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Characterizing groundwater flow at Fort Leonard Wood using universal cokriging with trend removal

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CHARACTERIZING GROUNDWATER FLOW AT FORT LEONARD WOOD

USING UNIVERSAL COKRIGING WITH TREND REMOVAL

by

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ABSTRACT

Groundwater elevation interpolation is necessary for the prediction of groundwater flow direction and contaminant transport. Kriging is a geostatistical tool commonly used to interpolate groundwater elevation. Kriging requires a relatively large number of monitoring wells at the site of interest. The variogram model is a crucial element to the kriging equations. The variogram modelling process is an iterative procedure that is often very time consuming. This study presents a literature based approach that provides a point of departure for the variogram modelling process as well as other kriging parameters. A literature database is developed in order to provide insight and a measure of reasonableness to the variogram parameters developed at a groundwater interpolation site. A case study was performed on the Fort Leonard Wood Military Reservation located in Missouri. A data quality analysis was performed on the dataset and spatial outliers were removed. The results from before and after spatial outlier removal are shown. Compliance points were developed using data gaps observed from the standard error maps produced during kriging. The number of wells for the Fort Leonard Wood site were reduced from 61 wells to 45, 30, and 15 wells. Three realizations were performed for each well reduction and results were averaged. Results indicate that when the number of wells are reduced to 15 wells the contour maps are inconsistent with the baseline contour map, each other, as well as the conceptual model. The literature based approach can be easily applied as a point of departure for kriging groundwater elevations.

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1. INTRODUCTION

1.1 GEOSTATISTICAL CONCEPTS

Kriging is a least-squares linear regression geostatistical tool commonly used for interpolation. Kriging is known for producing estimates that are unbiased and have minimum variance. A perk of the kriging process is that it also produces an estimate of error at the prediction point. Multiple forms of kriging are used within the literature to develop a potentiometric surface of groundwater. The different forms of kriging are detailed in Goovaerts (1997). The most commonly used forms of kriging include: simple kriging (SK), ordinary kriging (OK), universal kriging (UK), cokriging (CoK), and kriging with external drift (KED). SK is kriging in which the mean is assumed to be known and to be constant throughout the site area. OK assumes that the mean of the dataset is not stationary and is unknown, allowing for one to account for local variation. UK assumes that trend is present in the dataset. This trend is removed from the dataset, and the residual is used within the modelling process. The trend must be added back to the interpolated results. CoK incorporates both a primary and secondary variable that are often related, such as groundwater elevation and ground surface elevation. KED also incorporates secondary variable information, but uses the secondary information to characterize the spatial trend of the primary variable.

A variogram model is required for the kriging interpolation process. Olea (2003) defines the unbiased estimator of the variogram as

$$\gamma(h) = \frac{1}{2n(h)} \sum_{i=1}^{n(h)} (Z(x_i + h) - Z(x_i))^2 \tag{1}$$

Where:

Z = an intrinsic random variable

h = the separation distance between measurements

$n(h)$= the number of pairs of variables at distance h apart

x_i = location of i^{th} variable

The variogram model relates variance to the separation distance of the points. The variogram model is first developed by plotting the separation distance (lag) on the x-axis of the graph and the variance on the y-axis. This produces a variogram cloud. A lag distance is chosen to produce a total of three to six total lags on the variogram plot (Olea, 2003). A lag tolerance is then chosen, and the cloud points are binned according to the tolerance. An acceptable tolerance is typically chosen as less than half the lag distance, and should produce more than 30 pairs of data per binned point (Olea, 2003). The binned variogram takes a shape that can be modelled with a theoretical variogram.

The most commonly used theoretical variogram models are Gaussian, exponential, and spherical. These models are defined using parameters from the binned variogram. The nugget of the variogram is the variance seen as the separation distance approaches zero. The sill is known as the variance that is reached asymptotically by the binned variogram. The range of the variogram is the separation distance that the sill is reached. Each theoretical variogram model has an equation dependent on the separation distance (h) built from the sill (C) and the range (a) developed from the binned variogram. The Gaussian model approaches the sill asymptotically, but is parabolic in shape near the origin. The Gaussian model is defined as

$$\gamma(h) = C\left(1 - e^{-3\left(\frac{h}{a}\right)^2}\right) \quad (2)$$

The exponential model increases exponentially and also approaches the sill asymptotically. The exponential model is defined as

$$\gamma(h) = C\left(1 - e^{-\frac{3h}{a}}\right) \quad (3)$$

The spherical model increases in a linear fashion near the origin. It reaches a finite sill at a finite range. The spherical model is defined as

$$\gamma(h) = \begin{cases} C\left(\frac{3}{2}\frac{h}{a} - \frac{1}{2}\left(\frac{h}{a}\right)^3\right) & if\ 0 \le h < a \\ C & if\ \ a \le h \end{cases} \quad (4)$$

Figure 1.1 illustrates the three different variogram model plots. All three models shown have a nugget effect of 0.1, a sill of 1, and a range of 100.

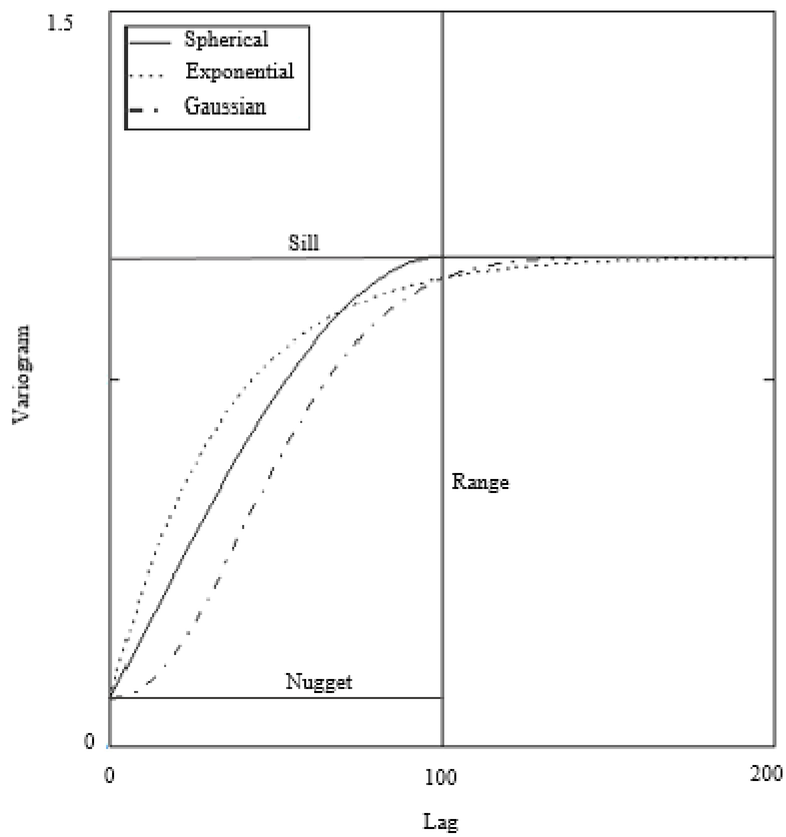

Figure 1.1. Theoretical variogram models and parameters

Variograms are often looked at directionally. When looking at a directional variogram an angular tolerance must be set. The average variance is calculated for each lag within the direction's angular tolerance. The presence of anisotropy is indicated by variograms that differ directionally. It is common practice to either model the anisotropy or to model the variogram in the direction with the largest variance (Kumar et al., 2005). Trend is commonly seen within datasets that are spatially dependent, such as groundwater or concentration data. Trend can be easily identified by observing the experimental variogram. If trend is present within the data, the variogram will increase in a parabolic fashion instead of reaching a finite sill. The trend is modelled using either a first or second degree polynomial and then removed from the original data. The removal of the trend leaves a dataset of residuals. The residuals are used to model the theoretical variogram and within the kriging process. The trend must be added back to the estimates in order to get reliable results.

1.2 REVIEW OF KRIGING APPROACHES

The literature is rich with applications of kriging groundwater elevations. Many authors have used a form of kriging with differing variogram models. Two of the most commonly used forms of kriging, when applied to groundwater, are UK and CoK. Kumar (2007) used UK with a spherical model on a site in northwestern India. The author used cross validation to determine the final trend removal order that best represented the site. It was found that a second order trend model produced the best statistical results. Prakash and Singh (2000), Ma et al. (1999), and Tonkin and Larson (2002) also used UK with a spherical model on their sites in Nalgonda District, India, South Central Kansas, and Cape Cod, Massachusetts. Prakash and Singh (2000) used their kriging results to design a monitoring well network. Tonkin and Larson (2002) compared regional-linear and point-logarithmic trend functions and found that point-logarithmic provided a more representative flow pattern. Nikroo et al. (2009) used UK with both a penta-spherical and spherical variogram model on their site in Fars Province, Iran. The authors also used CoK with a penta-spherical model. It was found that the UK with a spherical model produced the best statistical results for their site. Hoeksema et al. (1989) used CoK with a linear model on their site and found that CoK was effective for estimating the water table surface in hilly terrain. Fasbender et al. (2008) used CoK with a spherical variogram model on their site in central Belgium. The authors found that their Bayesian data fusion technique allowed for the incorporation of secondary information such as river geometry and digital elevation models. Boezio et al. (2005, 2006a, 2006b) used CoK with a Gaussian model for their site in Brazil. In these studies, the authors found that collocated CoK produced more representative results than other methods.

Many authors have used kriging as an approach to develop a potentiometric surface of groundwater. However, a reliable point of departure for variogram modelling has not been found within the literature. Typically, an individual performing kriging would start with the variogram modelling process. This process is iterative and therefore time consuming. If CoK is to be used, the process becomes even more rigorous with the addition of two extra variogram models. The focus of this study is to provide a reliable point of departure for the variogram modelling process within kriging in order to reduce the amount of processing time associated with the iterative method. This process is compared to the commonly used iterative analysis to evaluate the method’s effectiveness.

2. METHOD DEVELOPMENT

2.1 GEOSTATISTICAL METHOD

When applying CoK, more than one variogram is necessary. A variogram model must be developed for each variable as well as a cross variogram ($\boldsymbol{\gamma_{jk}(h)}$) that relates the variables. Nikroo et al. (2009) defines the cross variogram as

$$\gamma_{jk}(h) = \frac{1}{2}\left[\gamma_{jk}^{+}(h) - \gamma_{jj}(h) - \gamma_{kk}(h)\right] \tag{5}$$

Where:

h = separation distance

$\gamma_{jj}(h)$ = the variogram of the primary variable at h

$\gamma_{kk}(h)$ = the variogram of the secondary variable at h

$\gamma_{jk}^{+}(h)$ = the variogram of the sum of the two variables at h

All three variograms ($\gamma_{jj}(h)$, $\gamma_{kk}(h)$, $\gamma_{jk}(h)$) are used within the kriging process to determine the kriging weights. The kriging weights are developed in such a way to minimize the mean square error.

Typically multiple theoretical variogram models are developed within the kriging process. The appropriate model is chosen through cross validation. Cross validation is an iterative process in which a singular measured point is removed from the dataset and is predicted using the developed model. The predicted value is then compared to the measured value to determine error. The model that produces the least amount of error is chosen as the representative model. The error can be defined using multiple statistics such as the coefficient of determination (R^2) or the root mean square standardized error (RMSSE). The R^2 is determined by plotting the predicted value versus the measured value. The R^2 ranges from zero to one, and is desired to be near one. The R^2 is defined as

$$R^2 = \frac{\boldsymbol{n(\sum Z(s_i) z(s_i)) - \sum Z(s_i) \sum z(s_i)}}{\sqrt{\boldsymbol{[n \sum Z(s_i)^2 - (\sum Z(s_i))^2][n \sum z(s_i)^2 - (\sum z(s_i))^2]}}} \tag{6}$$

Where

$Z(s_i)$ = Measured value at location s_i

$z(s_i)$ = Predicted value at location s_i

n = Number of observations

The RMSSE is also desired to be near a value of one. However, if the RMSSE is greater than one, the variability of the predictions is underestimated. Similarly, if the RMSSE is smaller than one, the variability of the predictions is overestimated. The RMSSE is defined as

$$\text{RMSSE} = \sqrt{\frac{\sum_{i=1}^{n}\left[\frac{Z(s_i)-z(s_i)}{\sigma(s_i)}\right]^2}{n}} \tag{7}$$

Where

$\sigma(s_i)$ = Predication error at location s_i

The application of CoK allows for the use of multiple variables, where the secondary variable is sampled more often or from a denser network. When applied to groundwater datasets, groundwater elevation is the primary variable and ground elevation is often the secondary variable. Ground elevation measurements are taken from the locations of each monitoring well as well as from a digital elevation model (DEM). Olea (2003) indicates that when developing a grid one should size the grid using the average of the minimum separation distances. The DEM points were extracted using the average of the minimum separation distance of the monitoring wells.

It is imperative to evaluate the quality of data before the application of geostatistics. This study applied a method developed by Helwig (2017) to determine potential outliers within a dataset of a study site. This method employs the use of the already developed variogram model and can therefore be used readily within the kriging process.

A perk to kriging is the automatic development of a standard error map along with the prediction map. The standard error map is often used to determine where significant data gaps exist. The interpolative nature of kriging lends to less reliable predictions farther away from sampling points. If an individual desires to develop a representative monitoring well network, the areas on the standard error map with the most error can indicate an appropriate location for a monitoring well.

2.2 LITERATURE BASED METHOD

Twenty-two works (19 sites) related to the kriging of groundwater were evaluated for variogram and kriging parameters. The parameters evaluated included: site area, number of monitoring wells, variogram model type, range, sill, nugget effect, trend removal, kriging type, and model verification statistics. These parameters were compiled into a database for use as a comparison tool in future kriging works. This database is located in Table 1 within the journal paper section.

The parameters within the database guided and confirmed the process used for this study. UK and CoK were the two most often used kriging types. Cross validation was used to as model verification. The verification statistics used most often included R^2 and RMSSE. Trend was removed in a majority of the studies (15 of 19).

In order to develop a point of departure for the kriging process, the parameters were evaluated for correlation. Site properties and kriging parameters were plotted against one another and a correlation between the site area in square miles (mi^2) and the variogram range in feet (ft) was developed. No other correlations were observed within the literature. The correlation found between the site area and the variogram range is defined as

$$y = 1348.6e^{0.0238x} \tag{8}$$

Where

y = estimated theoretical variogram range (ft)

x = site area (mi^2)

The correlation can be applied to a study site to quickly determine a representative variogram range or it can also be used as a comparison for an iteratively determined variogram range.

2.3 ITERATIVE METHOD

The iterative method was applied in order to compare the results from the developed equation method. The iterative method is the most commonly used method to develop theoretical variogram parameters. An individual performing the iterative method would begin by modelling the experimental variogram with a selected theoretical variogram model type. After modelling a theoretical variogram, the model is used within the kriging process. Cross validation statistics would be developed for the model. This process is repeated for multiple theoretical variogram models with multiple variogram parameters. The model that produces the best cross validation statistics is chosen as the underlying model. The underlying model is then used for any further and final kriging analyses.

2.4 QUANTITATIVE ANALYSIS

The comparison of the iterative and literature based method was performed using a quantitative analysis. Three comparison points were selected for the site. These points' locations were chosen by evaluating where data gaps exist within the current monitoring well network. The predicted groundwater elevation and the direction and magnitude of groundwater gradient were compared for the iterative and the literature based process. The direction and magnitude of the gradient were determined manually. In order to evaluate the performance of the literature based method when presented with limited data points, the number of well locations were reduced from 61 wells to 45, 30, and 15 wells. Three realizations were conducted for each well reduction case. The results for the realizations of each well reduction were averaged and compared to the baseline results of the 61 well iterative method results.

2.5 FLW-056 SUBSITE SEASONALITY ANALYSIS

The FLW-056 subsite is sampled more often than the rest of the FLW site. The FLW-056 subsite is typically sampled every spring and fall season. A seasonality analysis was conducted on this subsite to determine if there were any seasonal effects on variogram parameters. A total of 16 sampling events were fit with a Gaussian variogram model and kriged with universal CoK (2^{nd} order trend removal). The Gaussian theoretical variogram model was selected for the FLW-056 site due to the cross validation results. The Gaussian model produced an R^2 nearest to one for the majority of the sampling seasons. The ground surface elevation was used as the secondary variable. The variogram ranges were compared to determine if seasonality was present within the datasets.

PAPER

I. LITERATURE-BASED POINT OF DEPARTURE PARAMETERS FOR KRIGING GROUNDWATER SURFACES

Keywords: groundwater elevation, kriging, variogram, cokriging, digital elevation model

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ABSTRACT

Groundwater flow can be characterized by interpolating groundwater elevations using available water level data from monitoring wells. A literature review was performed to identify the typical kriging models and model parameters used for groundwater elevation interpolation. The review indicated that universal CoK with trend removal using ground surface elevation as the secondary variable was the most common model. The variograms typically used spherical models, and a relationship between the

total area being kriged and the variogram range was identified. An application at a Missouri study site showed that there was no significant benefit to using the area/range relationship relative to the typical iterative process used to identify appropriate kriging parameters. Instead, the application showed that it was more important to use a sufficient number of water level measurements. This finding was consistent with the results of the literature review which showed that most applications used a minimum of 30 monitoring wells.

1. INTRODUCTION

Groundwater contamination is a prominent issue that has adverse effects on locations worldwide. One of the first steps in characterizing the nature and extent of potential contamination and designing any subsequent remedial action is identifying the groundwater flow direction. Groundwater monitoring wells are typically installed to collect both water quality data and groundwater potentiometric surface data. These groundwater level data are used to identify flow direction (Yang et al., 2008). Any planar surface, including a groundwater potentiometric surface can be defined using three data points. However, groundwater surfaces are seldom planar, and additional data are needed for reliable characterizations (Kumar, 2010; Theodossiou and Latinopoulos, 2005; Varouchakis and Hristopulos, 2012; Fasbender et al., 2008).

Geostatistical methods are often used to better understand groundwater surfaces. Kriging is a geostatistical interpolation tool used to predict groundwater elevations that preserves elevation data measured at the wells (Kumar, 2008). A critical element within the kriging process is the development of the variogram model. A variogram relates the variance between measured points to the separation distance between these points. The variogram model is used to predict the desired parameter at an unmeasured point by assigning weights to the neighboring points (Hoeksema et al, 1989). Many authors have applied a variogram model and a form of kriging to interpolate groundwater elevations (Pucci and Murashige, 1987; Kumar, 2008; Varouchakis and Hristopulos, 2013; Nikroo et al., 2009; Rivest et al., 2008; Gambolati and Volpi, 1979; Sophocleous et al., 1982; Prakash and Singh, 2000; Desbarats et al., 2002; Kumar et al., 2005; Boezio et al., 2006a, 2006b; Ahmadi and Sedghamiz, 2007). Kriging requires a relatively large amount of sampling points to develop a representative variogram model. This representative variogram model is typically developed using an iterative method.

The sparse and non-stationary nature of groundwater measurements can lead to a variogram model that is unrepresentative of the data set. However, there are variations of kriging that are better suited for groundwater data (Isaaks and Srivastava, 1989; Nikroo et al., 2009; and others). Universal kriging (UK) assumes that trend is present within the dataset and must be removed to satisfy the stationary requirements of kriging.

(CoK) incorporates both a primary and a secondary variable within the interpolation process. The primary variable is the prediction variable, and the secondary variable is more extensively sampled. For groundwater interpolation, the primary variable is groundwater elevation and the secondary variable is often ground surface elevation. Incorporating both primary and secondary information allows for a more representative variogram model.

Identifying the representative variogram parameters and model is often a difficult iterative process with no guidelines for reasonable parameters. A reliable point of departure for a site's variogram parameters could help reduce the effort involved in developing the variogram model. The study identifies a process to establish a point of departure for variogram parameters by summarizing the typical range of values as found in the literature. The use of the literature review results will be applied to a groundwater surface study at Missouri's Fort Leonard Wood Military Reservation (FLW), which contains many unique features such as karstic terrain and monitoring wells that are highly clustered according to anthropogenic features such as landfills and other potential sources of groundwater contamination. A quantitative analysis is performed to compare results using the full number of wells and reduced number of wells at the FLW site.

2. LITERATURE REVIEW

A literature review identified 22 peer reviewed papers addressing19 sites related to the kriging of groundwater. Each paper was reviewed for site properties (area and number of wells), variogram parameters (model type, nugget, sill, range, and trend model), and kriging properties (kriging type and validation procedure). These parameters are summarized in Table 1. The literature review shows that some parameters are used more often than others. The spherical and Gaussian theoretical variogram models are used more often than other models; UK and CoK are the kriging types that are used the most; trend was removed in 15 of the 22 studies.

Table 1. Literature review table

Reference	Number of Wells	Site Area	Variogram Model Type	Sill or Slope	Range	Nugget Effect	Kriging Type	Trend Model	Model Verification
		mi²		ft²	ft	ft²			
Pucci and Murashige, 1987	171	46.3	NG	17,900	66,400	2,690	UK	Yes	RMSE AE
Kumar, 2007	143	1,740	Spherical	362	162	51.7	UK	Yes	RMSE MSE
Varouchakis and Hristopulos, 2013	69	19.4	Spartan	1,980	NG	NG	UK	Yes	R^2
Nikroo et al., 2009	257	6.95	Spherical Penta-Spherical Gaussian	1,080	53,700	90.4	OK UK SK CoK	Yes	AE RMSE MSE RMSSE
Abedini et al., 2008	85	37,300	Power	15,100	NG	285	OK	No	PAEE NMSE R^2
Yang et al., 2008	23	928	Gaussian	1,940	16,100	0	OK	No	R^2
Theodossiou and Latinopoulos, 2006	31	34.7	Spherical	17,200	3,610	0	NG	No	R^2
Rivest et al., 2008	10	3.47	Ad-hoc Covariance	N/A	N/A	0	KED	Yes	NG
Gambolati and Volpi, 1979	40	154	Linear	3.23	N/A	0	UK	Yes	MSE
Sophocleous et al., 1982	327	5,000	Linear	0.071	105,000	0	UK	Yes	SD
Hoeksema et al., 1989	59	0.232	Linear	-2.75	N/A	0	CoK	No	NLL MSE
Prakash and Singh, 2000	32	69.5	Spherical	53.6	8,200	37.7	UK	Yes	MSE

Table 1. Literature review table (cont.)

