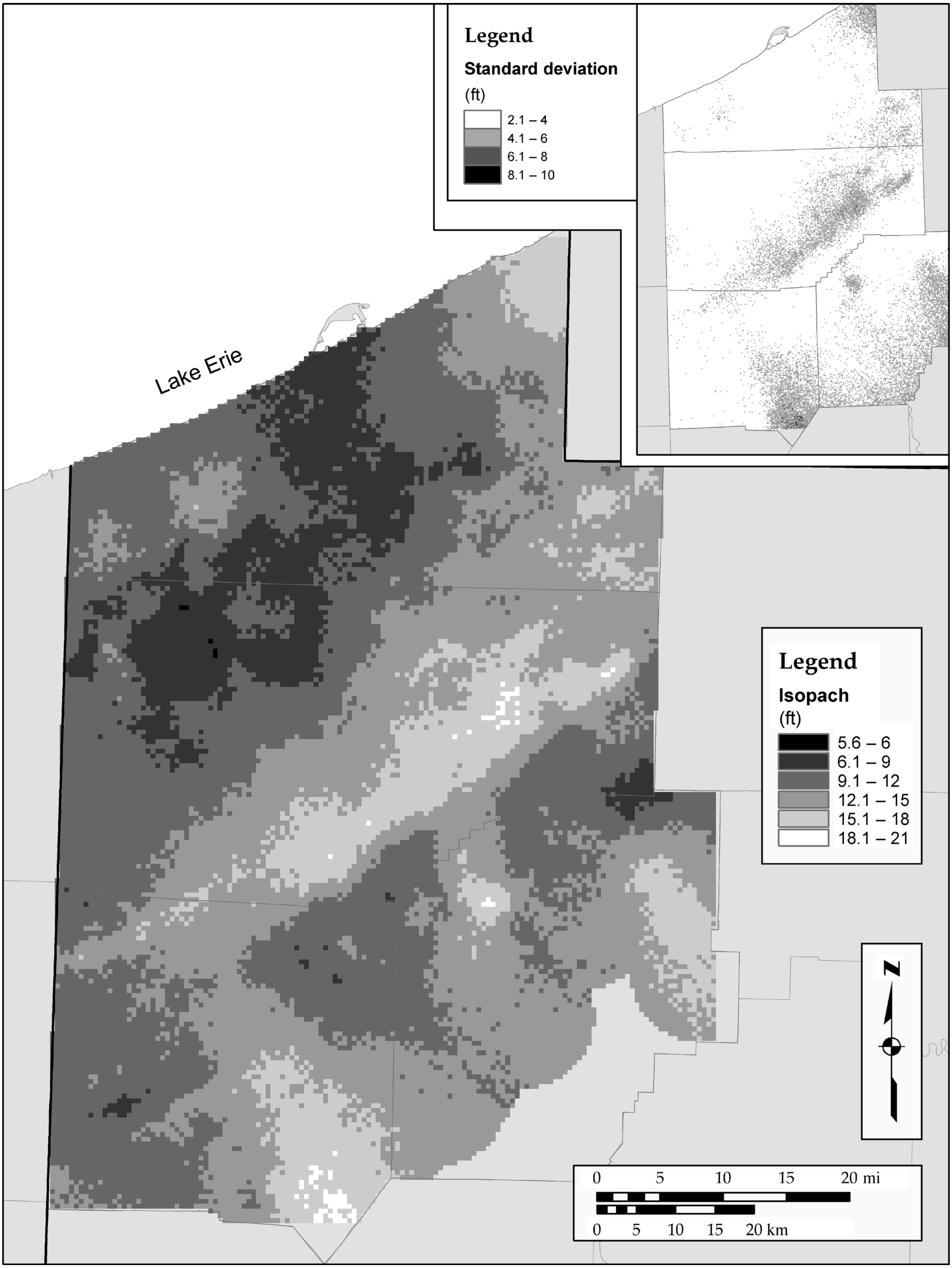


Figure 8. Results from 100 SGSIM runs showing the average thickness and standard deviation (inset) of the Whirlpool Sandstone.