Reference	Number of Wells	Site Area	Variogram Model Type	Sill or Slope	Range	Nugget Effect	Kriging Type	Trend Model	Model Verification
Desbarats et al., 2002	1,543	96.5	Gaussian	699	6,560	242	KED	Yes	AE MSE RMSE
Boezio et al., 2005	65	1.67	Gaussian	7,160	1,280	108	CoK	No	Mean Median SD R^2
Kumar et al., 2005	174	3,320	Linear	0.019	N/A	137	UK	Yes	R^2
Boezio et al., 2006a	65	1.67	Gaussian	2,050	1,310	108	KED CoK	Yes	R^2
Ahmadi and Sedghamiz, 2006	39	483	Spherical	1,150	31,900	1.08	UK CoK	Yes	R^2
Ahmadi and Sedghamiz, 2007	39	483	NG	Mult.	Mult.	Mult.	CoK	No	RMSE
Ma et al., 1999	50	618	Spherical	176	47,700	0	UK CoK	Yes	R^2
Tonkin and Larson, 2002	32	0.788	Spherical	0.226	3,610	0.022	UK	Yes	R^2
Boezio et al., 2006b	65	1.67	Gaussian	102	656	102	KED CoK	Yes	NG
Fasbender et al., 2008	135	129	Spherical	3,230	44,900	0	OK CoK	No	AE RMSE

Notes:
NG – not given
Mult. – multiple
N/A – not applicable
SK – simple kriging
KED – kriging with external drift
RMSE – root mean square error
AE – average error
MSE – mean square error
PAEE – percent average estimation error
NMSE – normalized mean square error
SD – standard deviation
R^2 - coefficient of determination
RMSSE – root mean square standardized error

Site properties and variogram parameters from the literature review sites were plotted against one another and analyzed for correlation. The only correlation observed within the literature review data was between the site area and the variogram range. The variogram range in feet (ft) was plotted against the site area in square miles (mi^2), and is presented in Figure 1. An exponential trend line was fit to the data with a R^2 of 0.9, indicating that the equation is a reasonable fit for the data. The equation can be used as a point of departure for individuals beginning the variogram modelling process or as a comparison for an iteratively determined variogram range. The equation for the trend line was determined to be:

$$y = 1348.6e^{0.0238x} \quad (1)$$

Where

y = estimated theoretical variogram range (ft)

x = site area (mi^2)

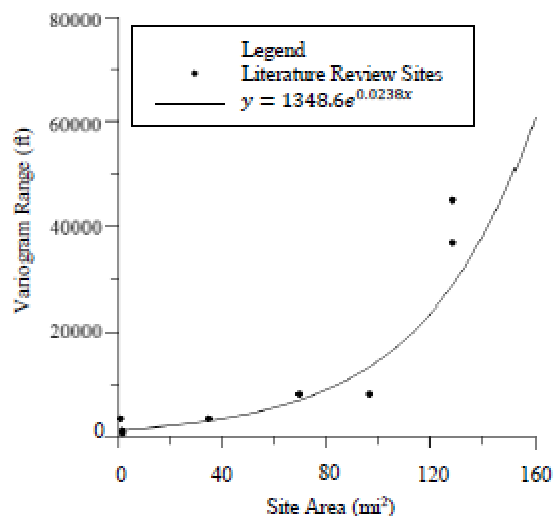

Figure 1. Site area (mi^2) versus variogram range (ft)

The literature review provides a suggested kriging procedure. A summary of the recommended kriging procedure is provided in Table 2. The literature shows a groundwater kriging site can have a minimum of 10 monitoring wells, but 30 or more wells is typical. Based on the literature review results, it is recommended to use CoK with trend removal (or universal CoK) to predict groundwater elevations (GWE). CoK makes use of two or more variables to improve the variogram model. The CoK estimate incorporates the spatial dependence of the primary variable as well as the dependence between the primary and secondary variables. It is suggested to use GWE as the primary variable and ground surface elevation as the secondary variable. A theoretical variogram model must be created for both the primary and secondary variables as well as a cross variogram ($\gamma_{jk}(h)$) to relate the two variables. In spatially correlated datasets, such as groundwater data, it is common to address trend within the dataset with the use of UK (Gambolati and Volpi, 1979; Nikroo et al., 2010, and others). The presence of trend creates a variogram that increases parabolically instead of reaching a finite sill. A trend model, typically not reaching above a second-degree function, is fit to the data and then removed.

Table 2. Summary of recommended kriging procedure

Number of wells	Minimum of 10 (typically 30 or more)
Kriging type	Universal CoK
Secondary variable	Ground surface elevation
Trend model	Second order polynomial
Polynomial parameters	Determine iteratively
Variogram model	Spherical or Gaussian
Variogram model parameters	Determine experimentally
Variogram sill	Determine iteratively
Variogram nugget	Determine iteratively
Variogram range	Determine iteratively or use Eq. 1

3. METHODS

It is common practice to evaluate the quality of a GWE dataset before the application of kriging. This study employs a method developed by Helwig (2017) that uses the variogram of the ground surface and GWE surface to identify potential spatial outliers in the dataset. The spatial outliers were removed from the dataset, and the censored dataset was then used for all kriging within the study. The variogram of the dataset before spatial outlier removal produced an unrecognized variogram pattern. After removal of the spatial outliers, a reasonable variogram was produced. These two variograms are shown in Figure 2.

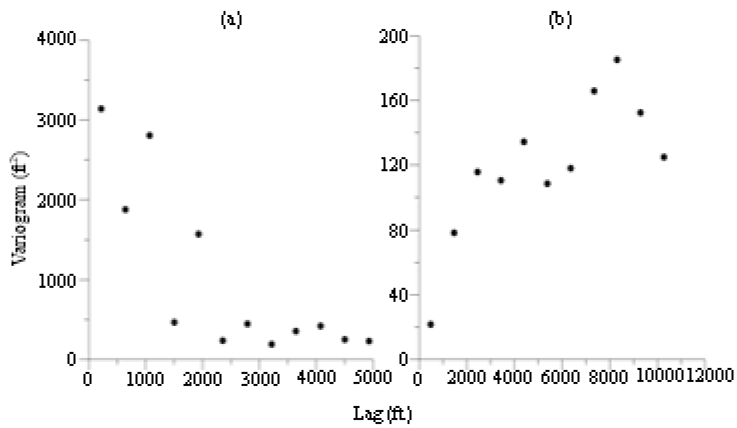

Figure 2. Variograms from before (a) and after (b) spatial outlier removal

The typical kriging process includes an iterative development of the variogram model. The iterative process consists of performing kriging with the different theoretical models as well as different variogram parameters. The parameters are changed within each model for each kriging iteration. The model that produces the best verification statistics is then chosen as the underlying variogram model and is used to produce the final kriging results. The theoretical variogram range was determined using the iterative process with a spherical, Gaussian, and exponential model. This was done by changing individual variogram parameters for each model type and then comparing verification statistics from cross validation. The model that produces the best verification statistics was chosen as the underlying theoretical variogram model for the site.

Comparison points were developed in order to compare the recommended literature approach to the typical iterative approach. At some sites there are specific locations where groundwater flow characterization is more important relative to other locations. For example, groundwater flow characterization will have a higher priority near water supply wells when considering wellhead protection. These comparison points were selected to bridge data gaps while remaining within the interpolative nature of kriging, but the locations could also serve to represent other potential points of interest such as water supply wells, remedial action locations, new sources areas, or other locations related to project objectives. The comparison points were used to predict groundwater elevation, flow direction, and magnitude of the gradient. These predicted values from the literature based method and the iterative method were compared. The number of wells were then reduced to compare the method's performances with fewer monitoring wells. Three realizations of the reduced number of wells were developed using a random number generator. Each realization was kriged using the iterative method and the literature based method. The predicted values for each realization were compared to the baseline results of a full well set kriged iteratively.

4. APPLICATION

A case study was performed at the Fort Leonard Wood Military Reservation (FLW), an active military base located in central Missouri. FLW consists of 64,000 acres and 71 monitoring wells. The geology at the site consists of the Jefferson City Dolomite Formation, the Roubidoux Formation, and the Gasconade Dolomite Formation. FLW contains a broad upland, northeast-trending ridge that is bounded by the Big Piney River to the east and the Roubidoux Creek to the west (Mugel and Imes, 2003). The groundwater flow direction at the site is typically controlled by regional topography. So there is a strong northeasterly flow component parallel to the topographic ridge with smaller discharges normal to and at the edges of the ridge into the two stream valleys (Kleeschulte and Imes, 1997). A figure depicting the conceptual flow directions for the site can be seen in Figure 3.

Groundwater flow is believed to be porous media flow with possible karst formations mainly in the Gasconade Dolomite formation (Kleeschulte and Imes, 1997). The 71 monitoring wells tend to be clustered around solid-waste management units and are split into numbered subsites. These subsites consist of FLW-002, FLW-003, FLW-012, FLW-056, and FLW-060. A map of the FLW site on top of a digital elevation model in feet above mean sea level (ft amsl) can be seen in Figure 4.

Universal CoK was applied to the FLW site where groundwater elevation was the primary variable and ground surface elevation was selected as the secondary variable. A second order polynomial was iteratively fit to the dataset and then removed. Universal CoK with a second order polynomial was chosen due to the number of uses of CoK and trend removal within the literature review study. All of the subsites were included within the modelling process, and 61 of the 71 wells were retained after the spatial outlier analysis. A kriging area of 32.7 square miles (mi^2) was determined for the FLW site. The variogram nugget, sill, and range were determined iteratively using the widely available ArcMap 10.2.1. A spherical model was selected for the dataset due to the number of uses within the literature. A summary of the kriging parameters is included below in Table 3.

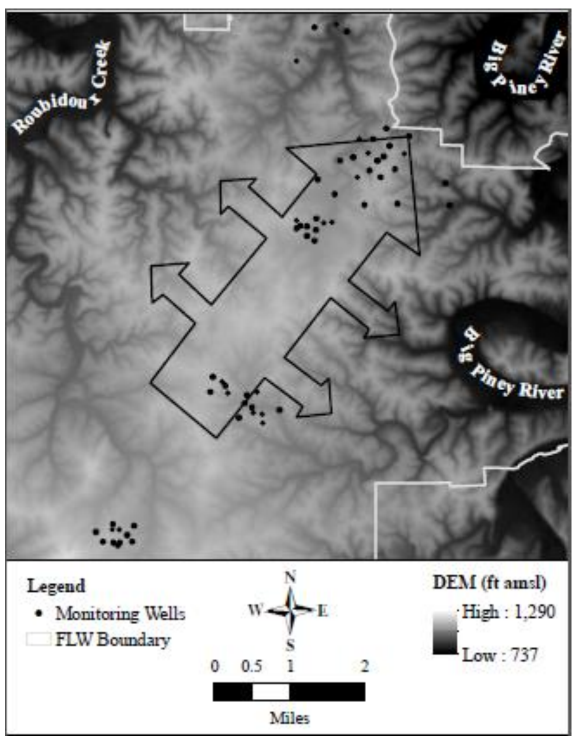

Figure 3. Conceptual groundwater flow direction

This iterative model was selected as the baseline case for comparison of the two methods. A contour map depicting the universal CoK results can be seen in Figure 5. The flow pattern observed in the contour map is reasonable given the conceptual model where the groundwater flows from the upland ridge towards the Big Piney River and the Roubidoux Creek.

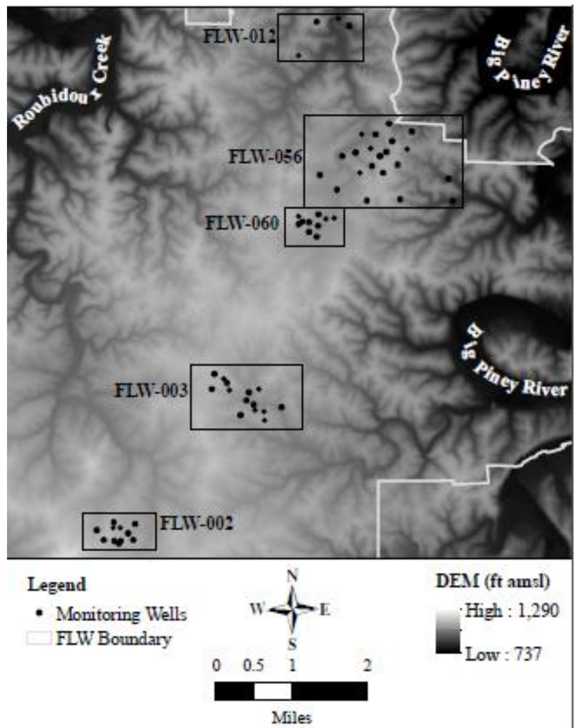

Figure 4. FLW site map

Table 3. Summary of FLW iterative kriging parameters

Site Area (mi^2)	32.7
Number of wells	61
Kriging type	Universal CoK
Secondary variable	Ground surface elevation
Trend model	Second order polynomial
Polynomial parameters	Determined using “trend tool” in ArcMAP 10.2.1
Variogram model	Spherical
Primary variogram sill	150.8
Secondary variogram sill	1,638.7

Table 3. Summary of FLW iterative kriging parameters (cont.)

Cross variogram sill	37.5
Primary variogram nugget	1.9
Secondary variogram nugget	1,251.0
Variogram range	5,334.2

The same process was repeated using the range from Eq. 1. A summary of the FLW kriging parameters for this application is shown in Table 4. A contour map depicting the universal CoK results for this case is shown in Figure 6. Inspection of the figures does not indicate that there is a significant difference in flow pattern between the iterative baseline case and the literature method.

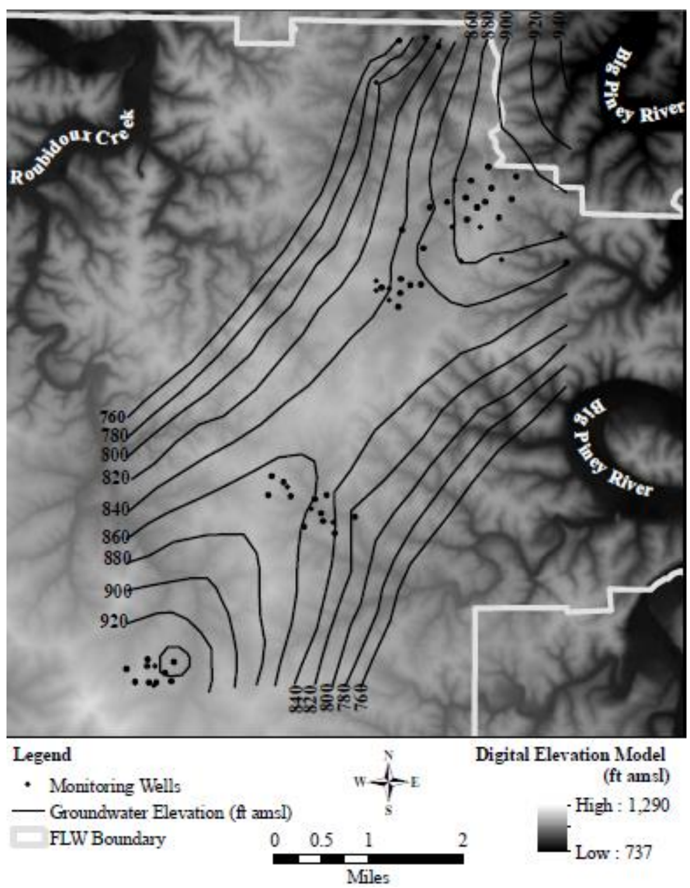

Figure 5. FLW baseline groundwater contour map

Table 4. Summary of FLW literature kriging parameters

Site Area (mi^2)	32.7
Number of wells	61
Kriging type	Universal CoK
Secondary variable	Ground surface elevation
Trend model	Second order polynomial
Polynomial parameters	Determined using “trend tool” in ArcMAP 10.2.1
Variogram model	Spherical
Primary variogram sill	150.8
Secondary variogram sill	2,889.7
Cross variogram sill	37.5
Primary variogram nugget	0
Secondary variogram nugget	0
Variogram range	2,940.0

This same comparison process was repeated for the site with a smaller number of wells. 45 wells were randomly selected from the baseline set of 61 wells. GWE surfaces were generated using the typical iterative process for the spherical model and the other variogram parameters. A second surface was generated using a specified range value of 2,940 ft (from Eq. 1), and the other variogram parameters were determined iteratively. The process was repeated for two more random realizations of 45 wells, and the resulting surfaces were compared. Visual inspection showed that the surfaces were not significantly different from Figure 5. The process was repeated for 30 wells and 15 wells. For some realizations of 15 wells, the resulting GWE surface was significantly different and was not consistent with the site conceptual groundwater flow model for the site and the flow patterns associated with surfaces kriged with 30 or more monitoring wells. An example of an inconsistent realization can be seen in Figure 7.

In order to perform a quantitative comparison of the interpolated GWE surfaces described above, three comparison points were identified. The comparison points selected for the FLW site can be seen in Figure 8. The points were selected to bridge data gaps between the FLW subsites.

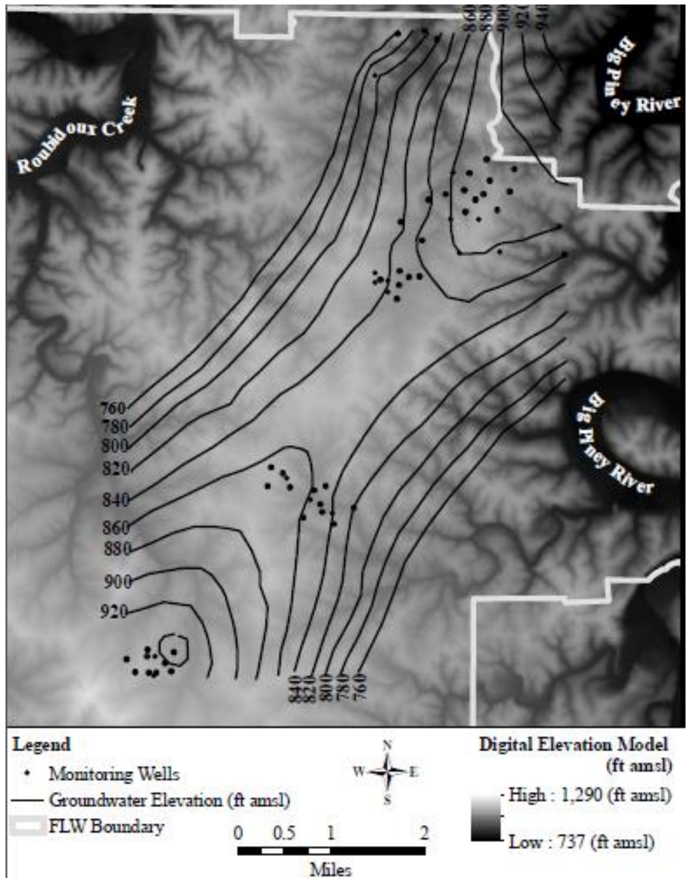

Figure 6. FLW literature based groundwater contour map

The average GWE elevation, gradient magnitude, and gradient direction were calculated for the 61, 45, 30, and 15 well scenarios for the typical iterative process and for the process modified to use the range value of 2,940 ft calculated from Eq. 1 and those results are given in Table 5. The results were averaged for the three realizations performed for each well scenario, and the differences from the baseline case are shown. The results indicate that the literature method does not significantly improve results of the reduced well scenarios when compared to the typical iterative method. Groundwater elevation values are shown to be predicted further away from the baseline prediction with fewer wells with a maximum difference of 15.7 ft. Flow direction remained constant for comparison point two, but changed rapidly for comparison points 1 and 3 with fewer wells. The magnitude of the gradient also showed greater differences in scenarios with fewer wells. Results for the 15 well scenario were typically inconsistent with the baseline case and the conceptual groundwater model.

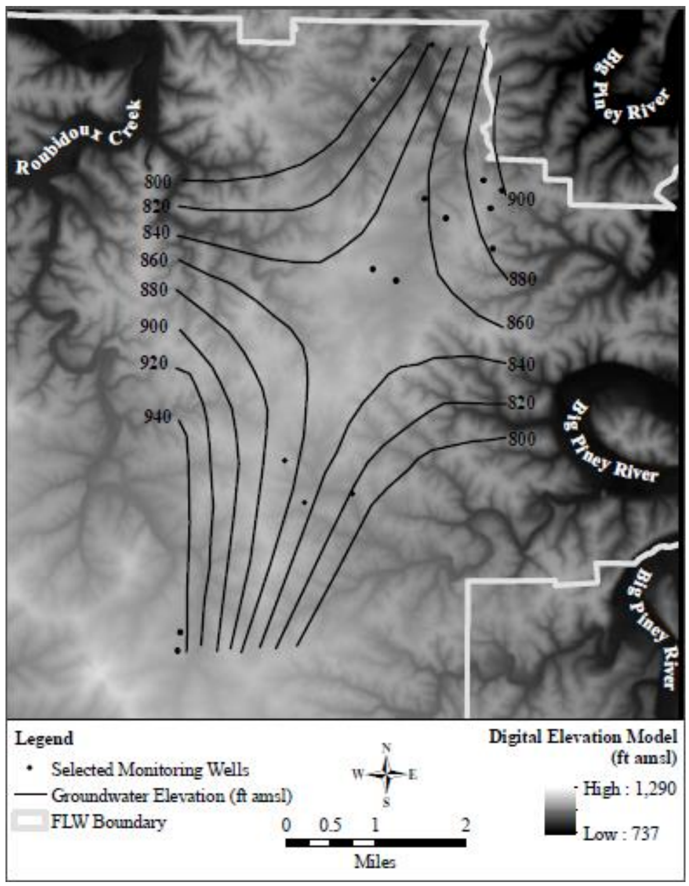

Figure 7. Inconsistent 15 well realization

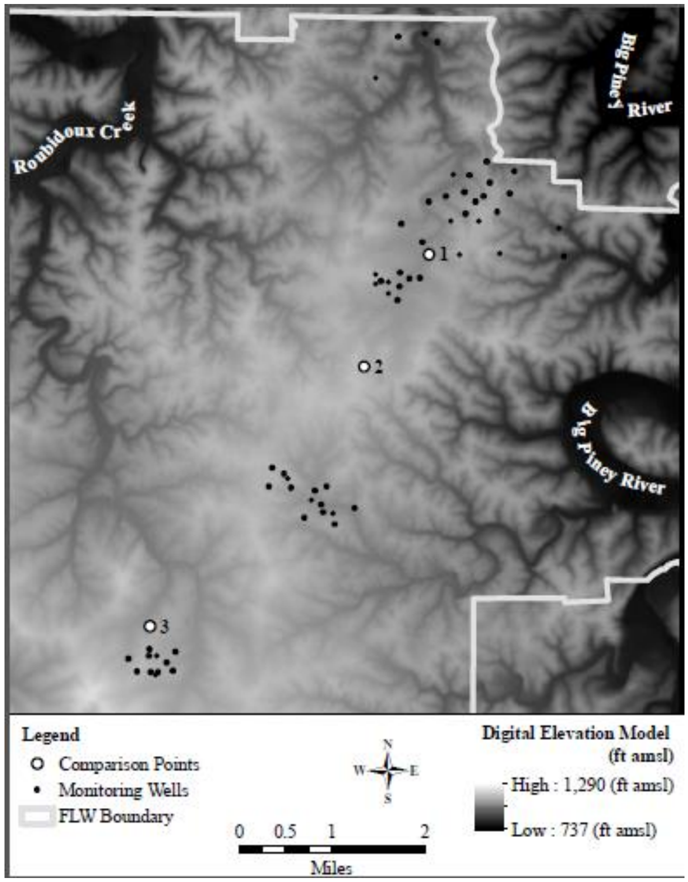

Figure 8. Comparison point locations

Table 5. Averaged results from 61, 45, 30, and 15 well scenarios

Comparison point		**1**			**2**			**3**		
		GWE	**Direction of flow**	**Magnitude of gradient**	**GWE**	**Direction of flow**	**Magnitude of gradient**	**GWE**	**Direction of flow**	**Magnitude of gradient**
Method	**No. of well**	**(ft amsl from base-line)**	**(° from base-line)**	**(ft/mi from base-line)**	**(ft amsl from base-line)**	**(° from base-line)**	**(ft/mi from base-line)**	**(ft amsl from base-line)**	**(° from base-line)**	**(ft/mi from base-line)**
Lit.	61	-0.9	0	-0.5	-0.2	0	1.8	2.4	0	2.0
Lit.	45	-0.1	10	12.1	1.1	0	8.0	5.9	23	4.6
It.		-0.7	10	-8.4	1.1	0	4.9	4.6	22	-3.9
Lit.	30	1.5	12	13.0	-1.2	0	6.2	3.5	32	5.9
It.		1.2	22	0.9	-1.5	0	6.0	3.7	33	10.7

Table 5. Averaged results from 61, 45, 30, and 15 well scenarios (cont.)

Lit.	15	2.9	17	32.5	-5.7	0	3.2	-15.7	70	-29.6
It.		4.0	53	36.4	-4.5	0	4.2	-14.3	77	-26.4

5. CONCLUSIONS

The literature provides the point of departure for kriging GWE in terms of the appropriate kriging method, trend removal model, and variogram model. A relationship between the area being kriged and the variogram range was identified from the literature, but an application at FLW showed that that relationship was not particularly useful. The more critical parameter was the number of wells used in the analysis. Although the literature review showed that others have used as few as 10 wells, 30 or more is typical for kriging GWE surfaces. For the application developed in this paper, GWE surfaces kriged with 15 wells resulted in surfaces that were inconsistent with each other, the baseline kriged surface, and the conceptual groundwater model for the site, while surfaces kriged with 30 or more wells generated consistent results that were consistent with each other and with the site conceptual groundwater flow model.

ACKNOWLEDGEMENTS

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SECTION

3. RESULTS

3.1 DATA QUALITY ANALYSIS RESULTS

A data quality analysis was necessary to include before the variogram modelling and kriging processes. This analysis was performed before the application of the literature based method and the iterative method. Variograms for the groundwater elevation and ground surface elevation were developed and used within the data quality analysis. The data quality study revealed multiple wells that were not representative of the FLW dataset and were deemed outliers. A total of 7 wells were removed: MW-1204, MW-1205, MW-1207, MW-211, MW-305, MW-307, and MW-401. Potential sources of error or causes of these outliers were reviewed and include long completion interval, shallow completion, solution features, perched zones, inconsistent initial water level, and seasonal variation. Four of these seven spatial outliers were identified as having shallow completion and were not completed in the targeted Gasconade Formation. It is suggested to complete future wells within the Gasconade Formation.

The removal of these outliers produced variograms that contained recognized variogram patterns. These variograms can be seen in Figure 3.1 and Figure 3.2. The variogram from before the outlier removal (Figure 3.1) experiences high variance at small separation distances and lower variance at larger separation distances. This is opposite from what is expected from a variogram of groundwater elevation data. The variogram from after the outlier removal (Figure 3.2) experiences small variance at small separation distances and high variance at larger separation distances.

The removal of the outliers from the kriging process did not produce contour maps that differed significantly from one another. Local variation in flow direction can be seen, but the overall flow schematic is unaffected. The groundwater flows towards the Roubidoux Creek and the Big Piney River in both cases, and both groundwater contour plots are representative of the conceptual model. The comparative contour plots can be seen in Figure 3.3 and Figure 3.4.

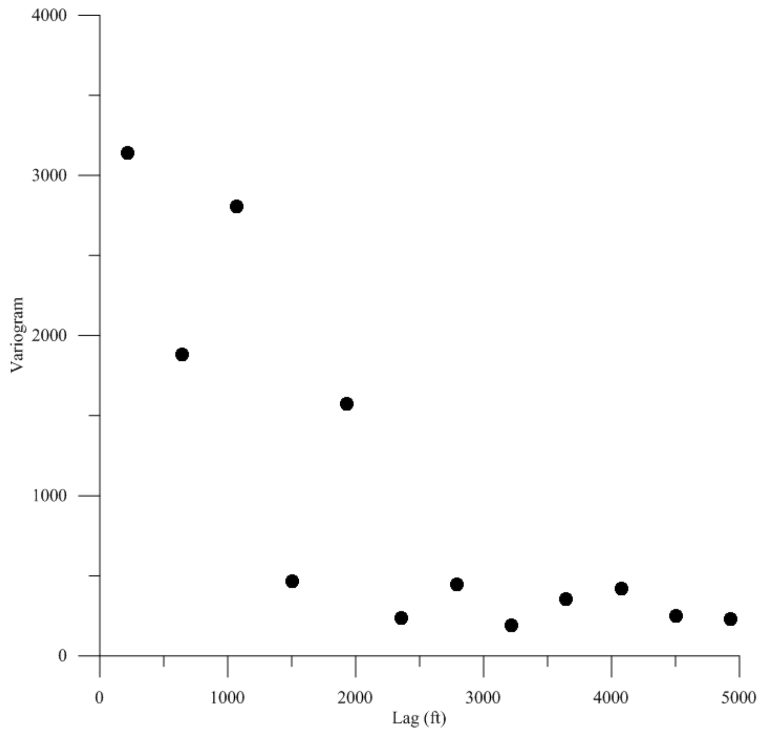


Figure 3.1. Experimental variogram from before the outlier removal process

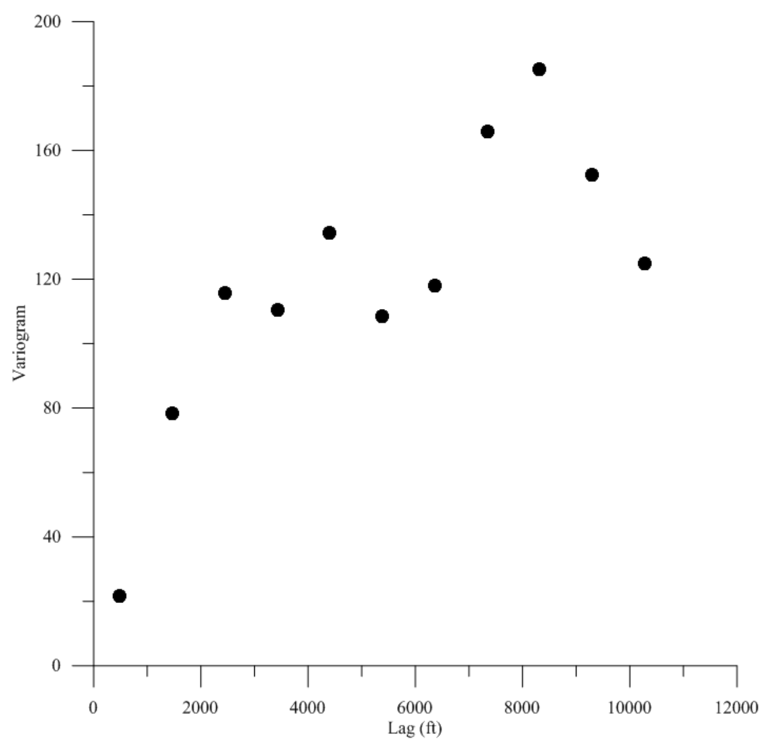


Figure 3.2. Experimental variogram from after the outlier removal process

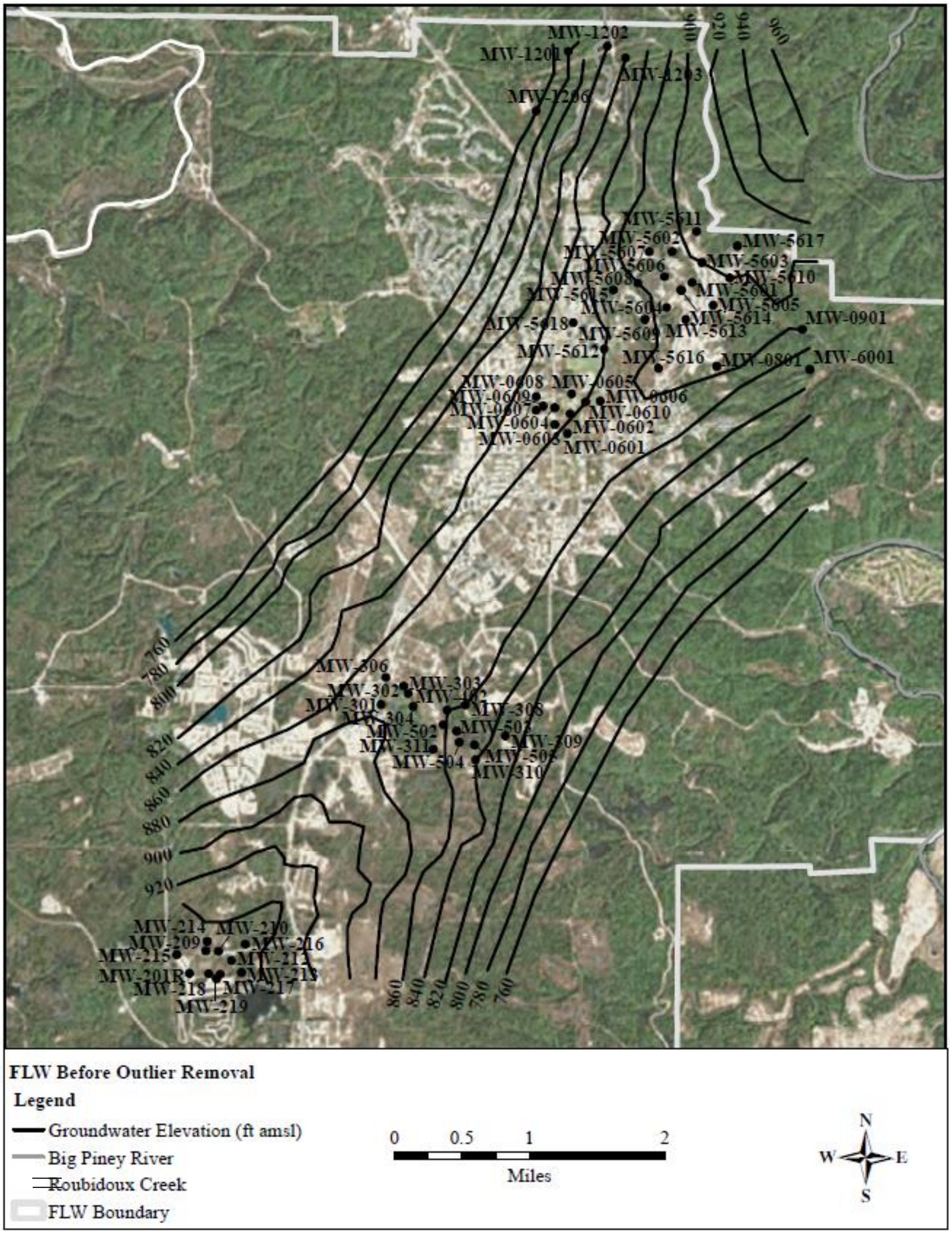


Figure 3.3. Contour plot from before outlier removal process

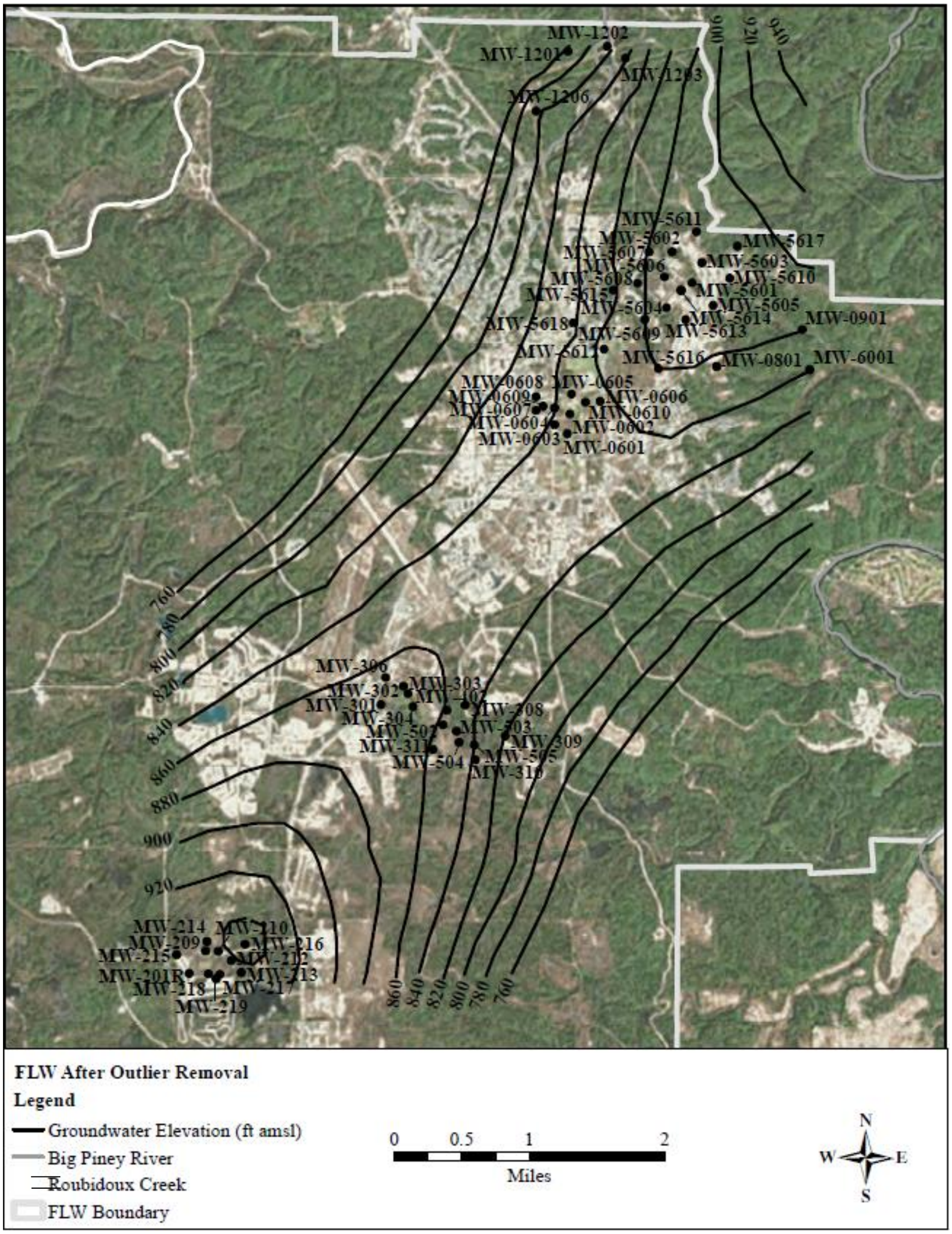


Figure 3.4. Contour plot from after the outlier removal process

3.2 DATA GAP RESULTS

Standard error maps are typically used to determine where significant data gaps exist. The standard error map for the FLW site can be seen in Figure 3.5. Small error (2-3 ft) is seen around the clustered wells sites, but increases rapidly to 15-16 ft farther away from the well clusters. In order to develop a more representative monitoring well network, it is recommended to place wells in locations with higher standard error to bridge data gaps between clustered sites.

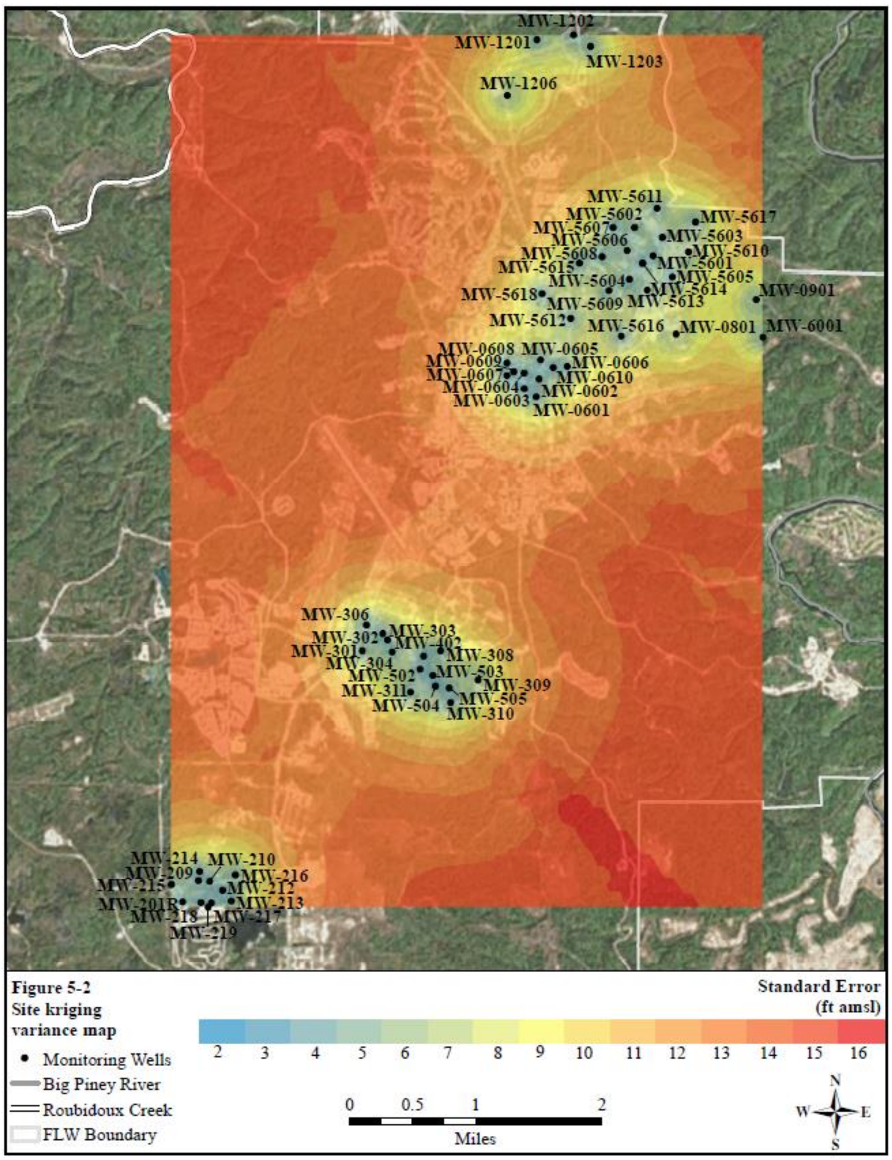


Figure 3.5. FLW full site standard error map

3.3 FLW-056 SUBSITE SEASONALITY RESULTS

A total of 16 seasons were kriged for the FLW-056 subsite. The iterative ranges for each season were recorded and compared to one another. The variogram ranges derived from the iterative process were plotted to evaluate any seasonal effects seen at the FLW-056 site. This plot of the seasonal ranges can be seen in Figure 3.6. It can be seen from this figure that the range fluctuates around 2,500ft. The low points on the graph tend to correlate with spring sampling dates indicating that there is slight seasonality within the data. The FLW-056 iterative seasonality study revealed that an individual performing kriging on this site in the future should use a Gaussian variogram with a range near 2,700ft for either a spring or fall sampling date. If the 2,700ft range does not represent the spring data well, a range of 2,400ft is then suggested.

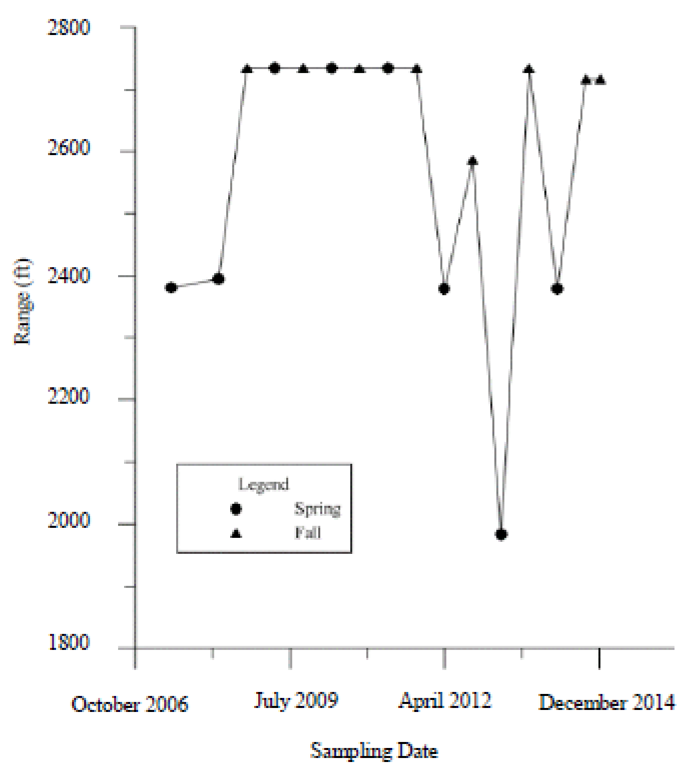


Figure 3.6. FLW-056 subsite seasonal ranges (ft)

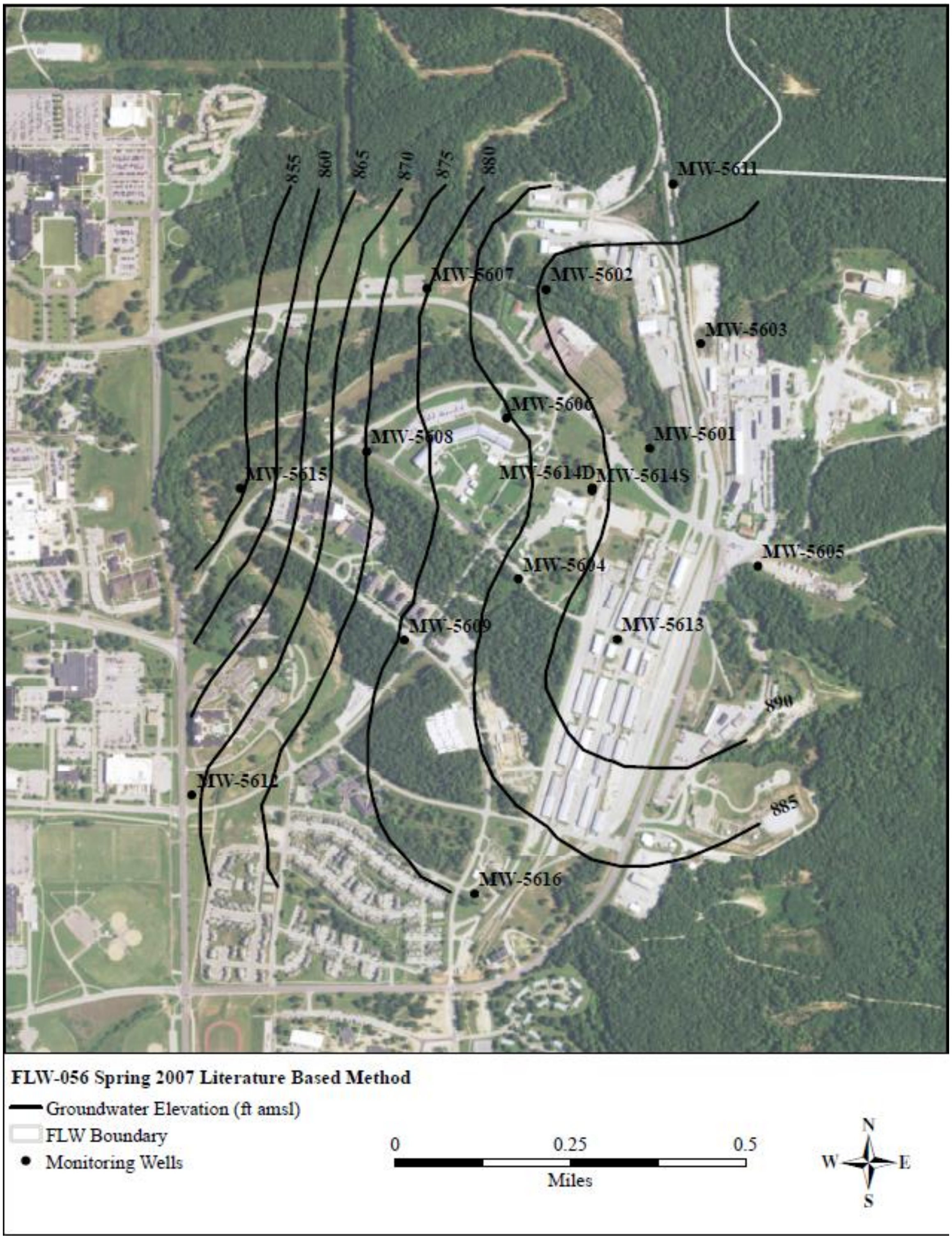
4. RECOMMENDATIONS FOR FUTURE WORK

The following ideas and topics are recommended to continue this research and to address assumptions made in the paper.

- Examine how larger site areas affect the developed range equation
- Evaluate effects of splitting the full FLW site into subsites and kriging each subsite
- Apply the range equation to other case study sites
- Sample the full FLW site for both spring and fall seasons in order to evaluate seasonality for the full site.
- Use standard error maps to create a denser monitoring well network and evaluate the effects on the groundwater elevation contour plot.

APPENDIX A.