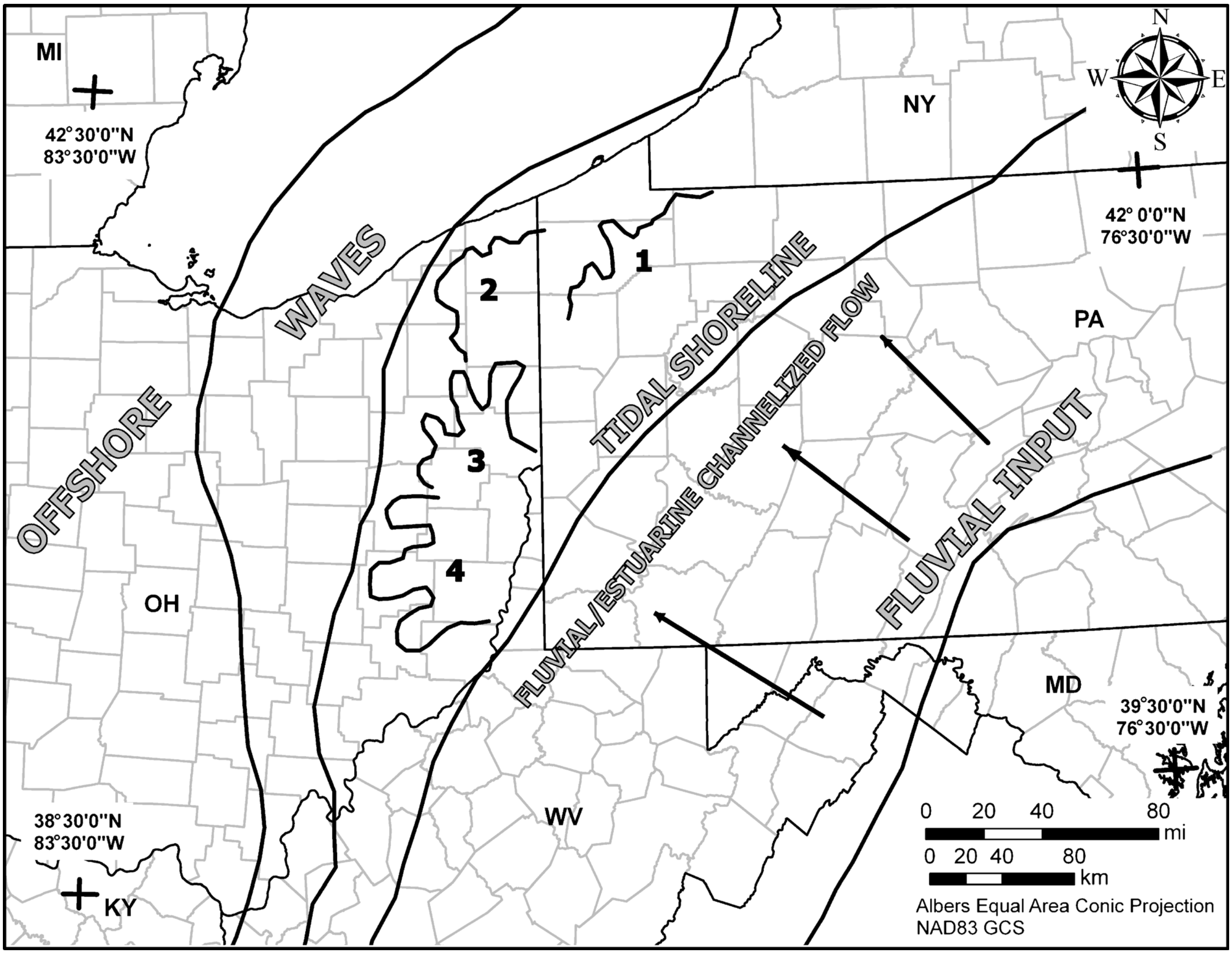


Figure 9. Regional paleoenvironmental interpretations for the Grimsby Formation (and equivalent units) of the Medina Group/"Clinton" Sandstone play. Four different shoreline configurations (labeled 1 through 4) have been proposed by Knight (1969), Pees (1987), Keltch et al. (1990), and Coogan (1991), respectively (modified from Castle, 1998).

capacity for Medina Group sands. The number of logs available for this study was ultimately limited by the availability of digital log curves for wells completed in the study area. The Commonwealth of Pennsylvania does not require the submittal of digital geophysical logs with completion reports; therefore, only paper logs are received by the Pennsylvania Geological Survey. Consequently, all of the digital-log curves used in this study were generated in house by the Pennsylvania Geological Survey.

Gamma-ray logs were evaluated for 360 wells throughout the study area. For those completely penetrating the Medina Group interval, a single clean sand cutoff of 60% (i.e., 80 API units) was selected as an average of what has been used previously for so-called clean Medina wells in northwestern Crawford and western Erie counties (Kelley, 1966; Kelley and McGlade, 1969; Piotrowski, 1981) and dirty Medina wells farther to the south and east in Crawford, Mercer, and Venango counties (Laughrey, 1984).

Density-porosity logs were available for 176 wells in the study area, all of which penetrated the entire Medina Group interval. Most of these were digitized directly from density-porosity curves provided by the operator, but in those instances where only bulk density curves were available, density porosity (ϕ) was calculated at 0.5-ft (0.15-m) intervals using the following formula, per Asquith and Krygowski (2004).

$$\phi = \frac{\rho_{ma} - \rho_b}{\rho_{ma} - \rho_f} \tag{1}$$

where ρ_{ma} and ρ_f are given as the grain density and fluid density, respectively, and ρ_b is the bulk density as recorded

Table 1. Univariate Statistics for Spatial Models Used in this Study

Data*	*N*	Min	Median	Max	Average	Standard Deviation
Depth top Medina	5598	2082	4593	6388	4542	783.7
Elevation top Medina	5598	−4933	−3315	−1512	−3237	735.0
Depth top Whirlpool (ft)	5295	2226	4784	6567	4731	775.95
Elevation top Whirlpool (ft)	5297	−5137	−3508	−1656	−3420	738.9
Elevation bottom Whirlpool (ft)	5375	−5153	−3508	−1668	3424	742.2
Isopach Whirlpool (ft)	5278	1	11	47	11.65	4.03
ISOCSWHIRL (ft)	329	1	8.5	23	8.48	3.98
MPWHIRL (%)	160	1.52	5.54	20.13	5.74	2.18
PFTWHIRL (ft)	122	0.03	0.33	1.69	0.41	0.32
PVWHIRL (ft^3)	160	0.04	0.47	1.79	0.47	0.32
Depth top Grimsby (ft)	5375	2082	4597	6388	4549	776.2
Elevation top Grimsby (ft)	5375	−4922	−3320	−1512	−3242	733.0
Elevation bottom Grimsby (ft)	3810	−5097	−3724	−1623	−3530	743.1
Isopach Grimsby (ft)	3798	5	120	195	118.1	22.0
ISOCSGRIM (ft)	243	3	41.8	128.5	45.2	21.6
MPGRIM (%)	155	1.49	6.25	22.78	6.42	2.16
PFTGRIM (ft)	152	0.07	1.69	6.97	1.94	1.30
PVGRIM (ft^3)	155	0.13	2.50	7.32	2.78	1.26

*ISOCSWHIRL, ISOCSGRIM = thickness clean sand (exceeding 60% sand) for Whirlpool Sandstone and Grimsby Formation, respectively; MPWHIRL, MPGRIM = average porosity in the clean sand portion; PFTWHIRL, PFTGRIM = feet of porosity in the clean sand exceeding 6% cutoff; PVWHIRL, PVGRIM = pore volume.

on the geophysical log. For this work, we used grain and fluid densities of 2.67 and 0.9 g/cm^3, respectively, as recommended by Castle and Byrnes (1998). Minimum porosity cutoffs, as are necessary for any volume-based sequestration calculations, were established at 6%, which is on the conservative side of previously reported values (i.e., 3 to 6%, per Laughrey, 1984, and Castle and Byrnes, 1998).

Pore space was estimated from the logs using a variety of approaches common in oil and gas exploration practice, which provided a range of parameters to investigate for spatial structure. Parameters calculated from the logs for further geostatistical evaluation include thickness of sand exceeding 60% (ISOCSWHIRL, ISOCSGRIM, for Whirlpool Sandstone and Grimsby Sandstone, respectively); average porosity in the clean sand part (MPWHIRL, MPGRIM); feet of porosity in the clean sand exceeding 6% cutoff (PFTWHIRL, PFTGRIM); and the pore volume (PVWHIRL, PVGRIM) calculated by multiplying the thickness of clean sand by the average porosity within the clean sand. The global use of a 60% sand cutoff combined with a 6% minimum porosity cutoff in our porosity-feet calculations necessarily excludes certain porous zones in dirty Medina wells of the study area. Consequently, the porosity-feet statistics in Table 1, particularly for the Grimsby Formation, may appear low to reservoir geologists who know the productive nature of the Grimsby in eastern Crawford, Mercer, and Venango counties.