LITERATURE BASED METHOD CONTOUR MAPS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FLW-056 Spring 2007 Literature Based Method
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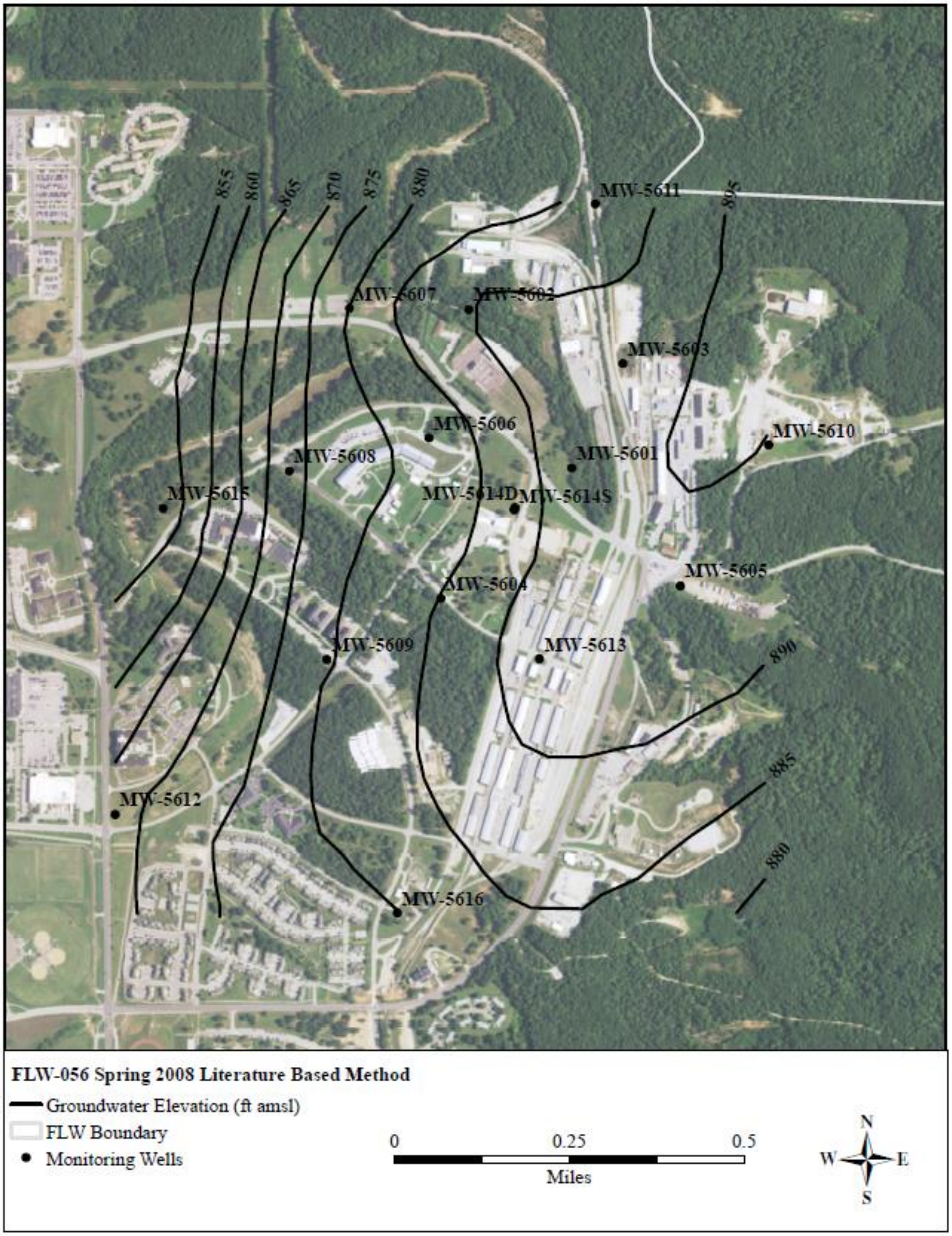
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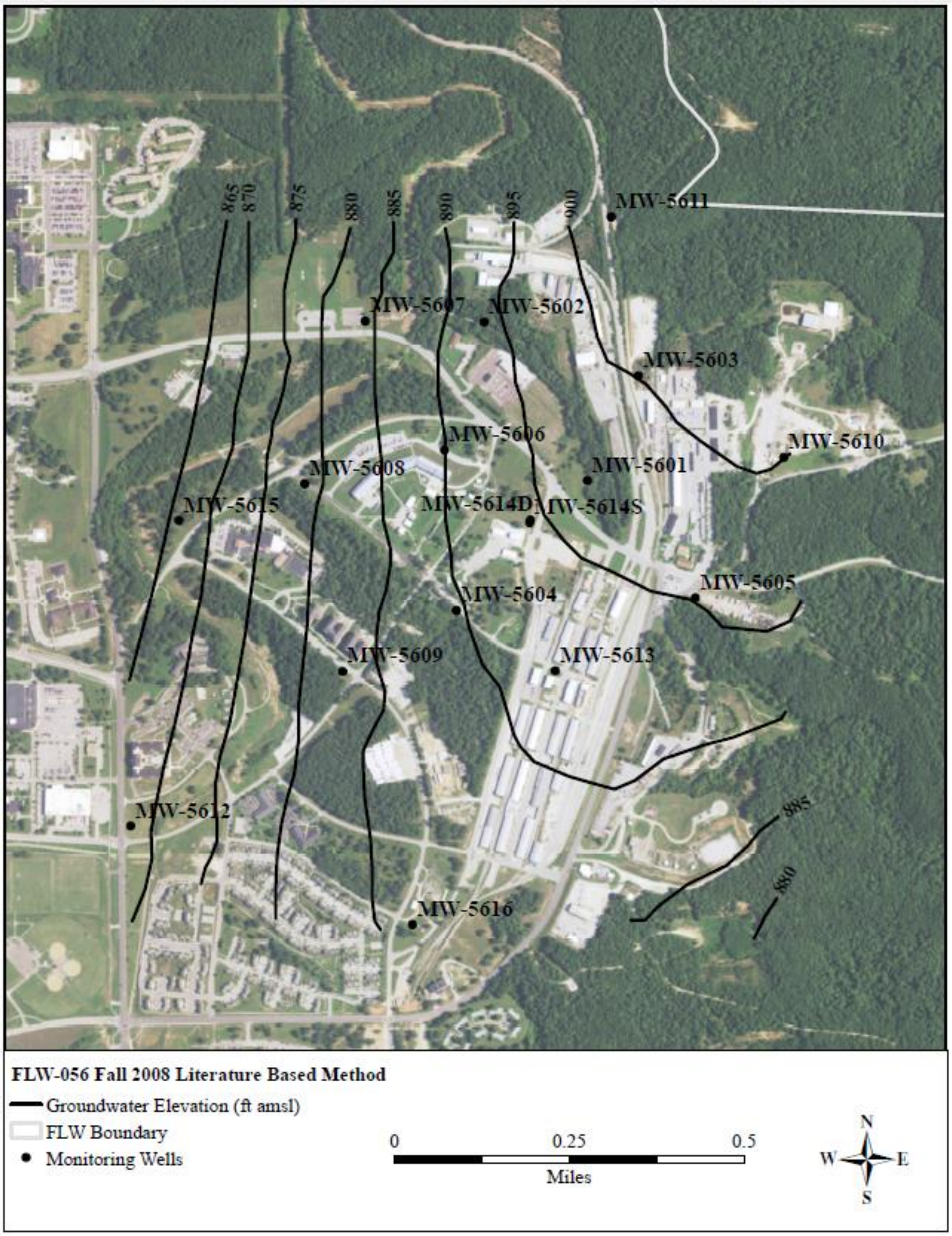
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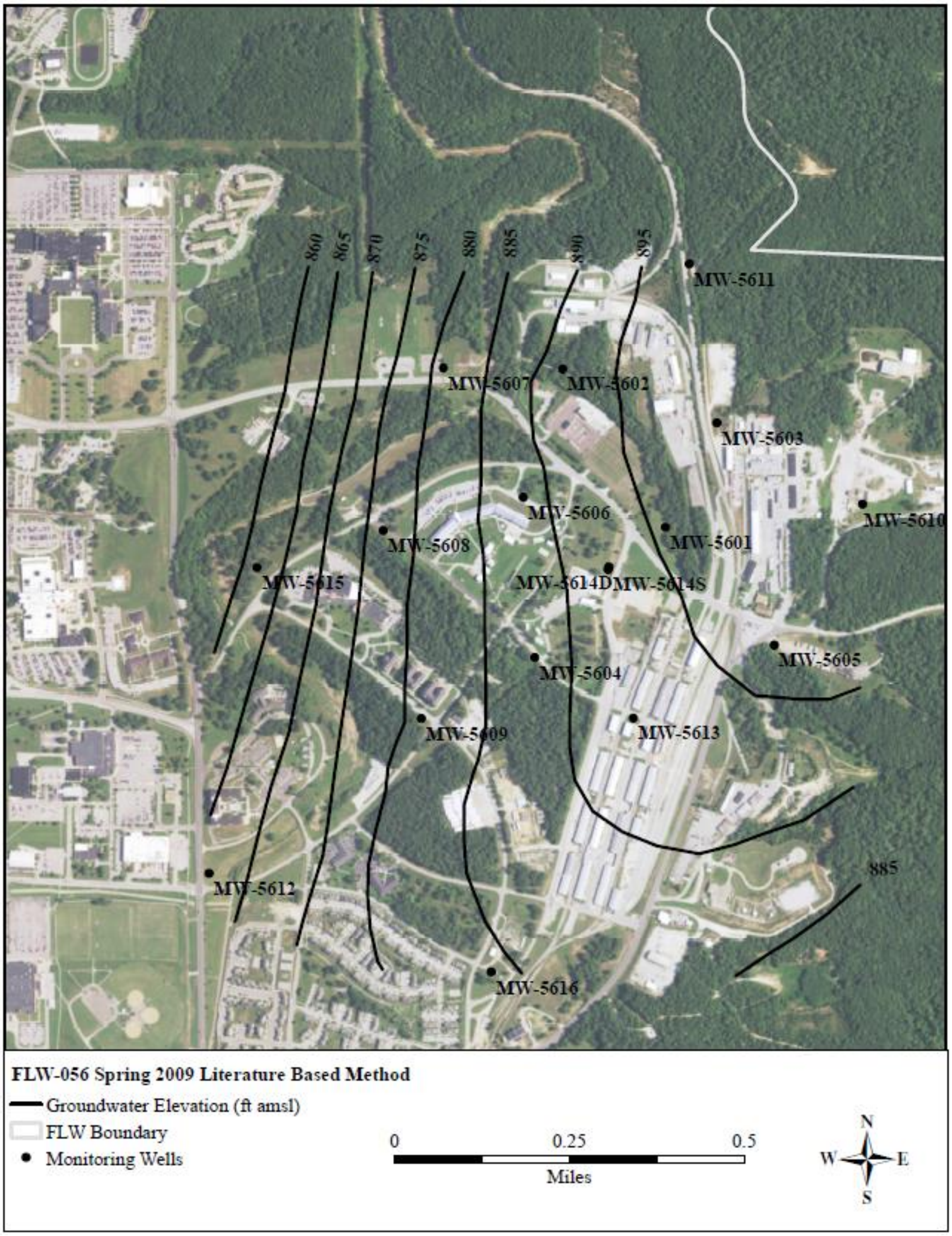
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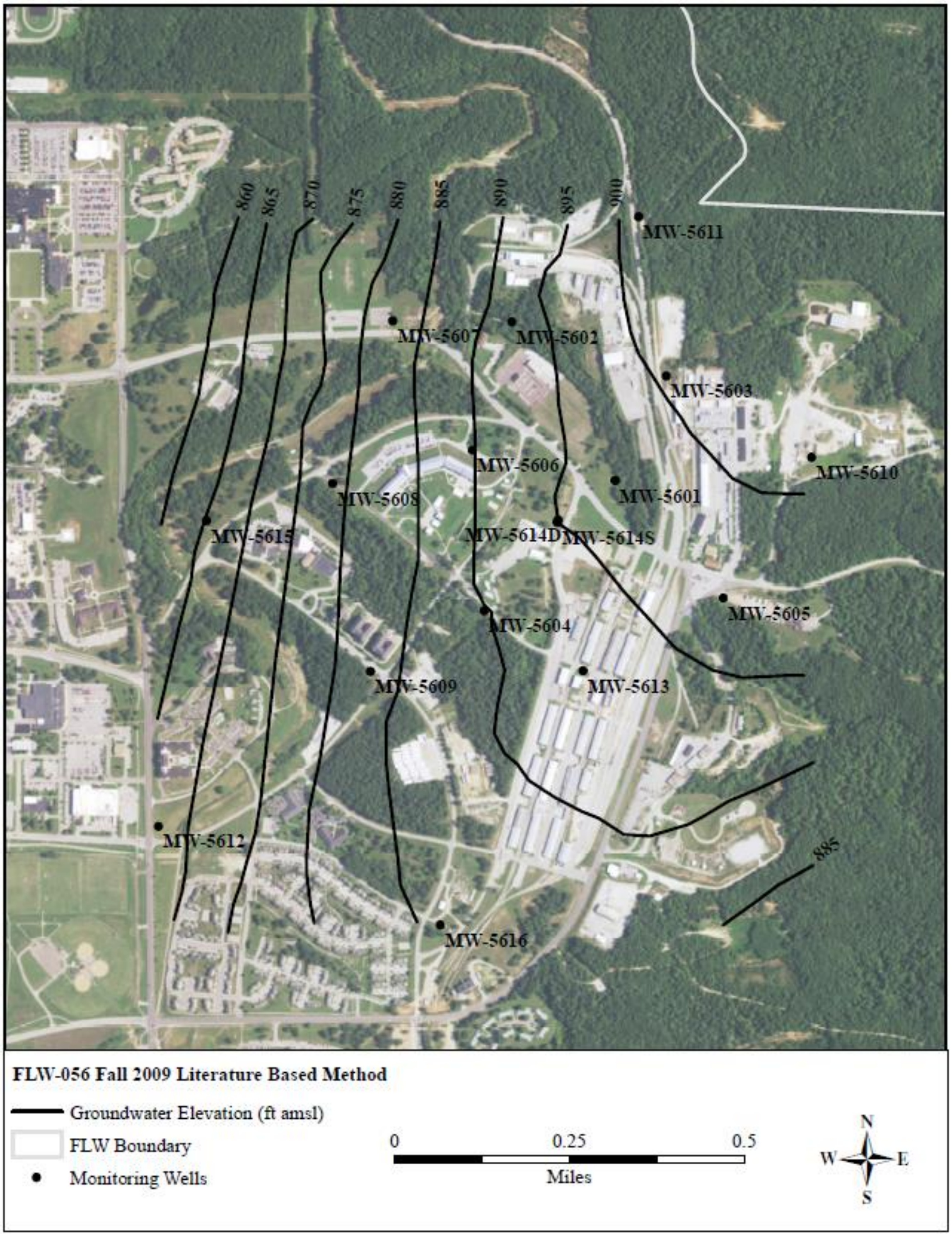
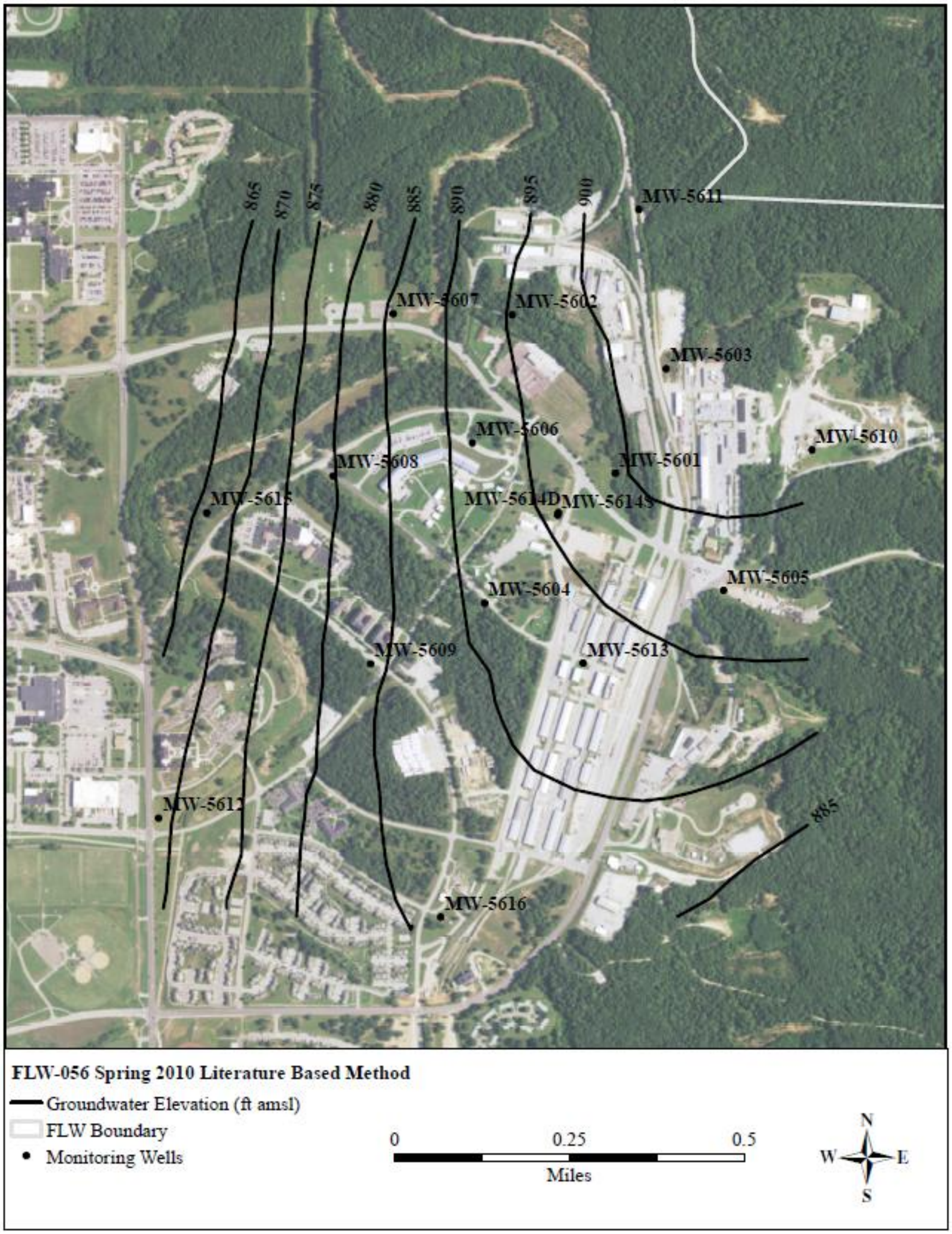


FLW-056 Fall 2009 Literature Based Method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FLW-056 Spring 2010 Literature Based Method
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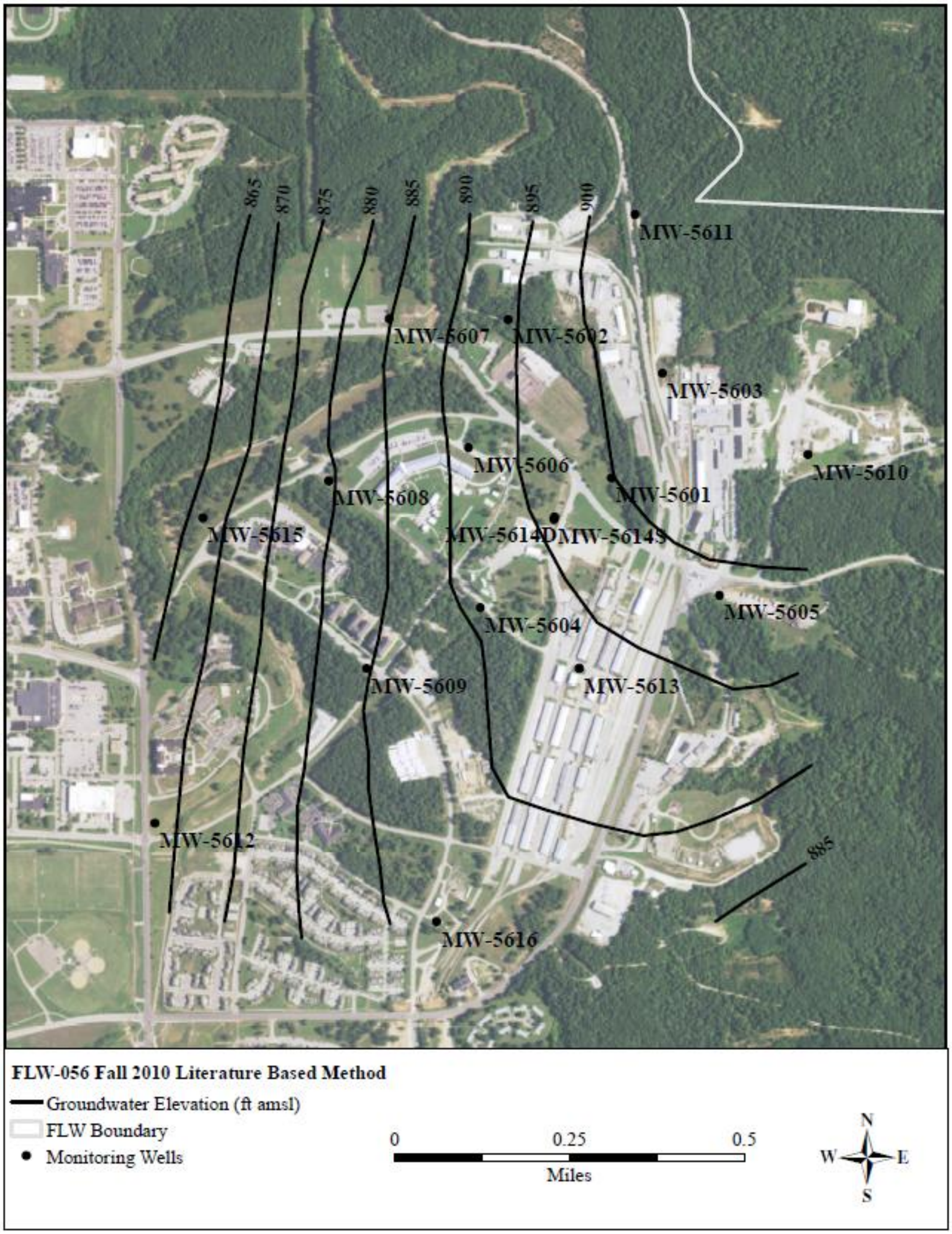
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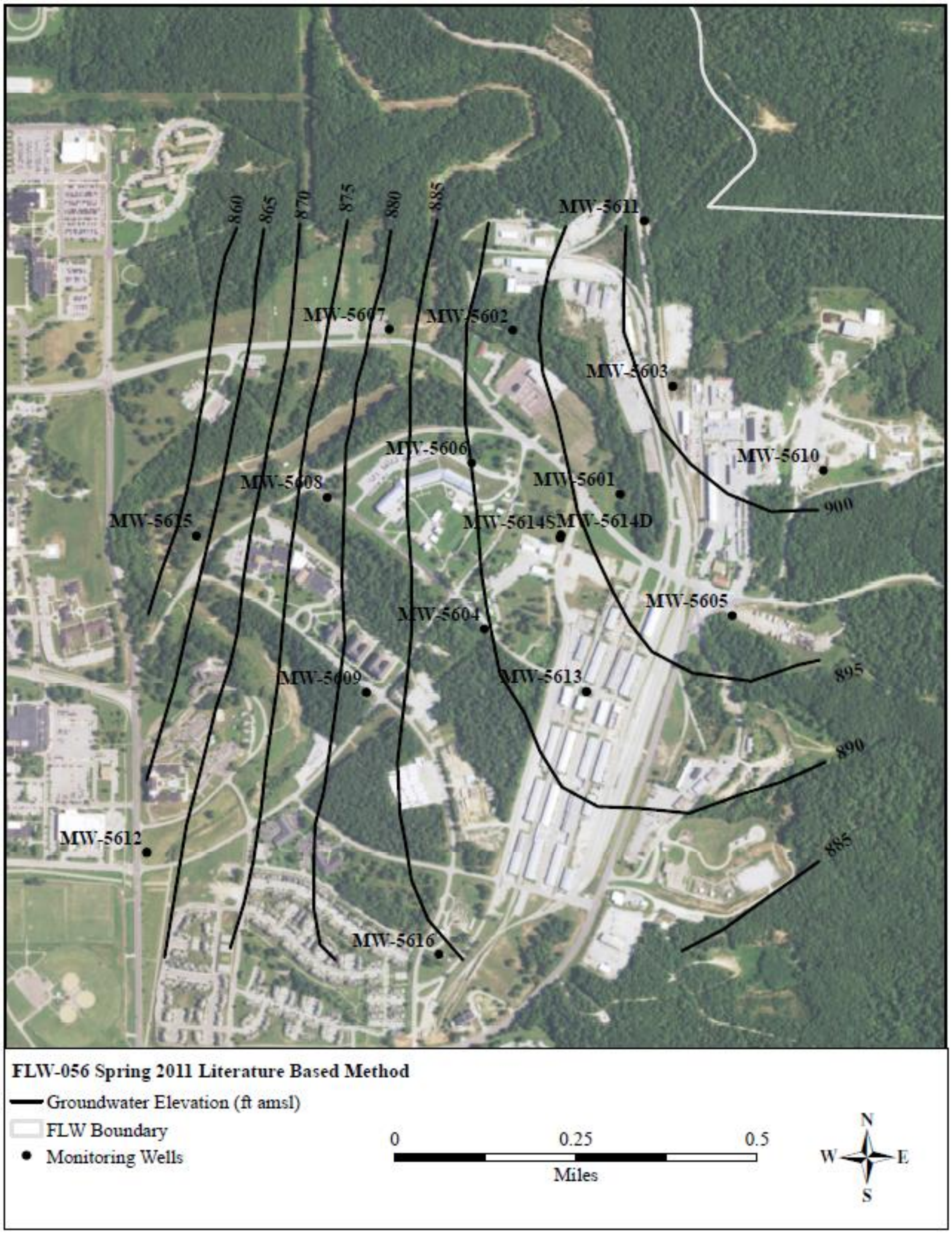

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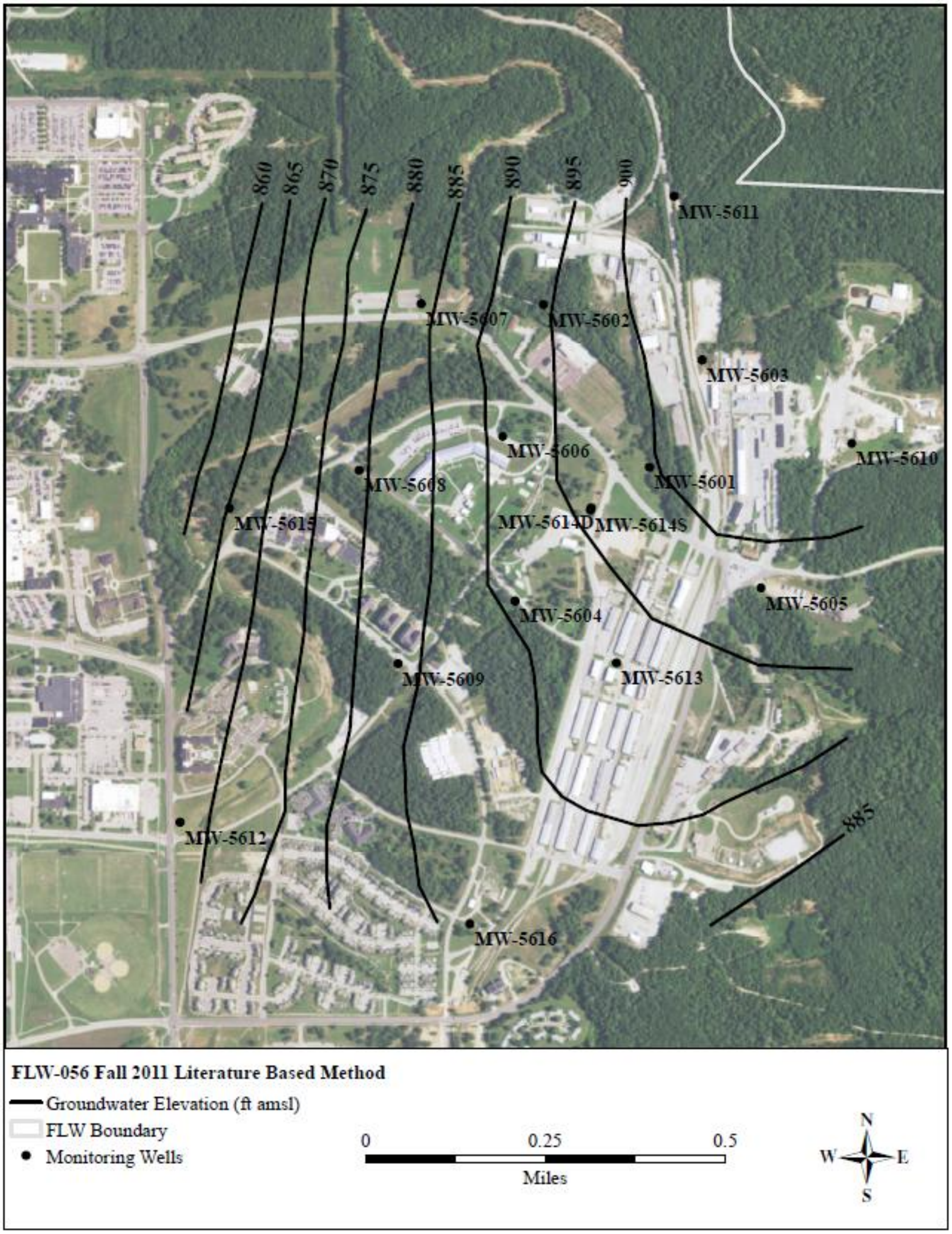
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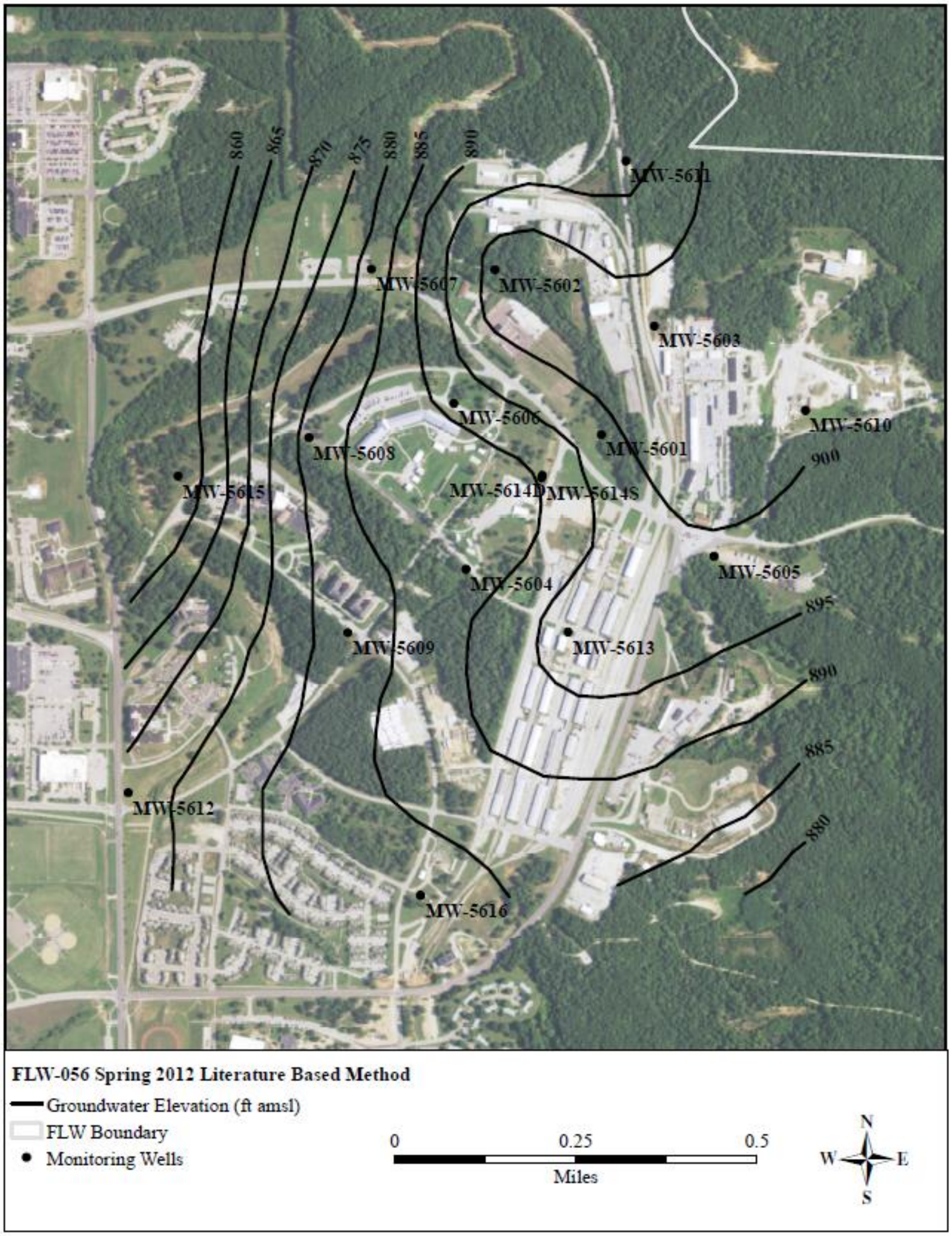