Geostatistical Modeling

The prediction at unsampled locations and the generation of continuous maps (rasters) were conducted using kriging (ordinary or simple kriging with or without detrending). In addition, geostatistical simulation (sequential Gaussian simulation [SGSIM]; Isaaks, 1990; Deutsch, 2002) was used to generate maps of uncertainty for cases where the spatial structure was weak. In addition to the availability of stochastic simulation, kriging was favored over other interpolation methods because of the additional information available through variogram modeling. The ratio of the partial sill to the nugget effect provided information on the strength and consistency of spatial autocorrelation within the data set. Experimental variograms without structure (pure nugget effect) demonstrate that the scale of spatial variation is less than the sample spacing and/or that the measurement error is large compared to spatial variability. In such situations (also revealed through cross validation), spatial prediction through interpolation provides little to no additional information, and the sample mean (or median for highly skewed data) is the best predictor at unsampled locations.

Geostatistical analysis proceeded using the following steps for each parameter modeled. Summary statistics (Table 1), histograms, and box plots were calculated using JMP® (SAS Institute Inc., 2008) software to identify outliers, check for skewed distributions, and obtain measures of center and spread. Spatial and geostatistical analyses were conducted using ArcMap and Geostatistical Analyst (GA) (ESRI, 2009), respectively. Each property was mapped as point data and investigated for broad trends using the trend analysis software available in GA. Trends, if present, were fitted and removed from the data using global, first-order polynomials (linear) in GA. Where simple kriging was used, the data were declustered using the cell method (Deutsch and Journel, 1998) and a normal score transformation was applied. Variogram modeling and kriging were conducted using GA. Experimental variograms were calculated and model variograms were fitted. For each data set, a heuristic procedure was followed where a range of variogram models were calculated and tested by one-out cross validation. Variograms were calculated over a wide range of scales by altering lag spacings (lag spacings from 500 to 50,000 ft [152 to 15,244 m]) and number of lags. Anisotropic effects, using or not using the nugget effect, and detrending or not detrending were tested. Weak anisotropy was detected in a few of the variogram models, but inclusion in the kriging models did not improve cross validation results. Without prior evidence to justify the more complex anisotropic model, isotropic variograms were used. We tested a range of model variogram functions as well; a spherical model was used for all because exponential and k-Bessel variogram models did not improve the results. The neighborhood search algorithm was held constant over all parameters. The points for each kriging estimate were chosen using a quadrant scheme, with five data points chosen per quadrant (for a total of 20 for each estimate). The maximum search range was set to the range of the model variogram. The choice of final variogram was not formally optimized, but the variogram providing the lowest root mean squared error (RMSE) from cross validation was chosen for the final kriging model. Side investigations showed similar error estimates between cross and external validation for the structure and isopach data, but the petrophysical parameters had too few data to permit external validation.

In addition to kriging, SGSIM was used to model the isopachs for both the Grimsby Formation and Whirlpool Sandstone and the pore volume for the Whirlpool Sandstone. This was done to further evaluate the uncertainty of these geostatistical models, which exhibited a large nugget effect and large cross validation RMSE (uncertainty mapping based only on the kriging variance provided information of limited use because the kriging variance is independent of the data values; Deutsch and Journel, 1998). The SGSIM uses kriging in conjunction with Monte Carlo simulation to produce a range of statistically compatible realizations, each reproducing the spatial structure (instead of the smooth kriging estimates) and the cumulative distribution of the data (Deutsch, 2002). In SGSIM, grid cells to be informed are selected along a random path. For each cell, the value is estimated from the simple kriging estimate plus a random residual drawn from normal distribution (with a mean of zero and a variance equal to the simple kriging variance). Each estimated cell is treated as a data point for subsequent estimates, ensuring that the model faithfully reproduces the variogram and distribution. Summary statistics calculated from the multiple spatial models can then be used to evaluate the quality of the spatial prediction. The SGSIM was performed in GA based on the simple kriging model (Table 2). The mean and standard deviation for each simulated cell was calculated from 100 simulation runs and mapped.

RESULTS

Results from exploratory and geostatistical analyses are presented in Tables 1 and 2, respectively. The spatial modeling results for each reservoir parameter are discussed below.

Formation Top and Overburden Thickness

The thickness of the rock above the target formation is crucial for sequestration planning. An overburden thickness of at least 2500 ft (762 m) (Wickstrom et al., 2005) is needed to maintain the injected CO_2 in a dense, supercritical state. Overburden thickness can be modeled either by kriging the depth data directly or by kriging the subsea elevation and then computing the difference between a digital elevation model (DEM) of the ground surface and the subsea elevation surface. For this exercise, the latter approach was preferred because it was more accurate. The variogram is stronger for the elevation of the top of the Medina Group (Figure 10, Table 2)

Table 2. Results from Variogram Modeling*

Data	Detrended?	Kriging	Lag	Partial Sill	Nugget	Range	Standard Deviation Mean	RMSE
Depth top Medina	Yes	OK	2500	13,146	1808	22,807	783.7	52.32
Elevation top Medina	Yes	OK	5000	1852.8	470.5	59,266	735.0	28.2
Depth top Whirlpool (ft)	Yes	OK	2500	13,943	1416	23,428	775.95	49.86
Elevation top Whirlpool (ft)	Yes	OK	5000	1657.9	269.5	59,266	739.5	25.17
Elevation bottom Whirlpool (ft)	Yes	OK	5000	1664.3	382.4	59,266	742.2	24.73
Isopach Whirlpool (ft)	No	SK	20,000	0.45	0.52	174,285	4.03	3.25
ISOCSWHIRL (ft)	No	SK	5000	0.45	0.30	59,266	3.98	3.23
MPWHIRL (%)	No	SK	5000	0.38	0.50	59,266	2.18	2.17
PFTWHIRL (ft)	No	SK	5000	0.64	0.30	41,977	0.32	0.29
PVWHIRL (ft^3)	No	SK	10,000	0.68	0.24	118,533	0.32	0.26
Depth top Grimsby (ft)	Yes	OK	2500	13,716	1811	23,521	776.2	51.78
Elevation top Grimsby (ft)	Yes	OK	5000	1813.6	452.7	59,266	733.0	26.86
Elevation bottom Grimsby (ft)	Yes	OK	5000	1691.5	585.1	59,266	743.1	29.5
Isopach Grimsby (ft)	No	SK	20,000	0.39	0.62	59,266	22.0	19.06/19.1**
ISOCSGRIM (ft)	No	SK	20,000	0.18	0.75	160,975	21.6	21.77/22.12**
MPGRIM (%)	No	SK	20,000	0.32	0.70	237,065	2.16	2.13/2.31**
PFTGRIM (ft)	No	SK	20,000	0.17	0.81	99,010	1.30	1.35/1.54**
PVGRIM (ft^3)	No	SK	10,000	0.03	0.94	No	1.26	1.25/1.36**

*ISOCSWHIRL, ISOCSGRIM = thickness clean sand (exceeding 60% sand) for Whirlpool Sandstone and Grimsby Formation, respectively; MPWHIRL, MPGRIM = average porosity in the clean sand portion; PFTWHIRL, PFTGRIM = feet of porosity in the clean sand exceeding 6% cutoff; PVWHIRL, PVGRIM = pore volume; RMSE = root mean squared error; OK = ordinary kriging; SK = simple kriging.