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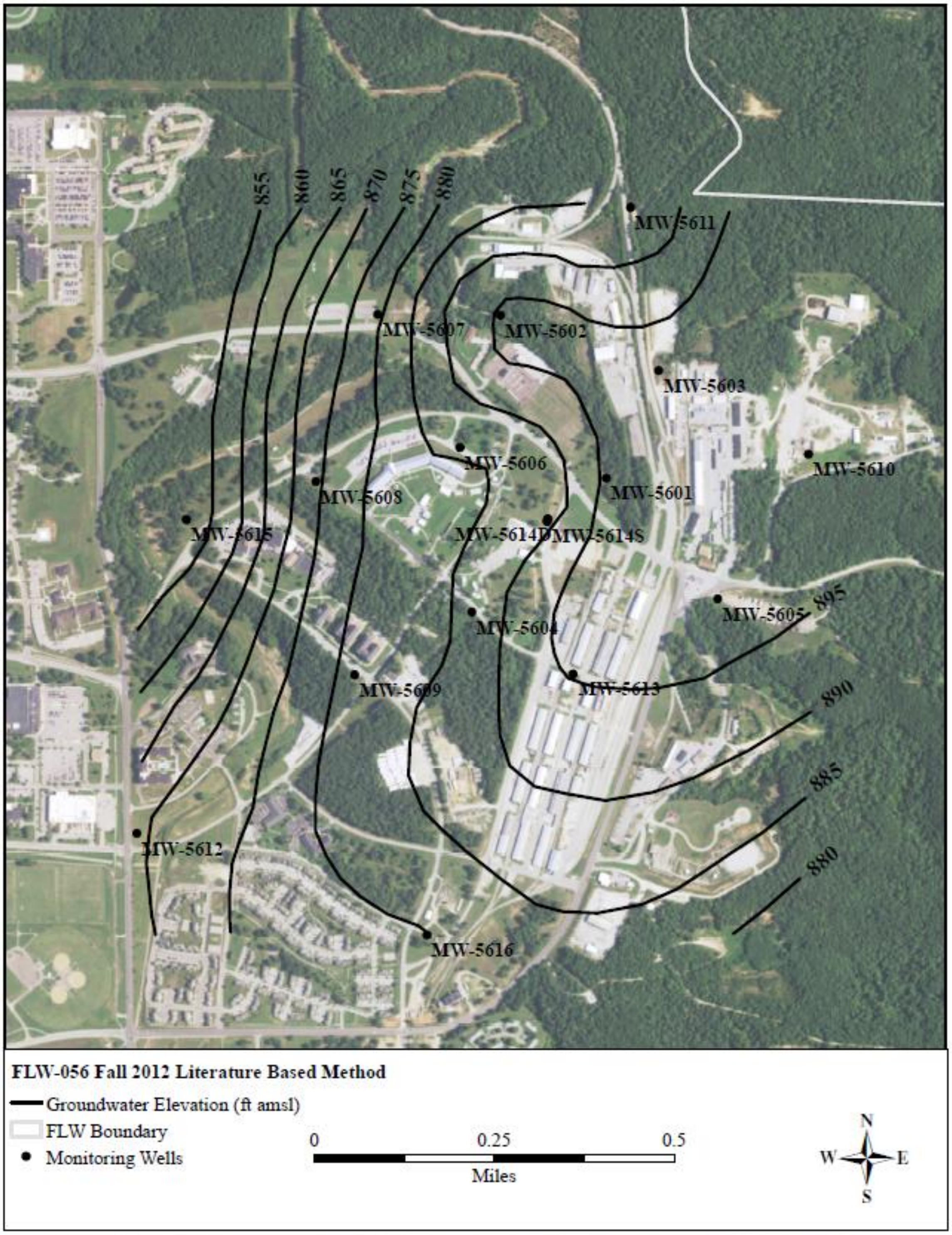
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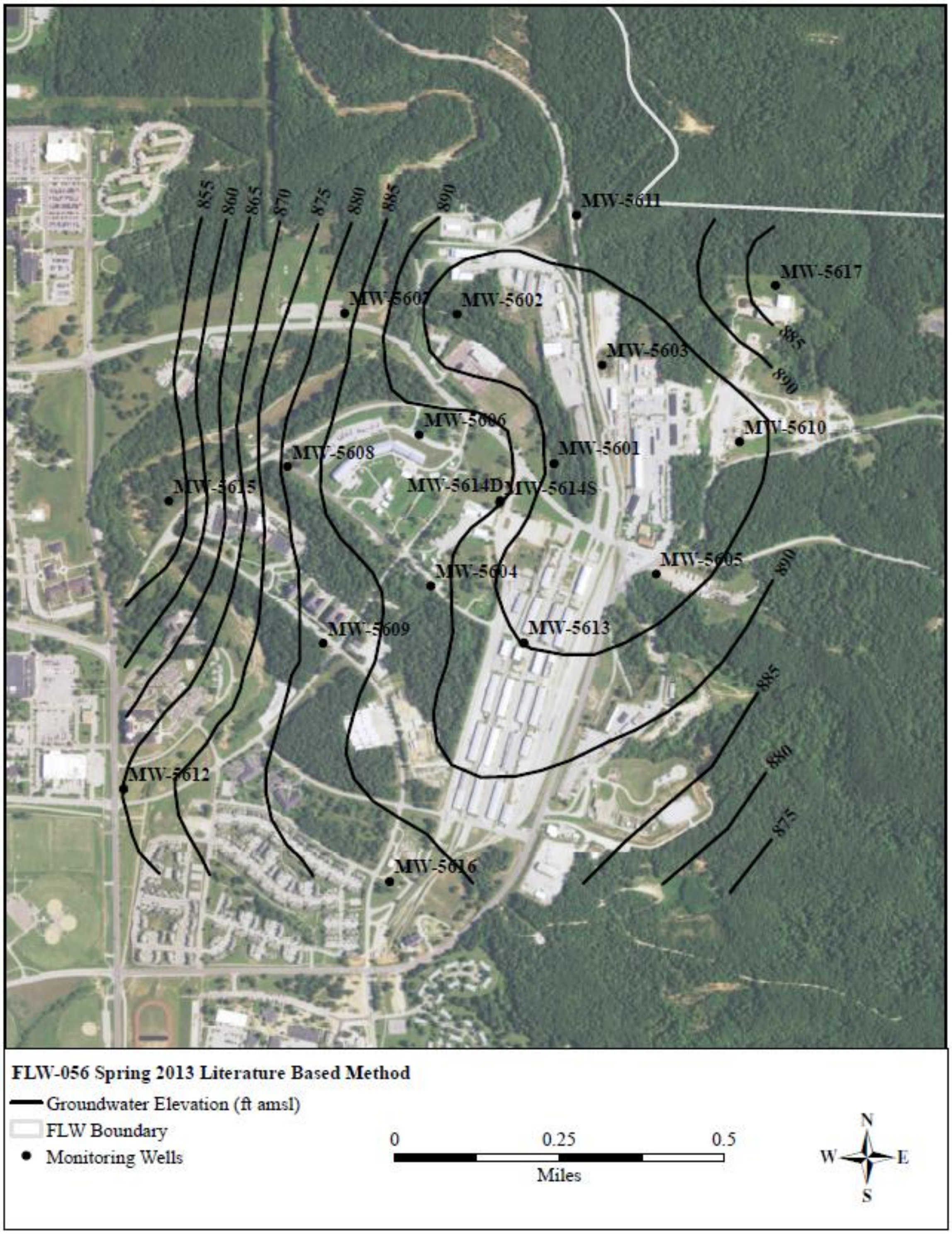
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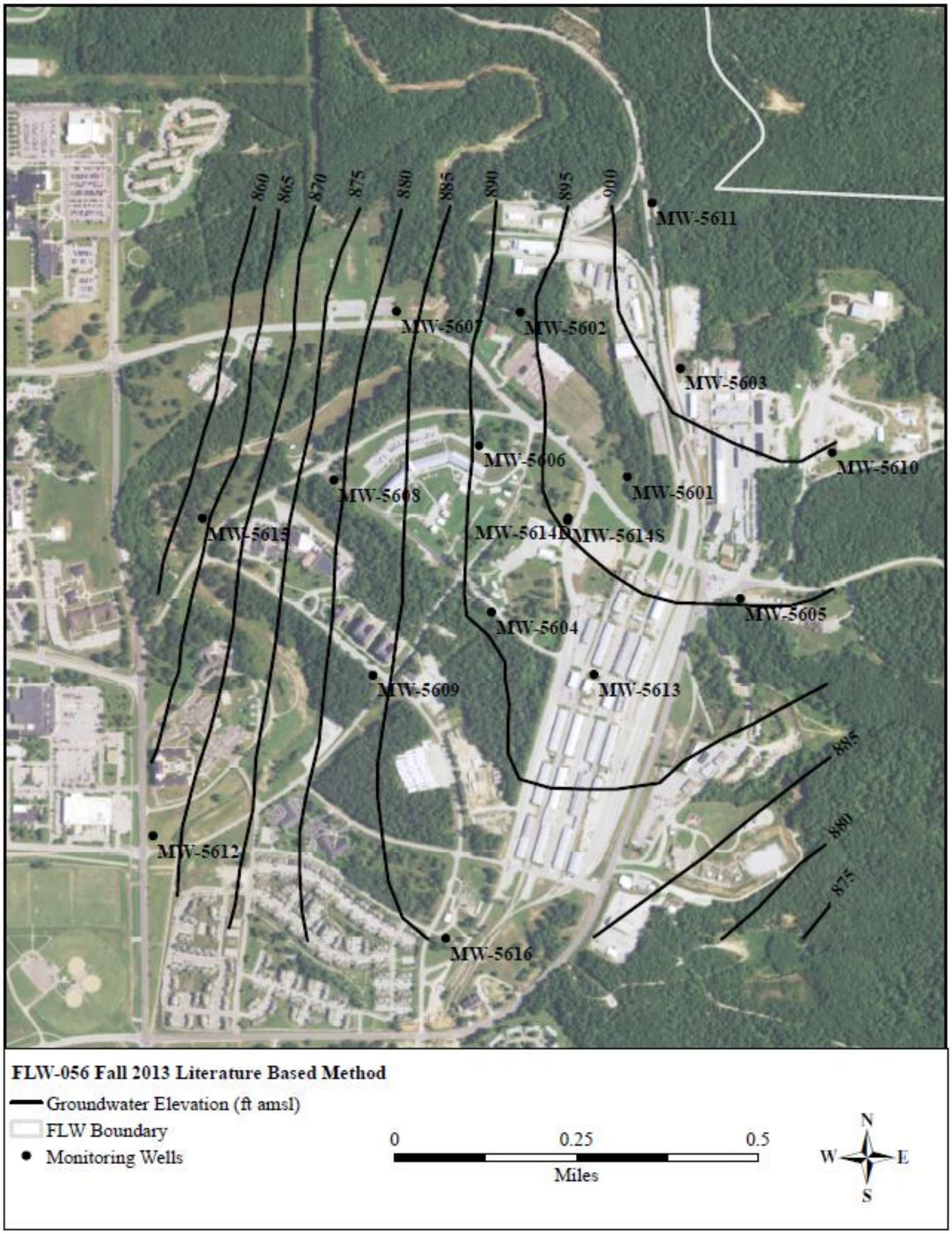
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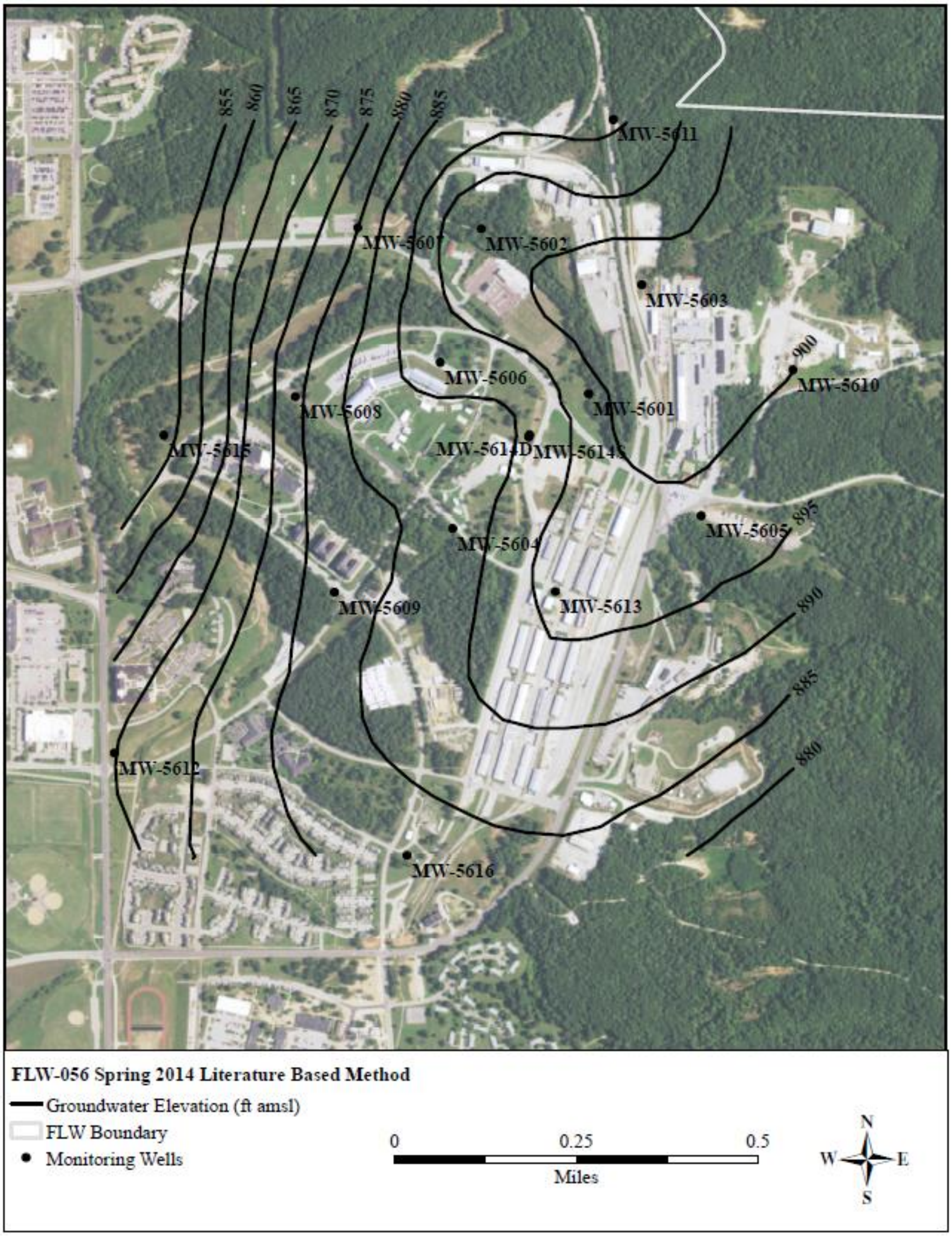
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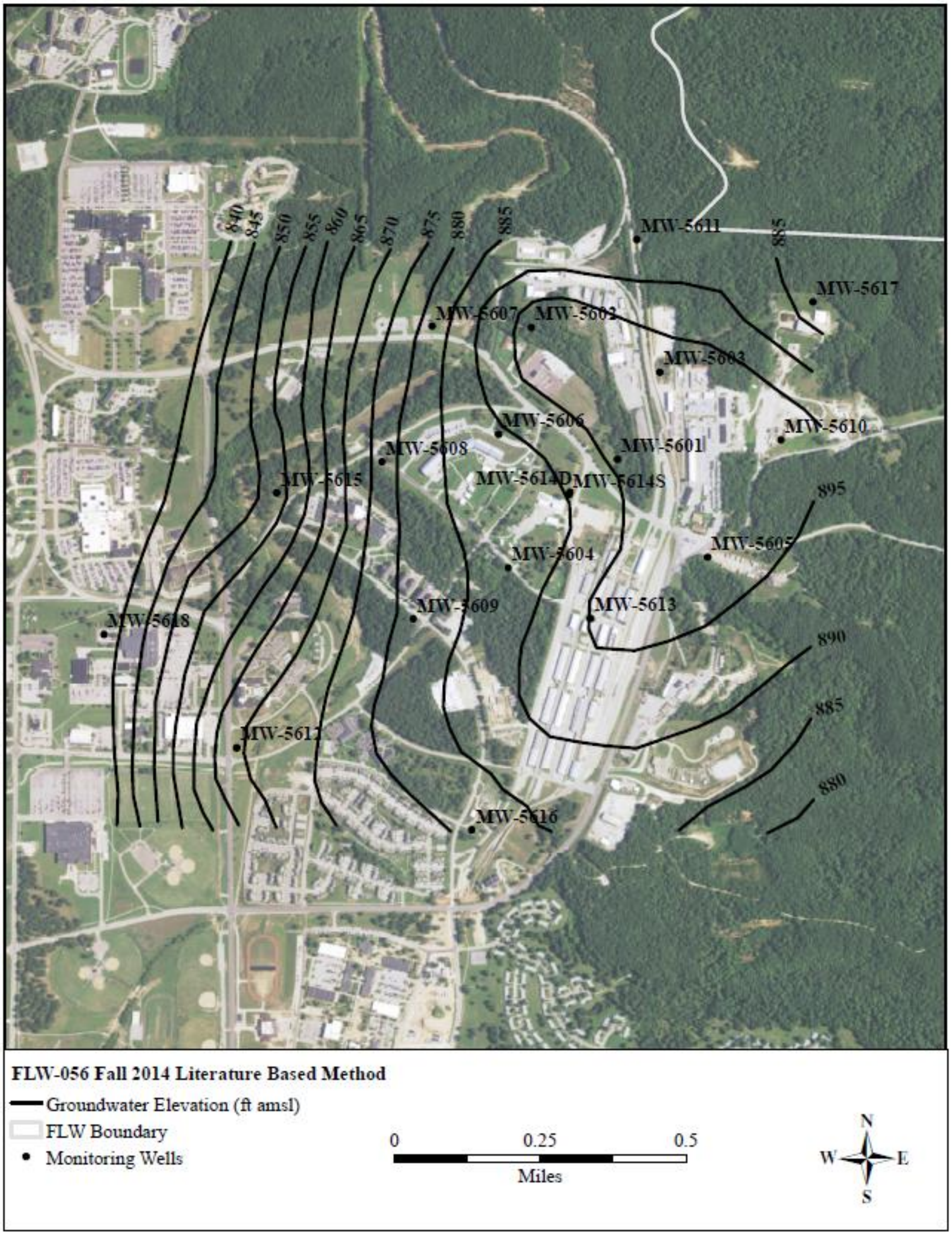
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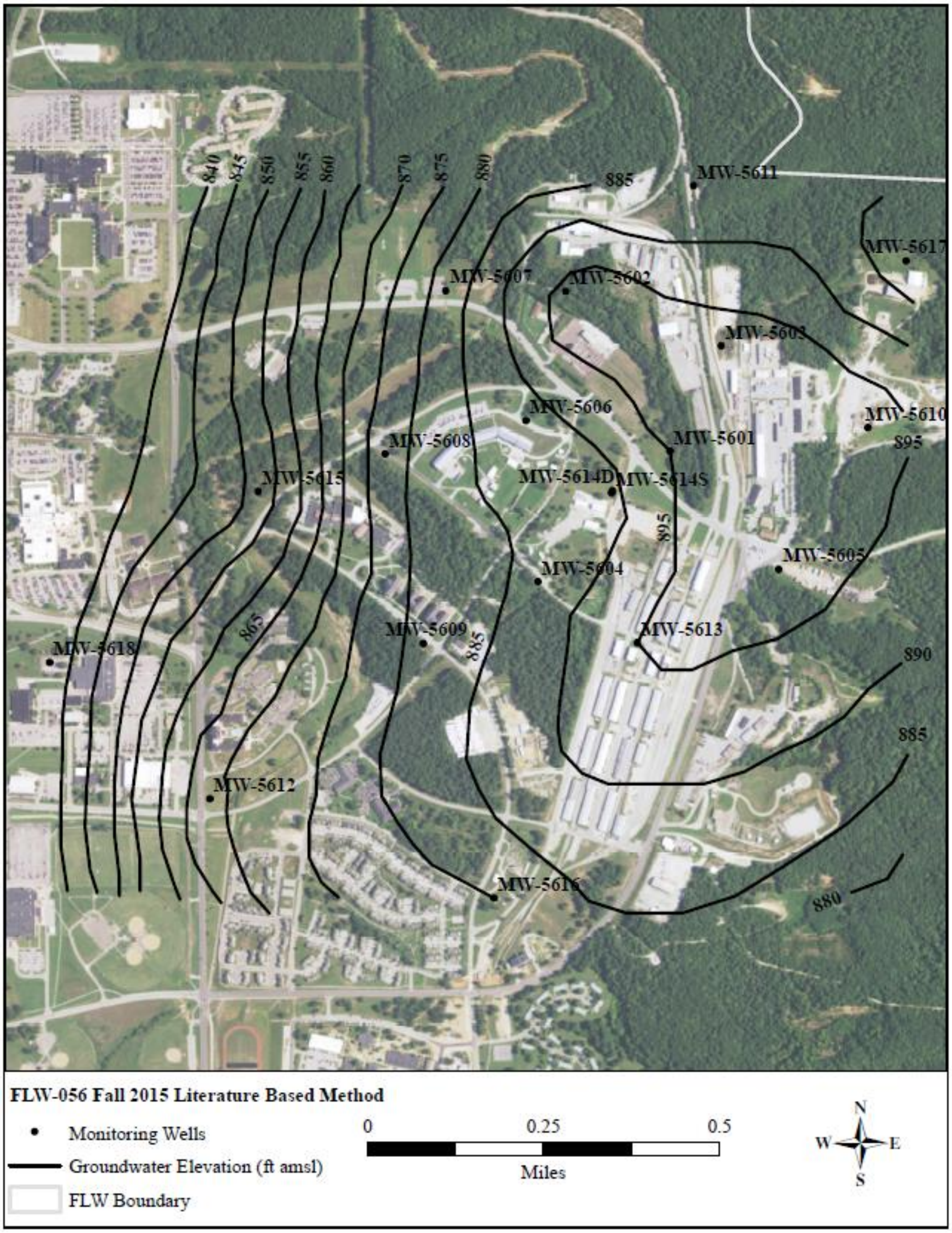
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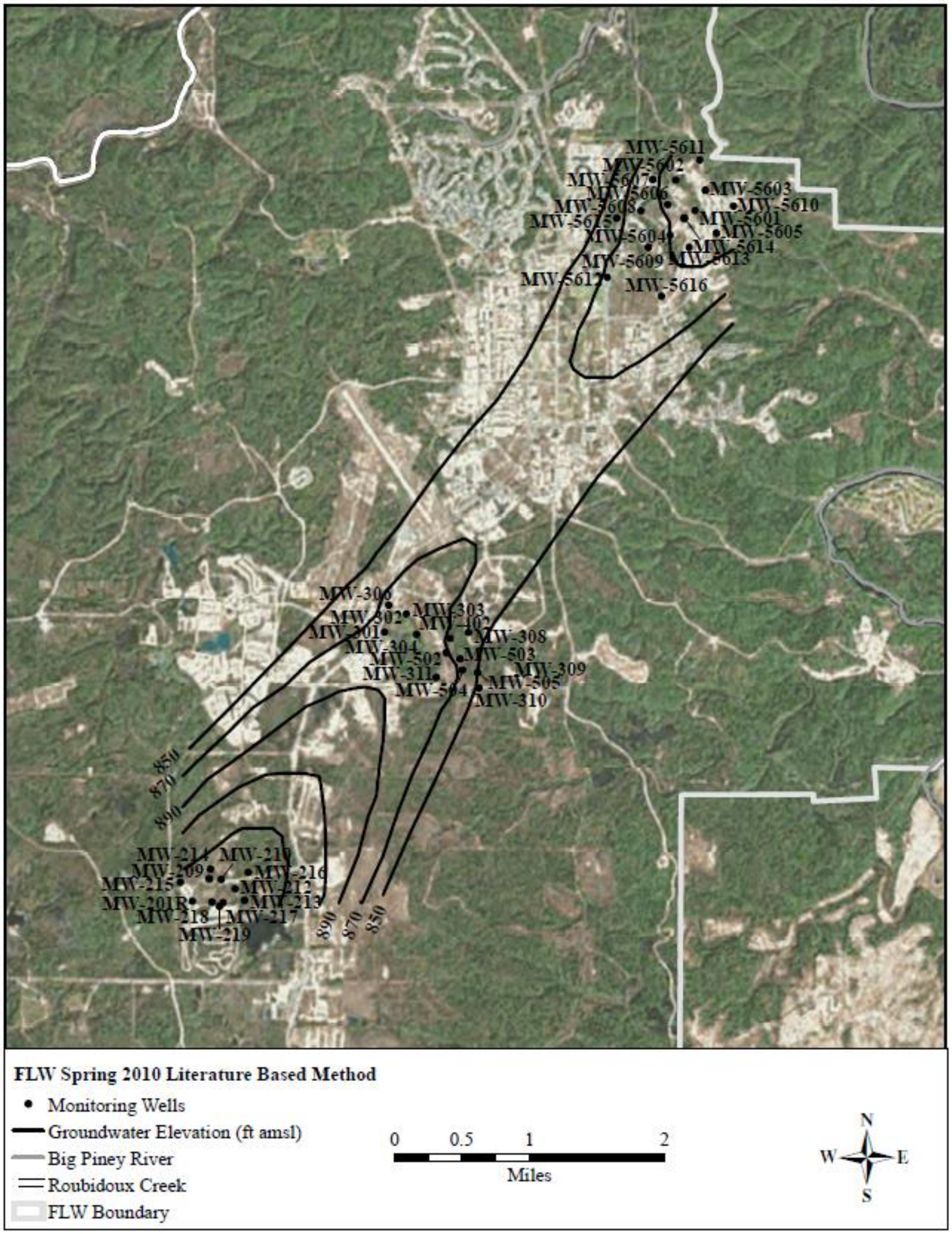
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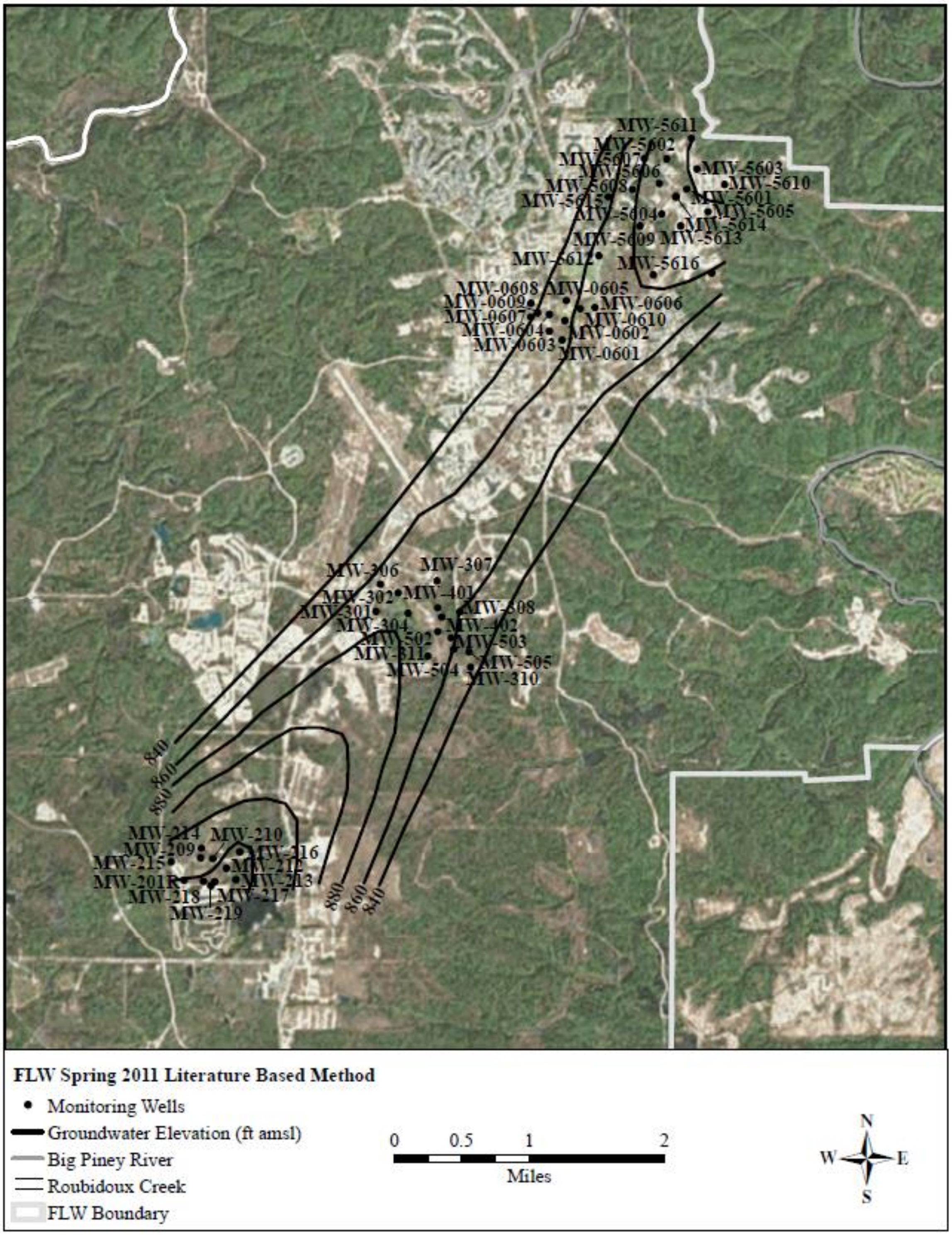
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Monitoring Wells
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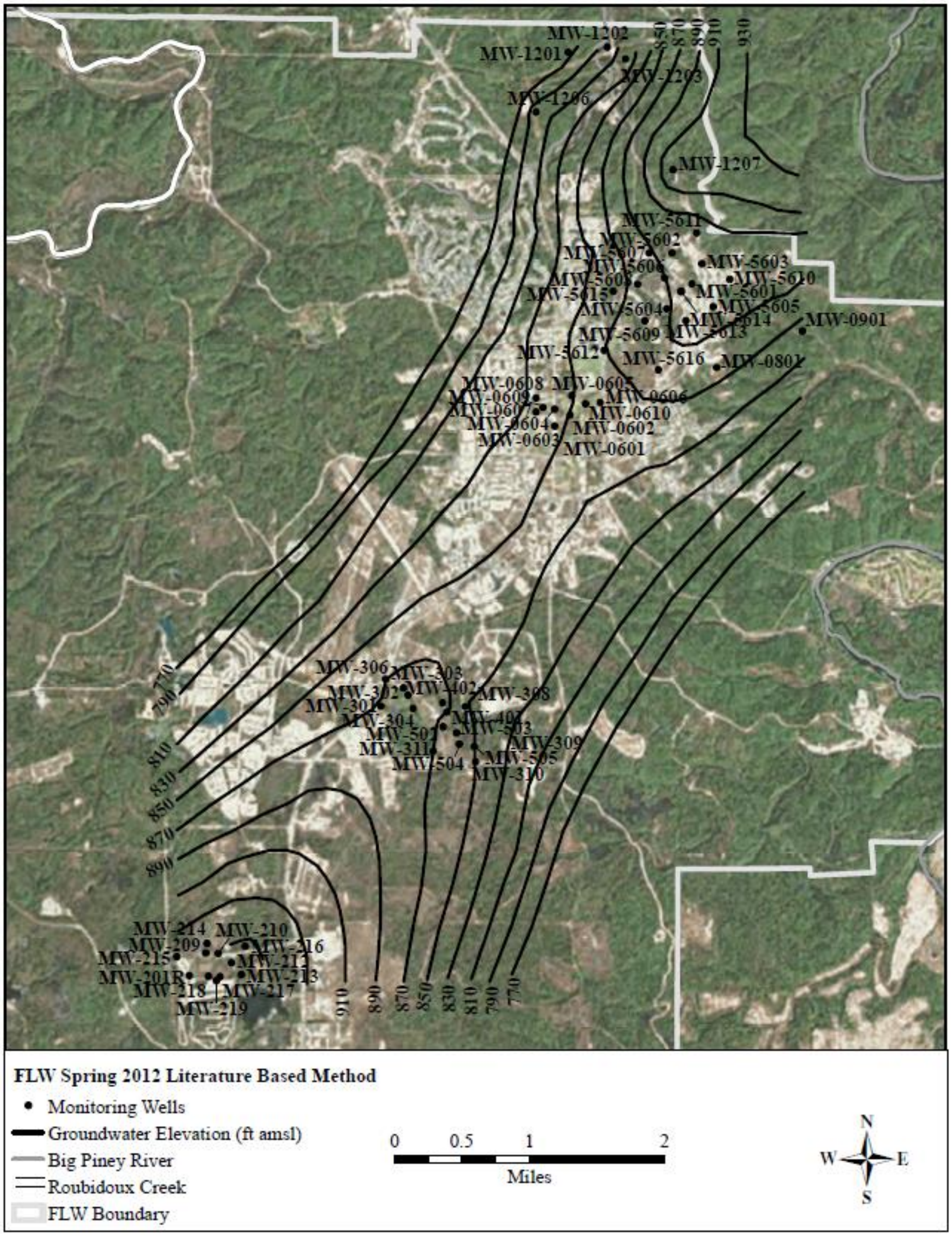
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FLW Spring 2012 Literature Based Method
Monitoring Wells
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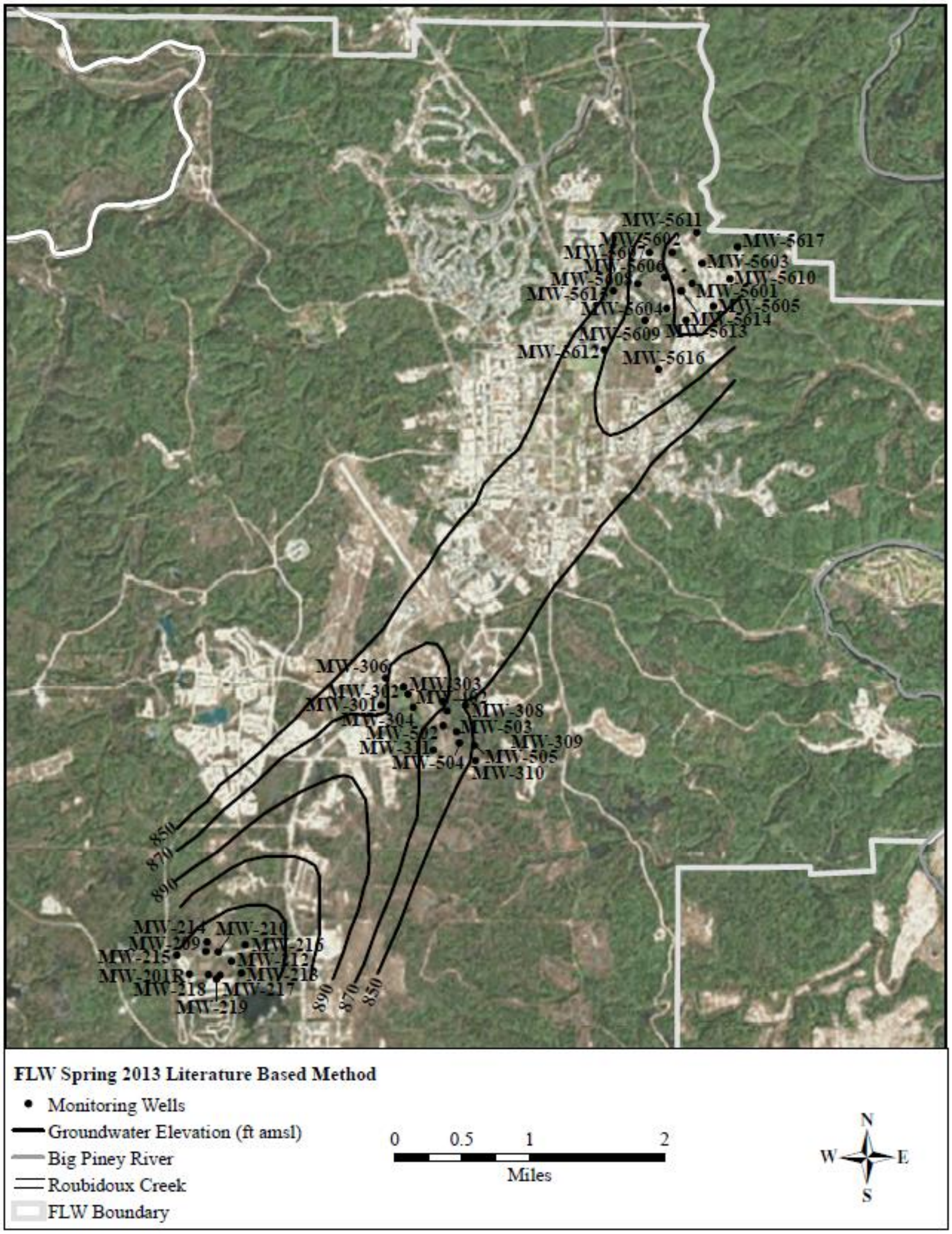
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Monitoring Wells
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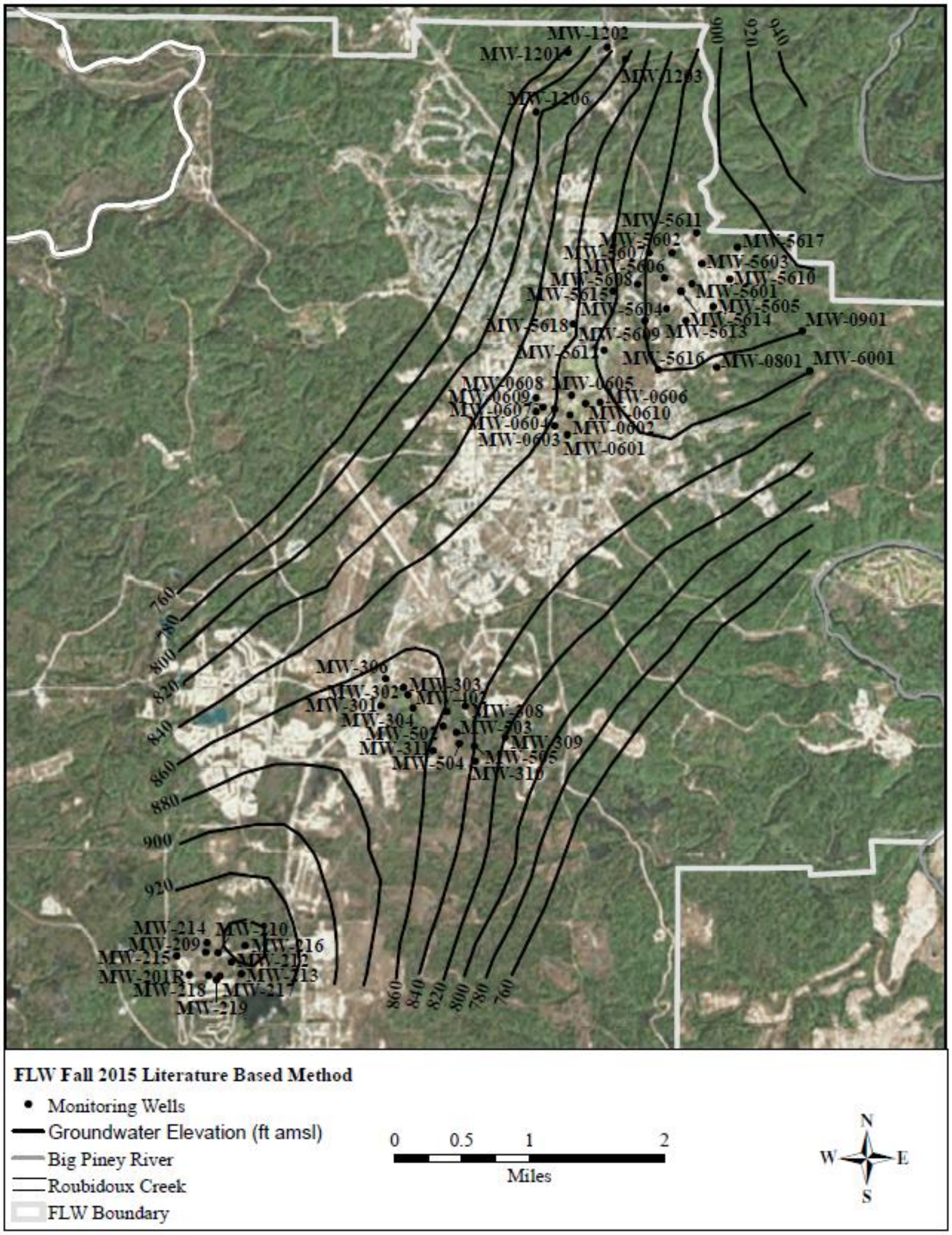
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Groundwater Elevation (ft amsl)
Big Piney River
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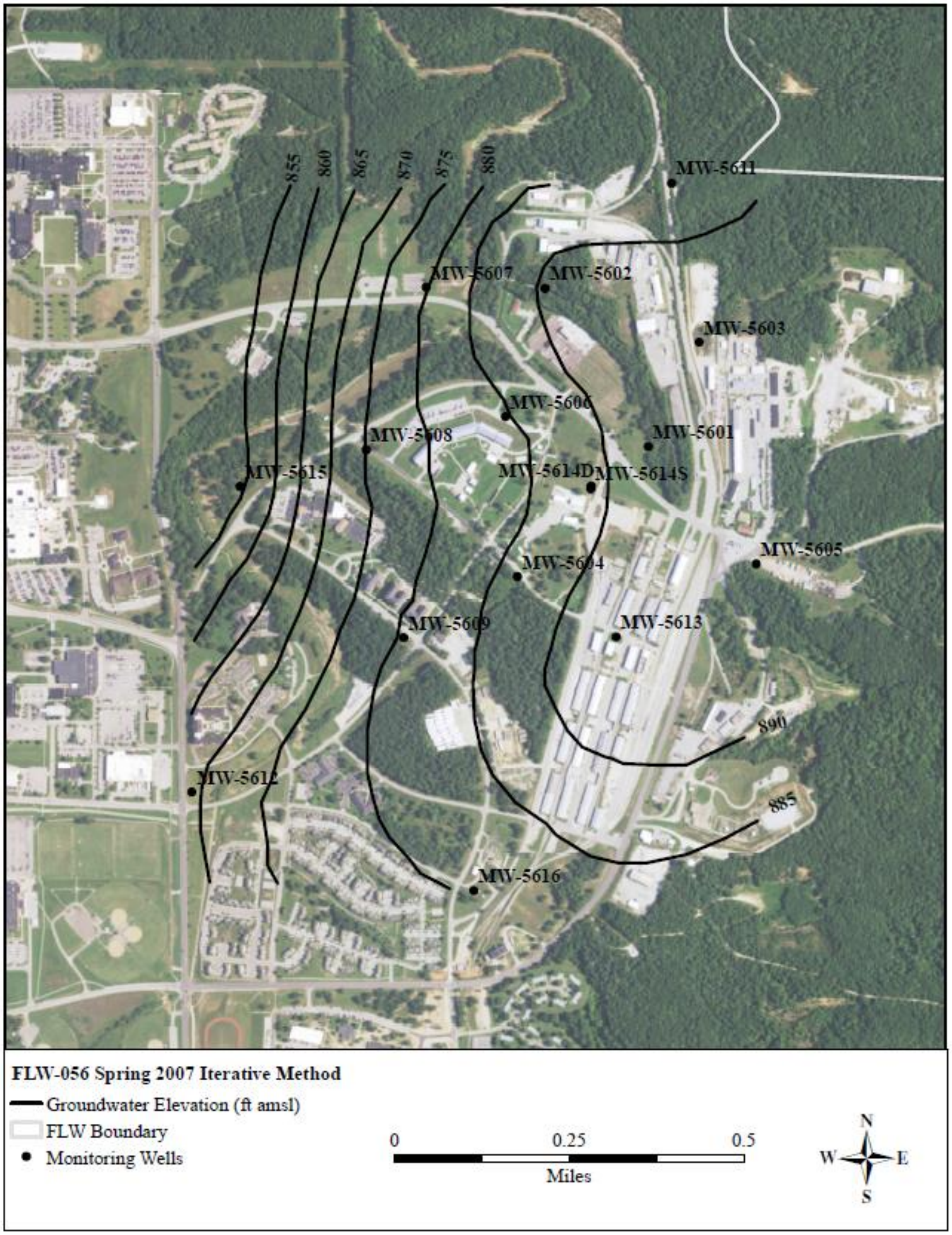
APPENDIX B.