**Denotes cross validation results for IDW instead of kriging because a reliable variogram was not obtained for the variable in question.

than for the depth data (Table 2). The cross validation error for the depth data is 52.3 ft (15.9 m, RMSE), whereas the error for the subsea top is 28.2 ft (8.6 m, RMSE), primarily because the subsea data contain only the variation in the stratigraphic boundary, but the depth data contain variability from both the stratigraphic top and the ground topography. The accuracy of the DEM in northwestern Pennsylvania was not measured directly, but for a DEM in eastern Ohio in similar topography, Venteris and Slater (2005) determined an accuracy of approximately 10 ft (3 m) at 30-m (98-ft) resolution when compared to elevation data obtained by precision global positioning systems. Assuming no covariance between the error sources, the total error in the second approach to determine the overburden thickness is 29.9 ft (9.1 m, RMSE).

The overburden thickness map (Figure 11) shows that, for most of the study area, the Medina Group has sufficient overburden for injection projects. Thickness steadily increases from the Lake Erie shoreline to the southeast toward the basin center. Only along the Lake Erie shoreline has the overburden thickness become insufficient to support sequestration projects.

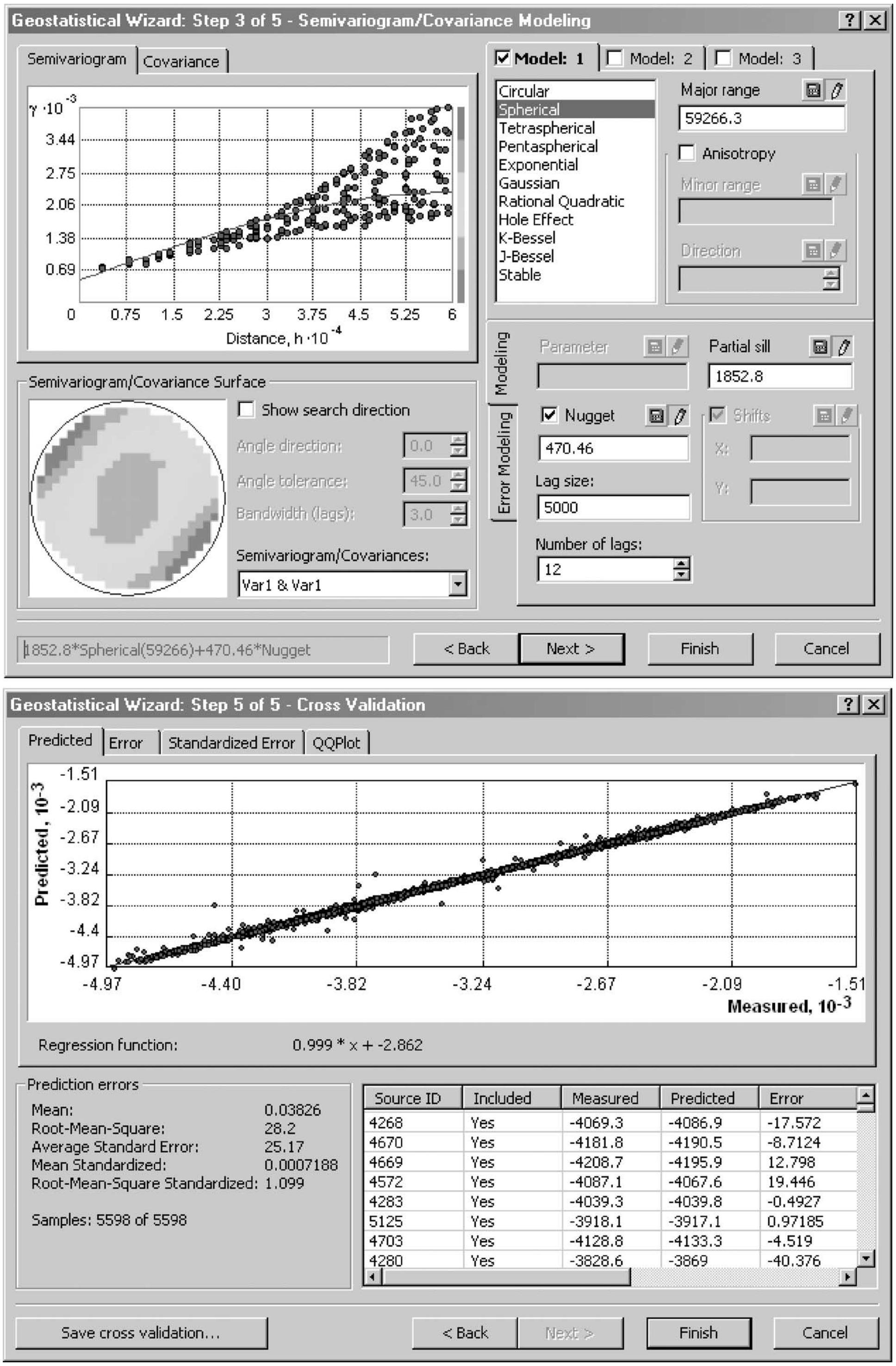
Isopach

As a first step in estimating the volume available for sequestration, we mapped the gross interval thickness for the Grimsby Formation and Whirlpool Sandstone, the two main targets within the Medina Group. Although not typically used directly in volumetric estimates, the isopachs were mapped because their calculation requires only two picks off geophysical logs. Thus, the isopach potentially contains less noise than the volumetric calculations, for which the measurements are more complex. Spatial variation in volume could potentially be mapped using a spatial isopach model and the average porosity if porosity proved difficult to map.

With isopach modeling, the question arises as to the best method of calculation. Two possible approaches exist: one involves calculating the thickness at each well and kriging the thickness; the other is to krig the top and bottom surfaces and then calculate the difference between them. The choice of method is based on the difference in error between the two approaches.

The kriging of the top and bottom of the sandstone contacts was not problematic, with strong variograms

Figure 10. Variogram model (top) and cross validation results (bottom) from ArcGIS Geostatistical Analyst (ESRI, 2009) for the elevation of the top of the Medina Group in northwestern Pennsylvania. This figure is illustrative of data with strong spatial structure, showing a distinct variogram and small RMSE from cross validation.



and small RMSE cross validation errors of around 25 ft (8 m) (only data points with both top and bottom picks were used in this part of the analysis). By contrast, the kriging models of thickness data showed relatively weak spatial structure (Table 2). One way to assess the strength of the spatial structure is the ratio of the partial sill (part of the semivariance with spatial structure) to the nugget effect (part without spatial structure because of spatial variation below the sampling distance and/or measurement error). For a good predictive model (elevation top Medina), this ratio is 3.6, but for the thickness data, it is less than 1.0. Another measure of the strength of the

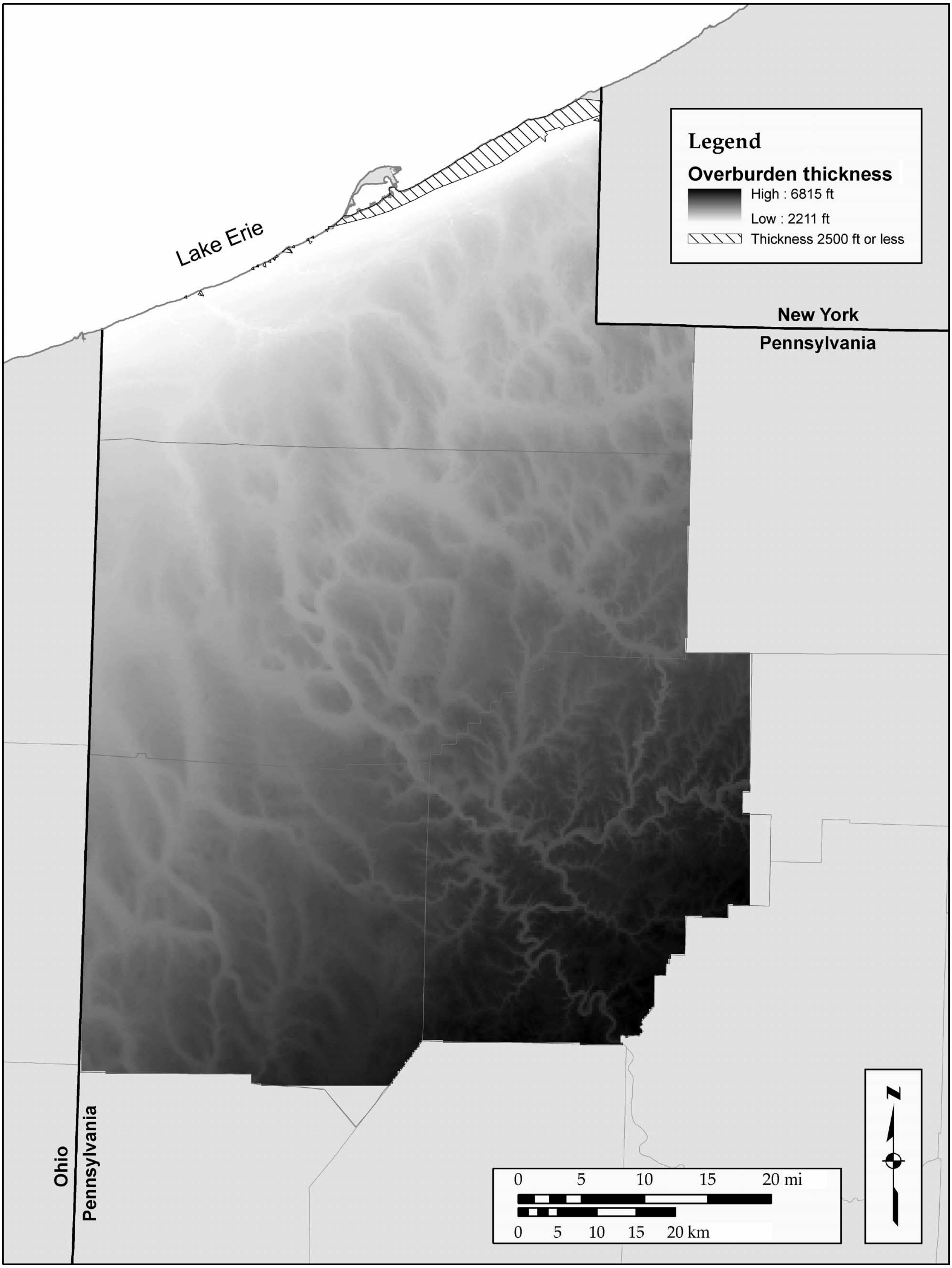


Figure 11. Thickness of overburden on top of the Medina Group, calculated from the difference in the U.S. Geological Survey 98.4-ft (30-m) resolution DEM and the structure map drawn on the top of the Medina Group (Figure 6).

model is the comparison of the standard deviation of the mean compared to the RMSE obtained from cross validation. For the isopach models, these statistics are nearly equal, indicating that the spatial model is adding only a small amount of additional information compared to using the mean thickness to predict unsampled locations. Also note that the issue is not a problem with geostatistical interpolation or with the attendant assumptions (stationarity); cross validation results from inverse distance weighting (IDW; for the Grimsby Formation, Table 2) gave nearly identical cross validation results.

The choice of approach to calculate the isopach is made on the basis of the relative error between the options. For the kriged thickness data, the error is estimated directly from the cross validation results. When calculating the isopach from the difference by the two surface methods, the errors propagate by

$$\sigma_{iso}^2 = \sigma_{top}^2 + \sigma_{bot}^2 - 2\mathrm{cov}(\mathrm{top}, \mathrm{bot}) \tag{2}$$

where σ_x^2 is the variance of the errors (RMSE for top and bottom) and cov(top, bot) is the covariance between the errors for the top and bottom surfaces. For the Whirlpool Sandstone, the cross validation errors (calculated for data points where both bottom and top surfaces are present) are as follows: σ_{top}^2 is 633.6 ft^2 (58.9 m^2) and σ_{bot}^2 is 601.3 ft^2 (55.9 m^2). The cross validation errors between the surfaces are highly positively correlated (Pearson coefficient $r = 0.94$) with a covariance of 581.04 ft^2 (54 m^2). By equation 2, the error (square root of σ_{iso}^2) in determining the isopach from the difference of the top and bottom surfaces is 8.5 ft (2.6 m). In this case, the error from the two-layer method is greater than the cross validation error from simple kriging (3.31 ft [1.01 m]). In contrast, the error for the Grimsby Formation isopach from equation 2 is 20.03 ft (6.11 m), which is not meaningfully different than the cross validation error (19.06 ft [5.81 m]). Accordingly, isopachs presented in this work (Figures 7, 8) are based on simple kriging models of thickness (presented as averages from SGSIM runs). Kriging of thickness data is favored over the two-layer method when the covariance (equation 2) is low (or negative) and the layer is thin (assuming, as in this case, a positive correlation between the magnitude of thickness and cross validation error). Such calculations could also be based on error estimates from SGSIM, which is a subject for future investigation.

Spatial Modeling of Petrophysical Parameters

We attempted to calculate spatial models for pore volume and its individual components (thickness of clean sand, average porosity within clean sand), and porosity feet (a metric popular in industry) for the Grimsby Formation and the Whirlpool Sandstone (Figure 12). As with the structure and isopach modeling, we adjusted a wide range of variogram calculation parameters in an attempt to find models of spatial structure. To be thorough, experimental variography was conducted in both GA and Stanford Geostatistical Modeling Software (SGeMS; Remy et al., 2009) because these softwares offer subtle differences in the variography approach. Most of these parameters exhibited a very small partial sill and large nugget effect (Table 2). The kriging model, therefore, provided little to no spatially predictive information for these parameters. As further verification, the parameters for the Grimsby Formation were also modeled using IDW in GA, which depends only on the relation of local data values to one another instead of a globally applicable model of spatial structure as kriging does. In each case, cross validation results from IDW did not improve the model over using the mean of the data to predict at unsampled locations (Table 2). As a final check, potential correlations between the isopachs and the measures of pore space were sought for use in mapping, but a predictive relationship was not found. With the exception of pore volume for the Whirlpool Sandstone (explored further below), the current data set is insufficient to make reliable spatial predictions of volumetric variables.

The model of pore volume for the Whirlpool Sandstone warranted further investigation because a clear variogram was observed and the comparison between the standard deviation of the mean and the RMSE from cross validation (Table 2) showed at least some potential predictive value. At question was the value of a rather weak predictive model for planning purposes. To address this issue, 100 conditional SGSIM runs were calculated (1000-ft [305-m] grid resolution), as were summary statistics for each grid cell. The average of 100 runs (the E type in geostatistical literature; Deutsch and Journel, 1998) is displayed in Figure 13. The model shows distinct areas of low (less than 0.5 ft^3 [0.014 m^3]) porosity volume in northwest Crawford and western Erie counties, as well as the central part of Venango County. Areas of relatively large porosity volume (>1.0 ft^3 [0.028 m^3]) exist in central Crawford and east central Mercer counties. At question is the reliability

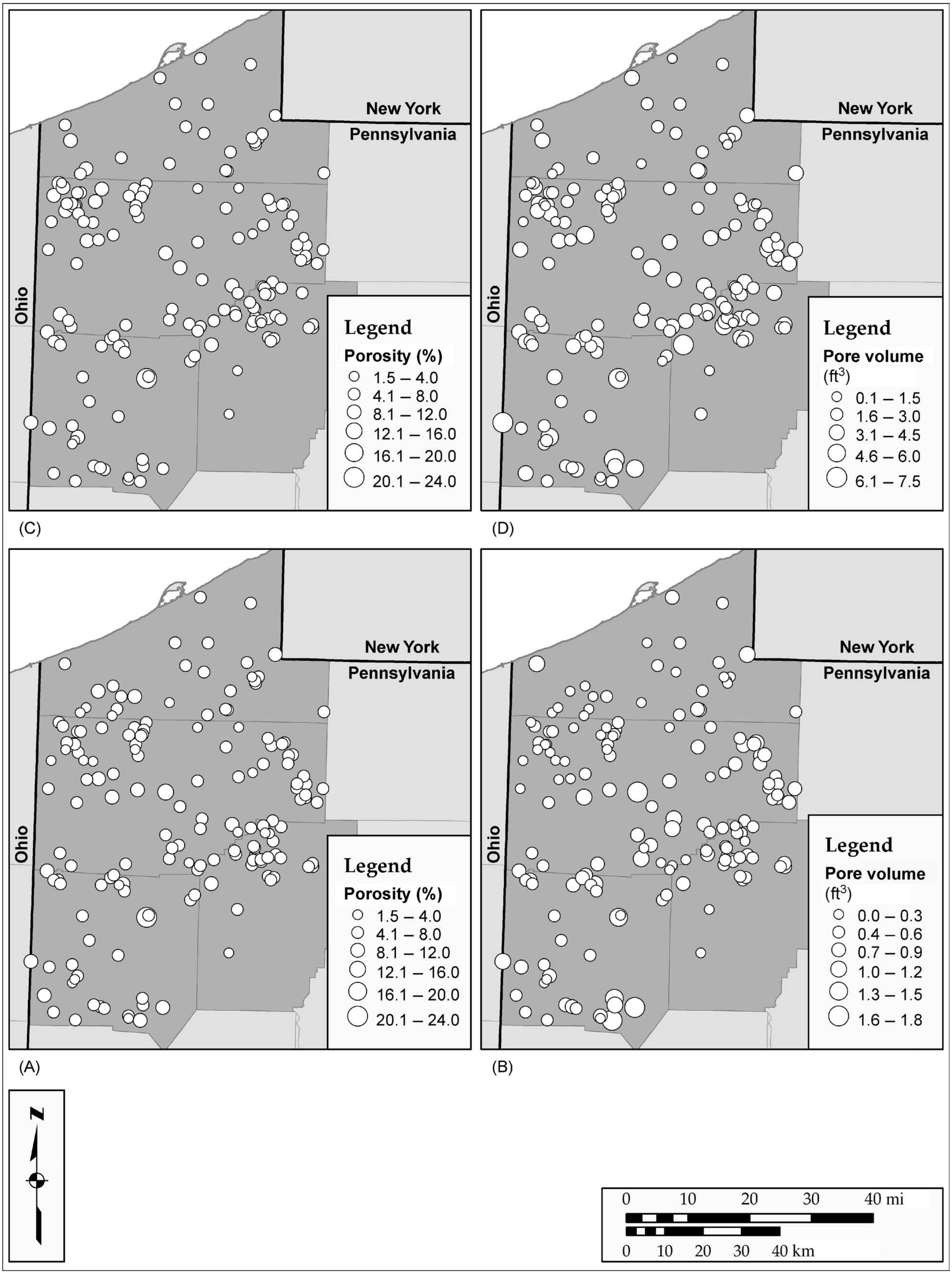


Figure 12. Maps showing the point values of parameters dealing with the estimation of pore volume for the Grimsby Formation and Whirlpool Sandstone: (A) MPWHIRL, (B) PVWHIRL, (C) MPGRIM, and (D) PVGRIM.

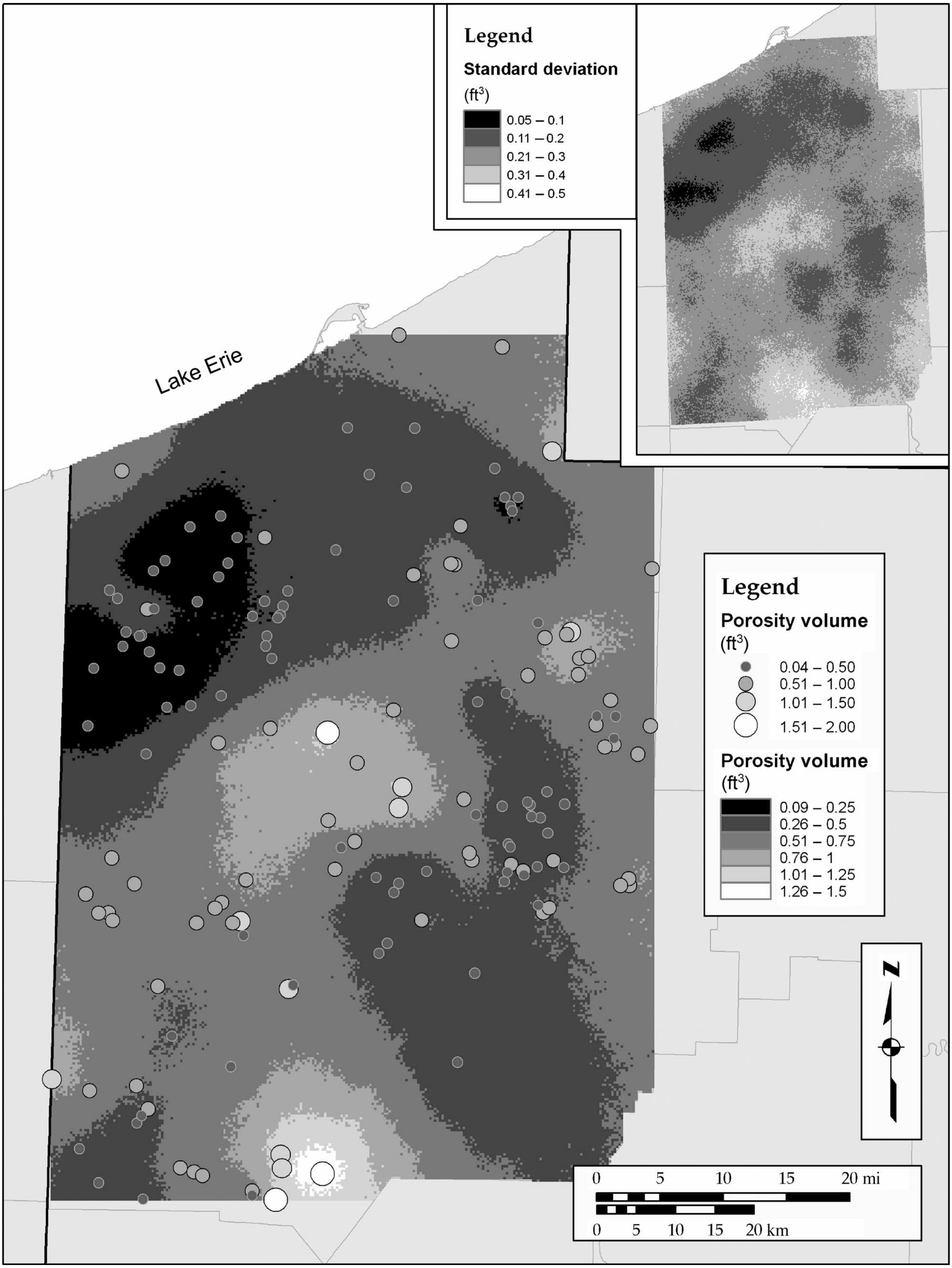


Figure 13. Results from 100 SGSIM runs showing the average porosity volume (ft^3) and the standard deviation (inset) for the Whirlpool Sandstone.

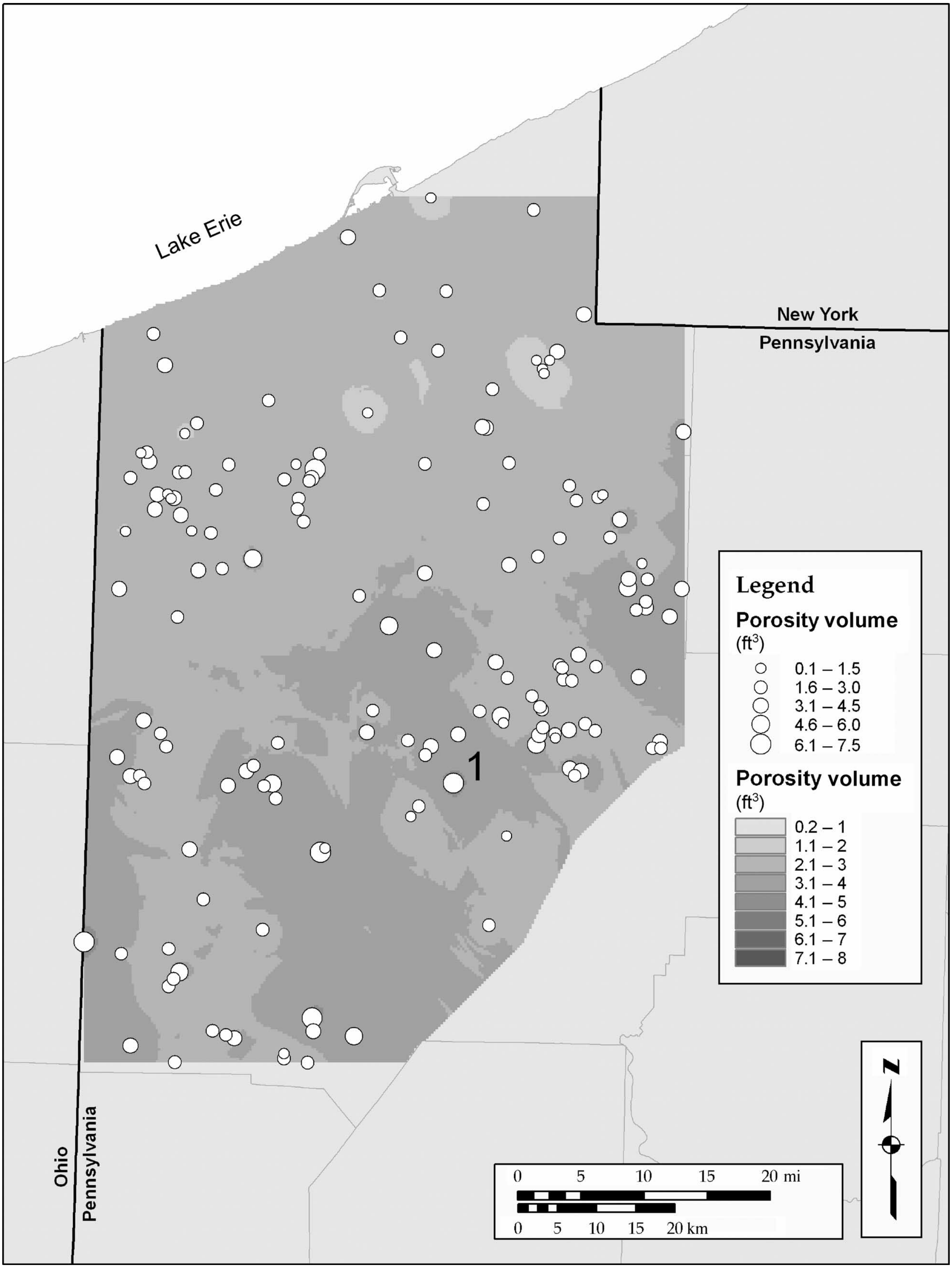


Figure 14. Map of porosity volume (ft^3) for the Grimsby Formation drawn using IDW. The interpolated values around the marked location (number 1) appear to predict an area of elevated pore volume.

of prediction for unsampled locations in these areas. The map of the standard deviation of the model runs shows that uncertainty increases with pore volume and, to a lesser extent, as the data become sparser. Low-porosity areas do not significantly exceed zero (2 sigma or 95% confidence level), whereas the areas of larger porosity volume exceed zero at a minimum of 0.4 to 0.8 ft^3 (0.011 to 0.023 m^3). Despite the noise present in the model, it provides useful information on the spatial distribution of pore volume within the Whirlpool Sandstone.

DISCUSSION

This case study shows the difficulty in mapping reservoir parameters with a typical amount of data available from existing public sources available to state geological surveys in the Appalachian Basin. For the Medina Group, this study and others (Wickstrom et al., 2005; Venteris et al., 2008) demonstrate that the data are sufficient to reliably predict reservoir architecture (especially in areas lacking intensive faulting). The spatial prediction of volumetric parameters, however, is not always possible. The key issue is the interaction between the scale(s) of spatial variability and the distances between well data. The prediction of the elevation of stratigraphic tops is typically more accurate because there are many more formation top and bottom picks than porosity measurements. This is because formation contacts can be derived from detailed drillers' logs and/or gamma-ray logs, which are collected for most wells by most operators; however, porosity measurements require that the rarer porosity log be obtained. Accordingly, the median distance to the closest well is 1643 ft (501 m) for the top of the Medina, but for the porosity volume measurements, the median distance is 7934 ft (2419 m). The magnitude and scale of spatial variation are also important. For example, the quality of prediction for the two isopach models is less than the quality of the structure models despite being based on similar amounts of data. Possible reasons include the decreased range in thickness values compared to the elevation of stratigraphic tops (signal to noise) and possibly more spatial variation below the sampling distance because of sedimentary processes. Similarly, our geostatistical analysis for the Grimsby Formation shows that the spatial scale of variability for pore space occurs at distances below the sample spacing or that measurement errors are too large to detect an existing structure. Castle and Byrnes (1998) investigated the calibration between porosity measured in lab samples and from logs and showed strong correlation, thus large measurement errors are not expected. In contrast, spatial variation occurred at a broad enough scale in the Whirlpool Sandstone to support meaningful mapping with the same data spacing. The variety in model quality illustrates the need for best statistical and geostatistical practices to ensure that spatial predictions are meaningful and potential spatial structures are not missed. Care in choosing geologic modeling units is also important because initial pore volume modeling in this contribution was based on the Medina Group as a whole without success. Dividing the model into Whirlpool and Grimsby components resulted in the exposure of spatial patterns in pore volume for the Whirlpool Sandstone.

Furthermore, these results illustrate the potential dangers in using black-box mapping algorithms or hand contouring. Generating a map of pore volume for the Grimsby Formation is possible (Figure 14), but the map gives unsubstantiated and potentially misleading information as cross validation results (Table 2) cast doubt on the validity of the spatial trends implied by the map. Figure 14 features a map drawn using IDW. At location 1, a well with a large PV value (7.3 ft^3) is observed. The IDW model shows a circular area of elevated PV surrounding this point, suggesting that this area is one of the most favorable locations for a project. The spatial model it is based on is unreliable, however, and no other information on the spatial distribution of geologic processes controlling thickness and porosity exists. Therefore, the lateral extent of the increased porosity volume surrounding location 1 is unknown, and the map is misleading.

For cases such as the Grimsby Formation, the best spatial predictor of pore volume at unsampled locations is the sample mean. When a reliable spatial model is absent, site locations should be selected in the immediate vicinity of existing wells with porosity measurements. When choosing sites for targets such as the Grimsby Formation, a question remains (how close is close enough?) for which the currently available data offer little guidance.

CONCLUSIONS

Site selection for carbon sequestration projects is a complex process involving a wide range of geologic, logistical, and political issues. The current case study and earlier mapping efforts (Wickstrom et al., 2005; Venteris et al., 2008) demonstrate the complex range of issues involved in the making of geologic spatial models and maps to support carbon sequestration planning. These studies show that careful consideration of geological, statistical, and geostatistical issues is needed to address the challenges presented by the limitations of the data relative to the complexity of the sedimentary geology of the north central Appalachian Basin.

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