ITERATIVE METHOD CONTOUR MAPS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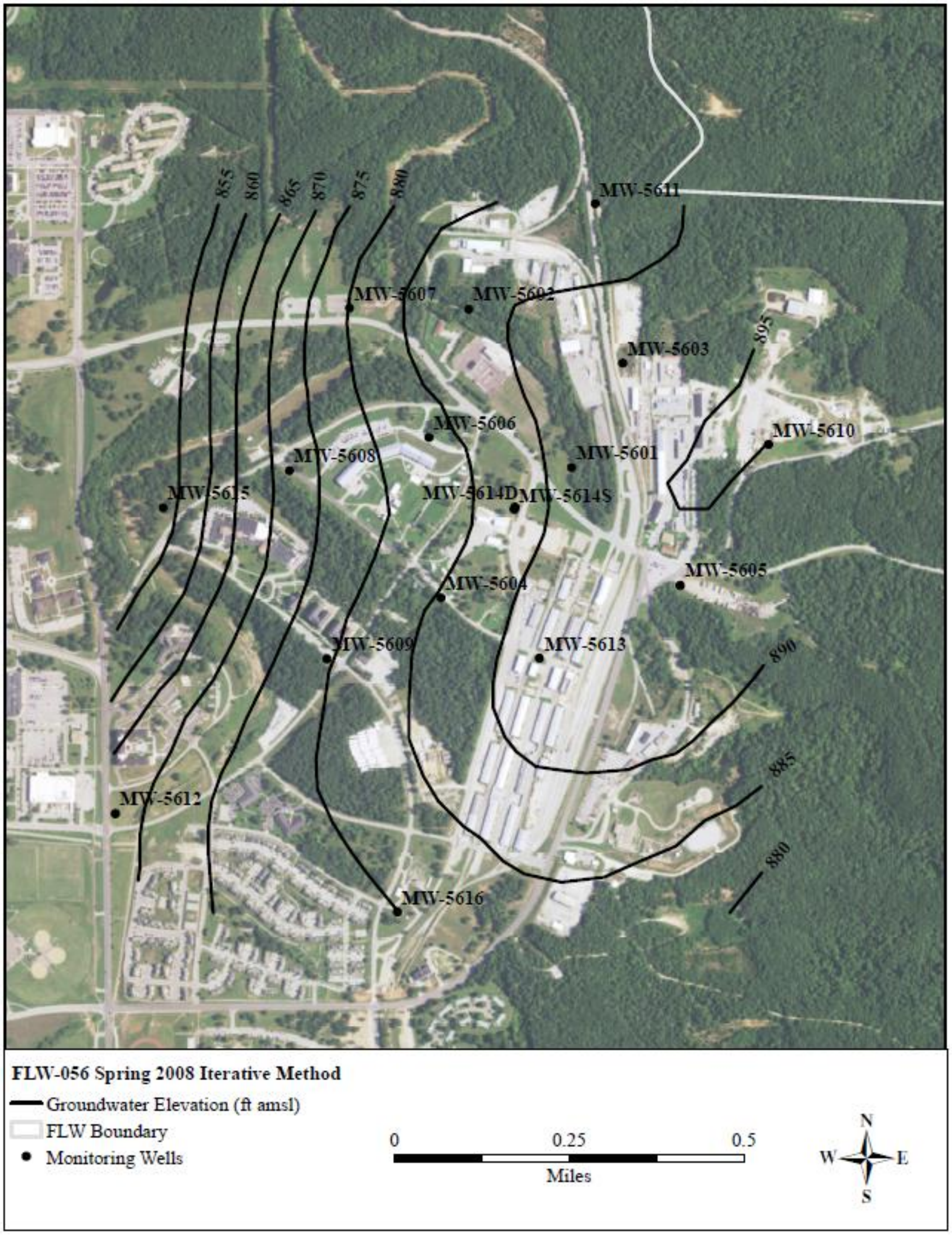
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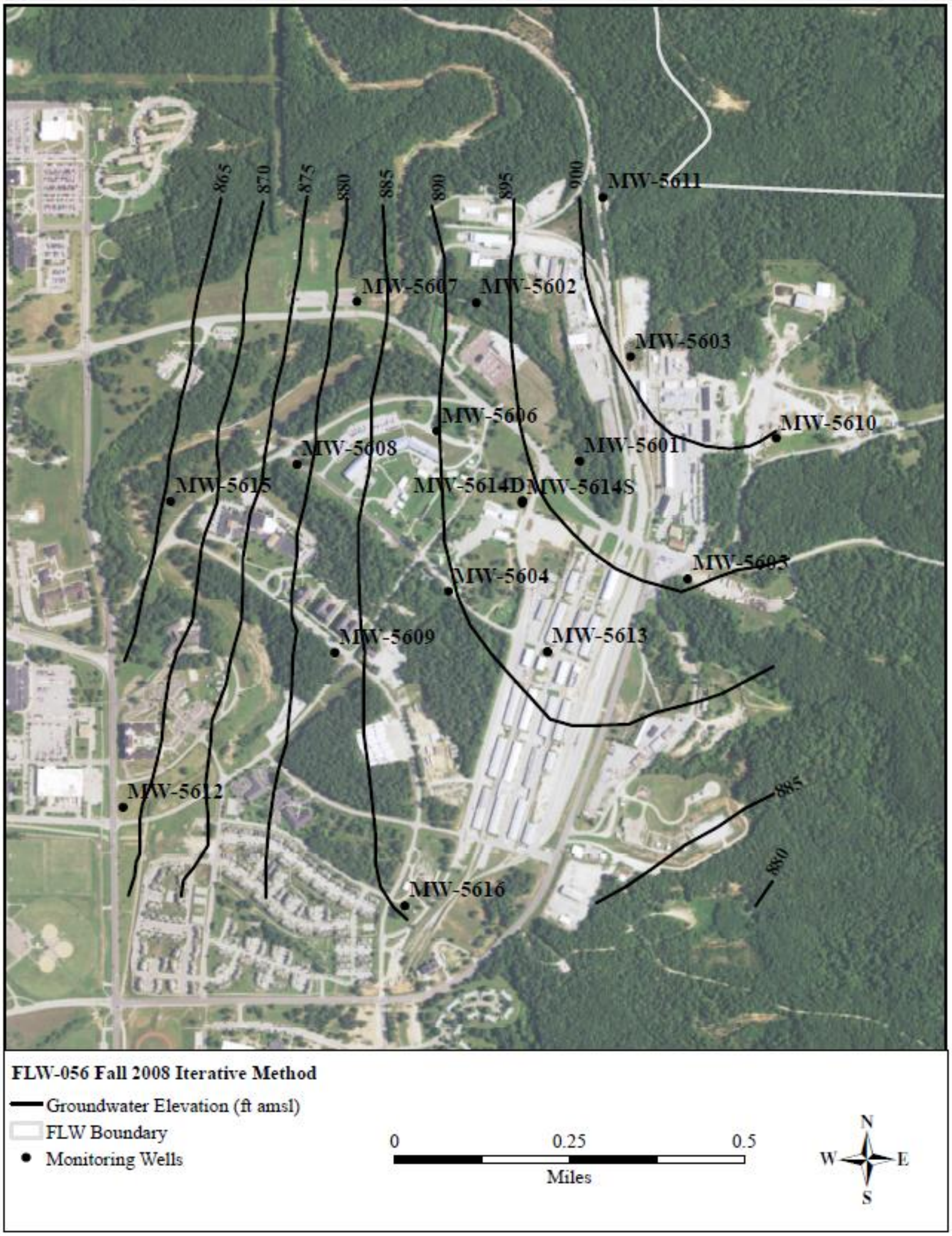
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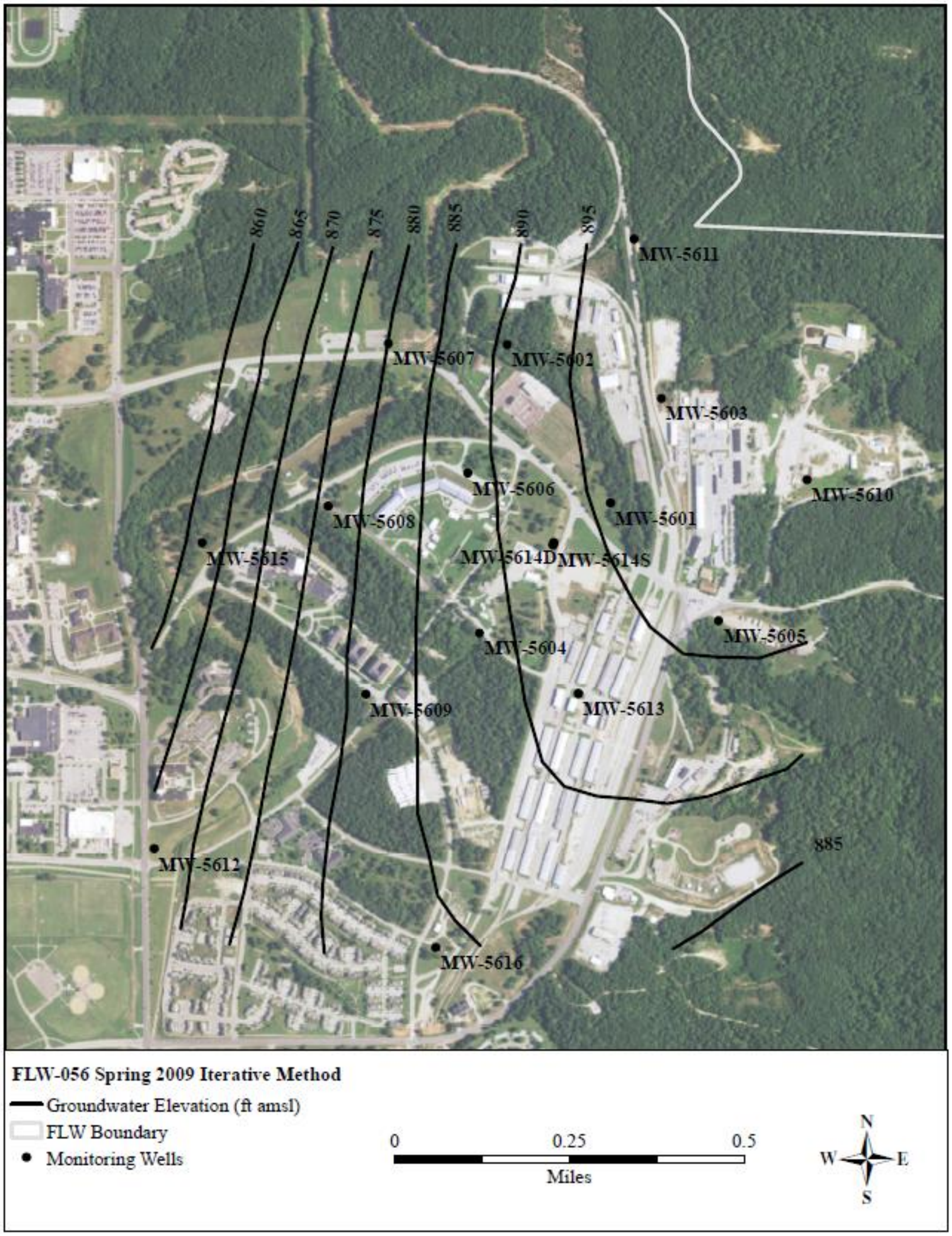
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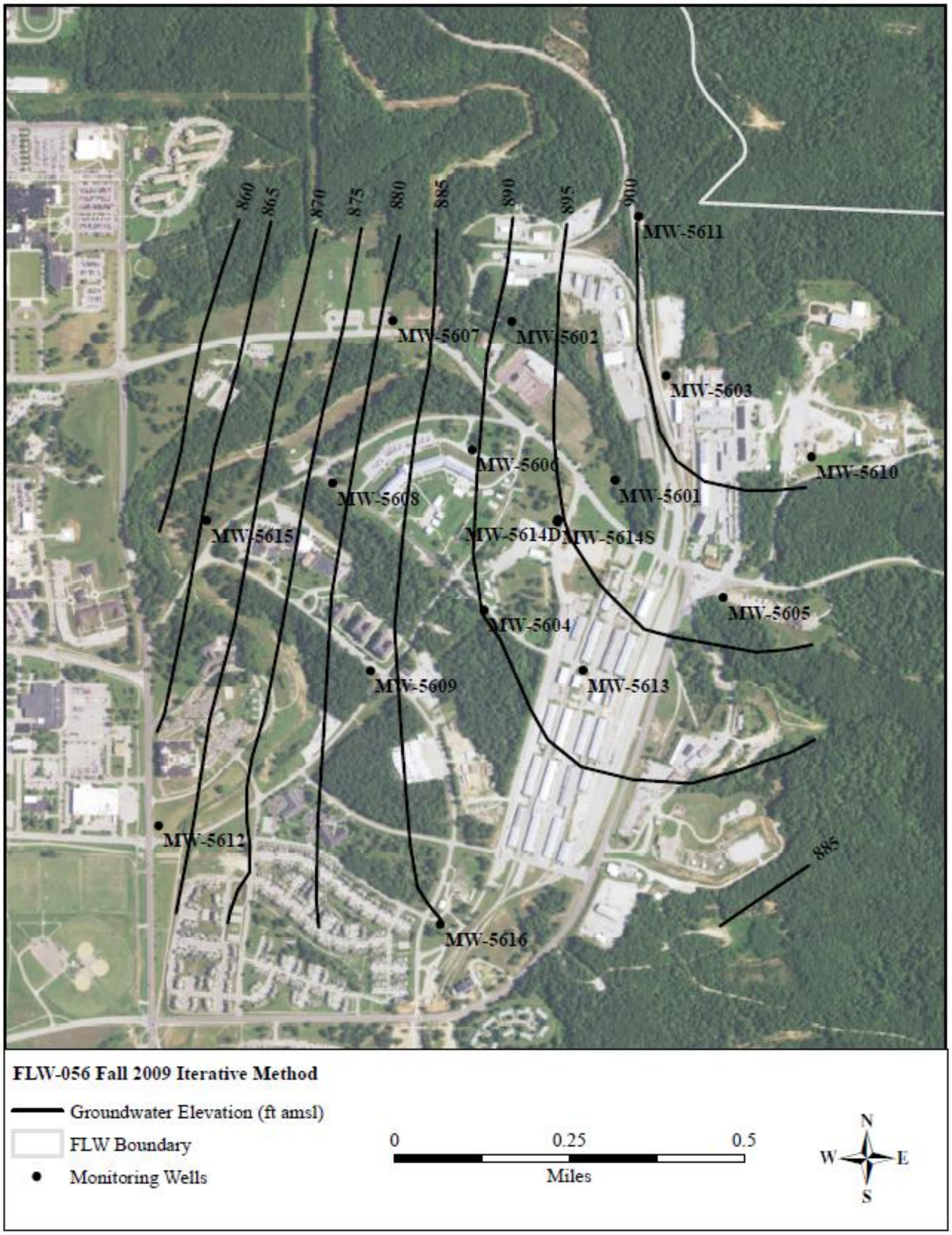
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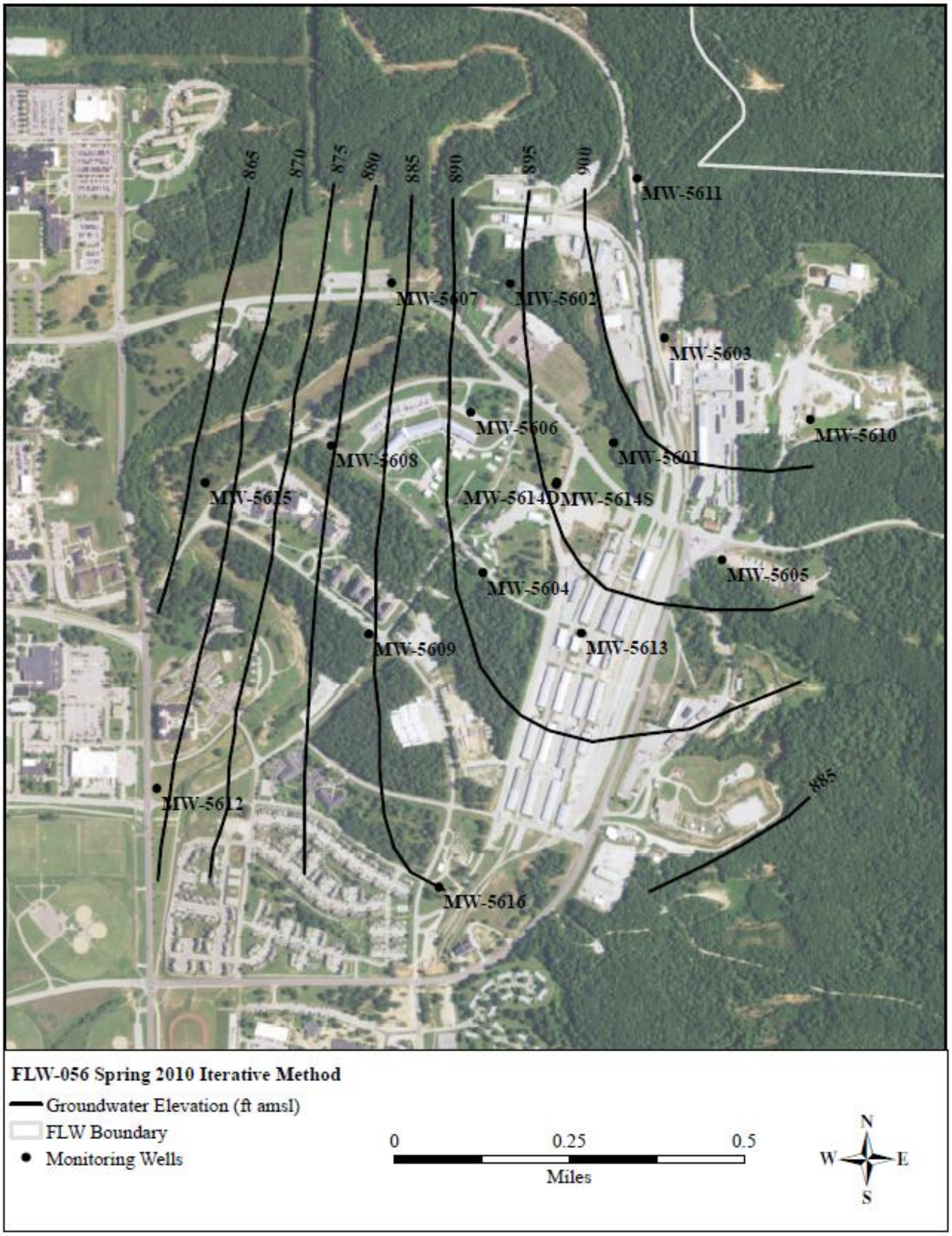
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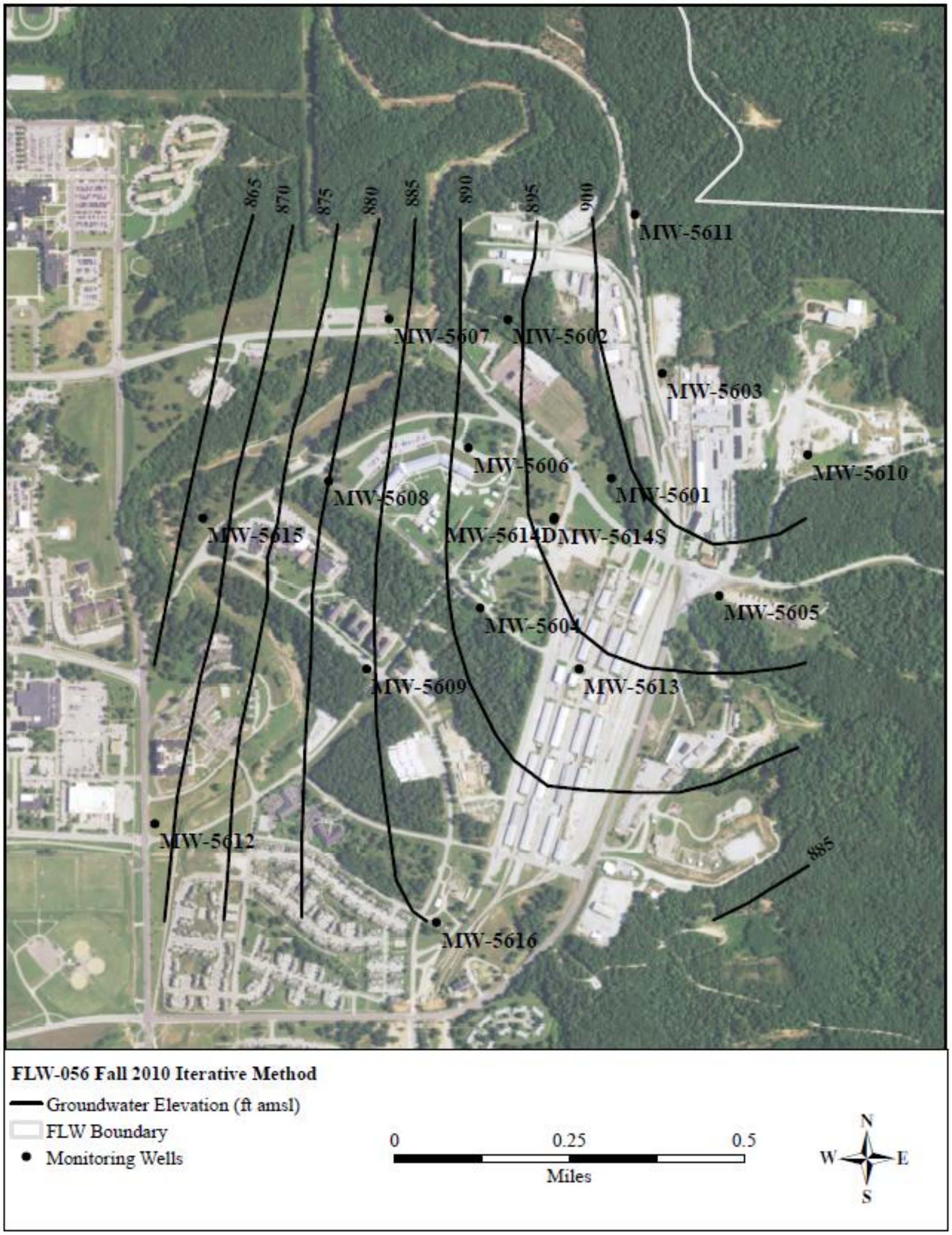
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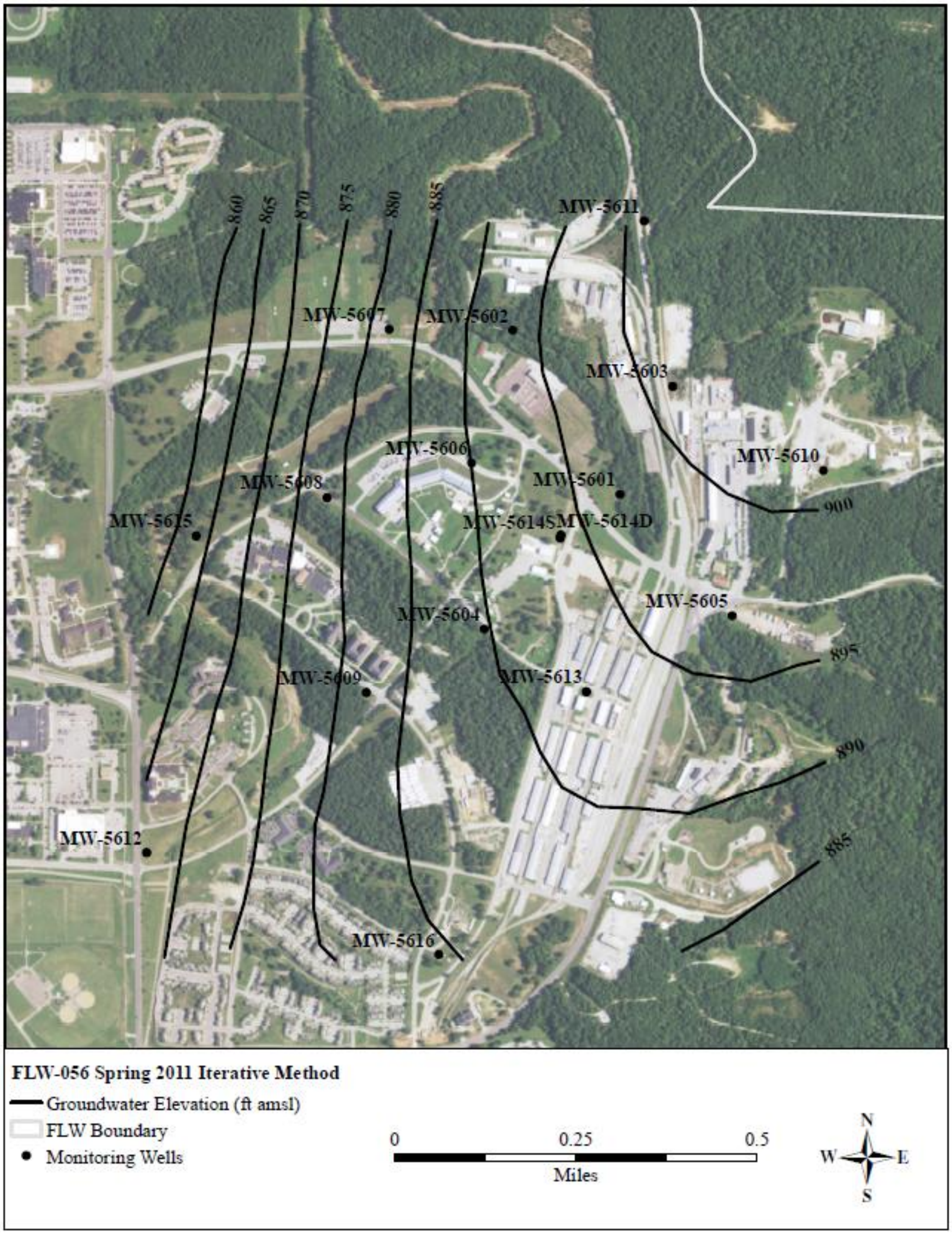
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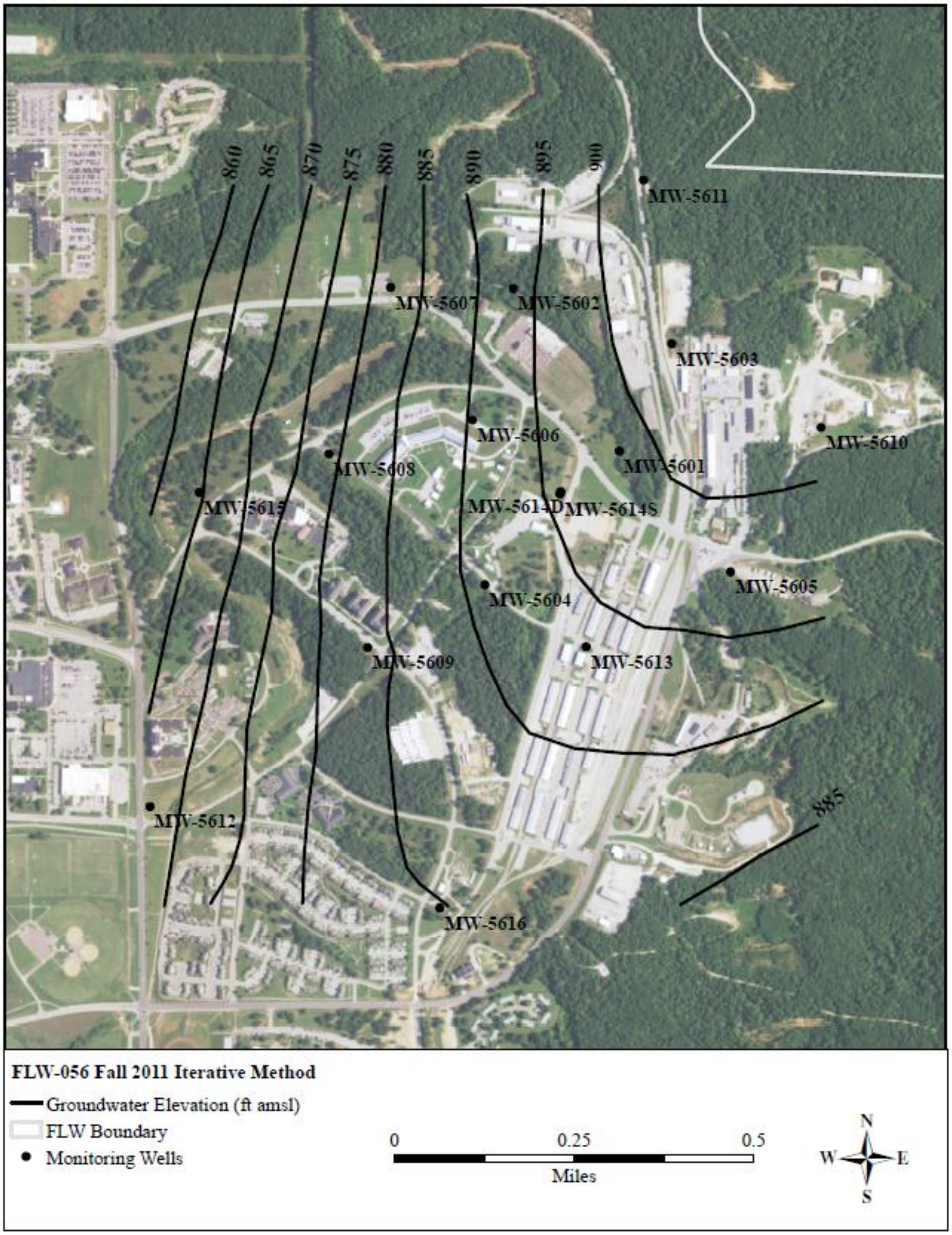
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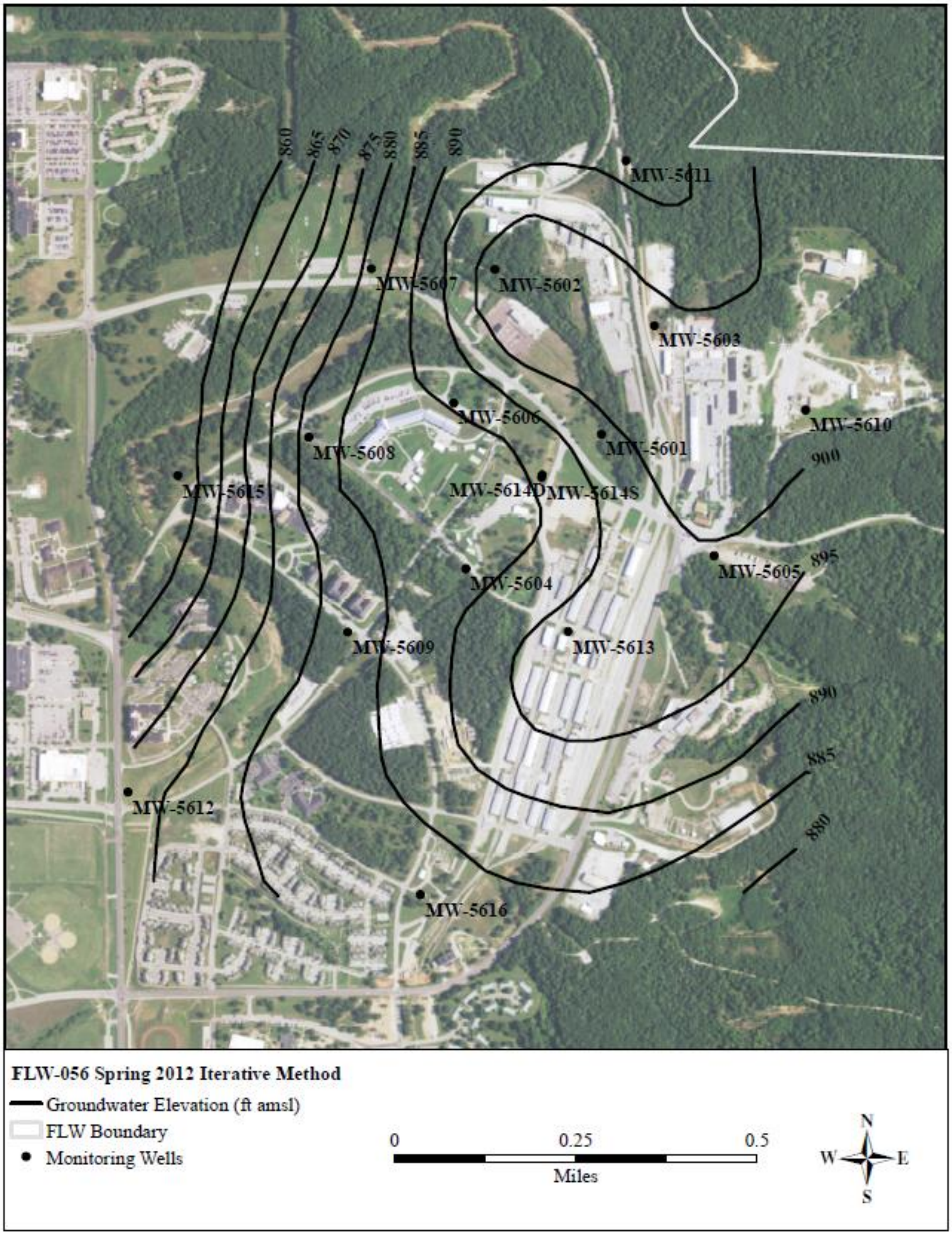
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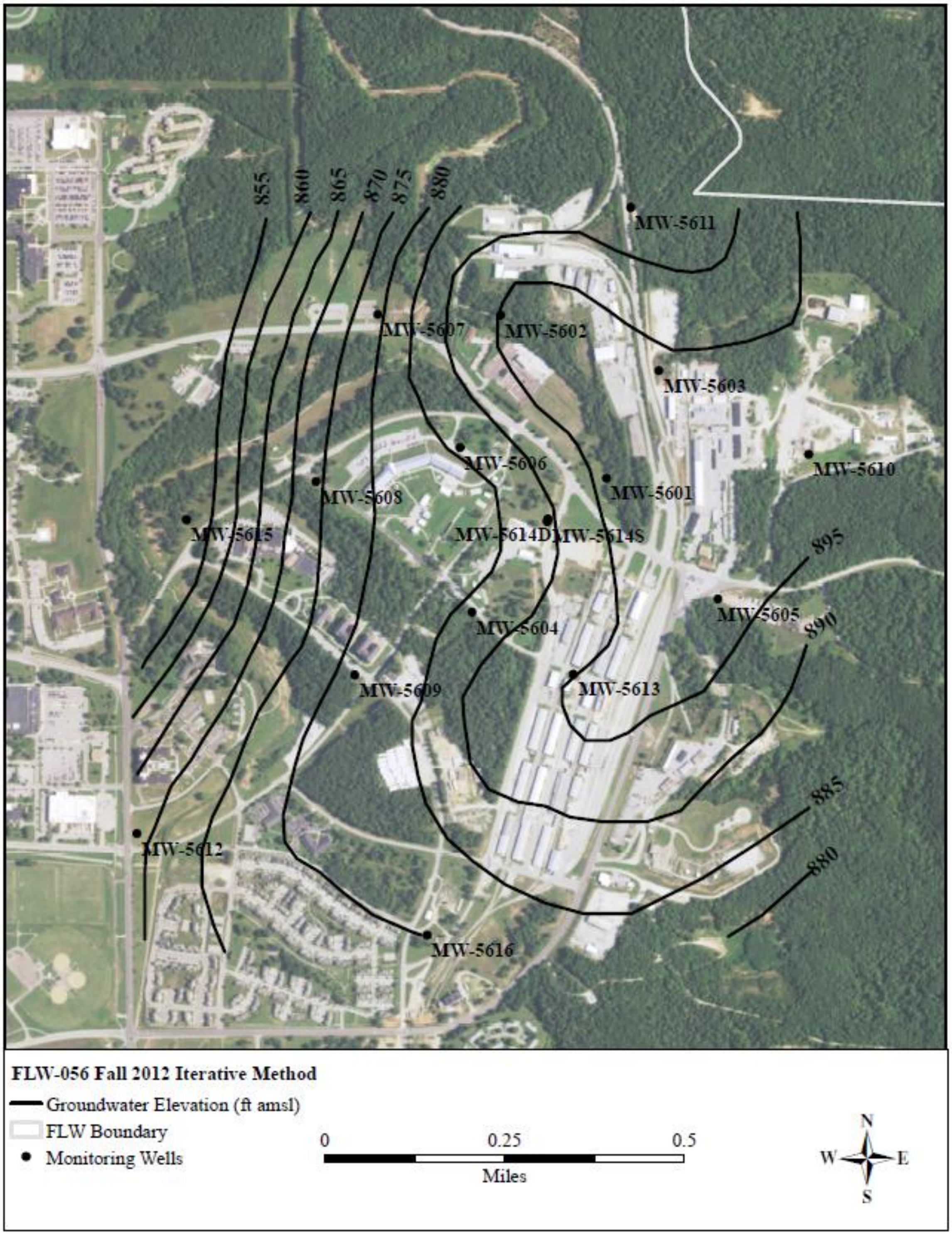
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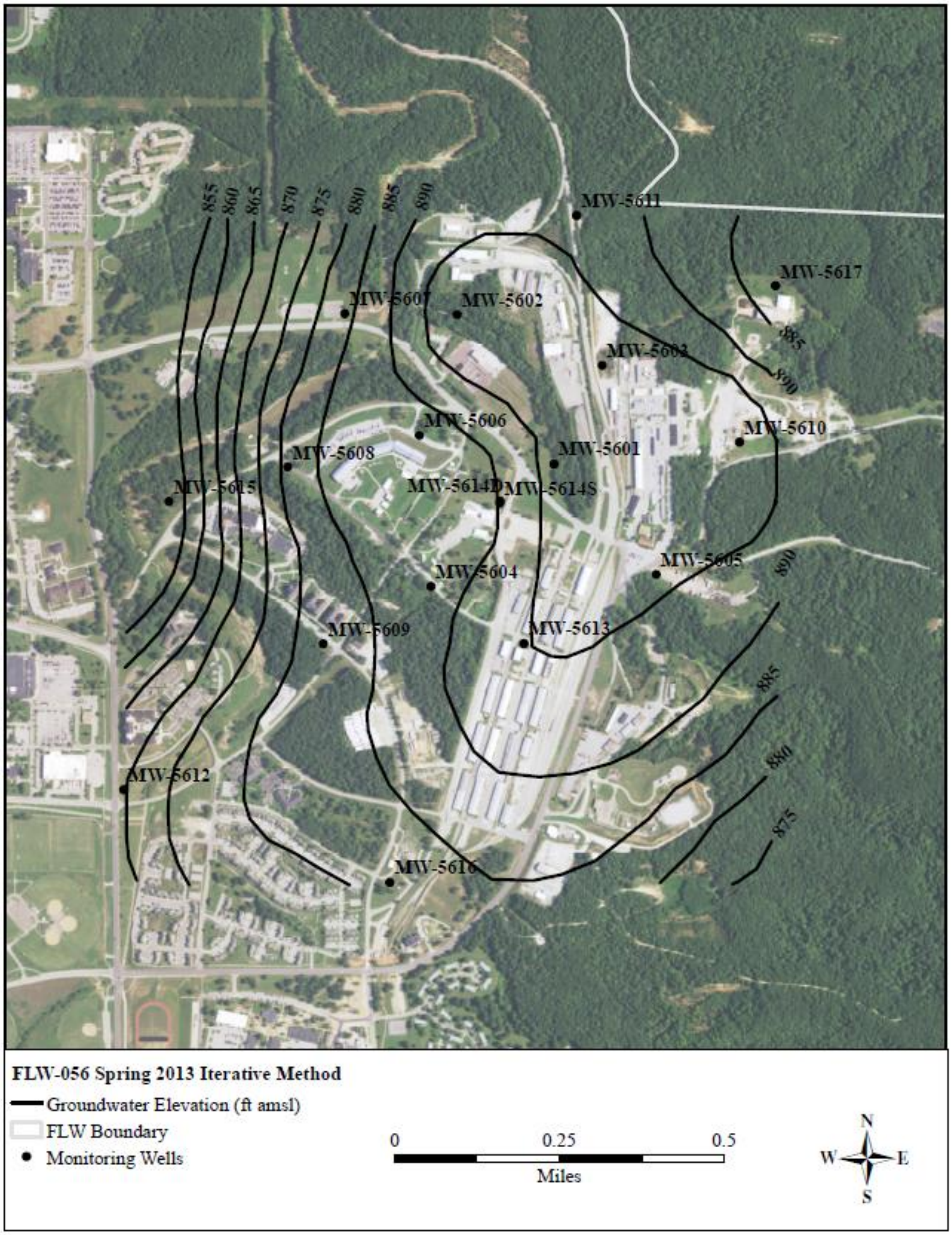
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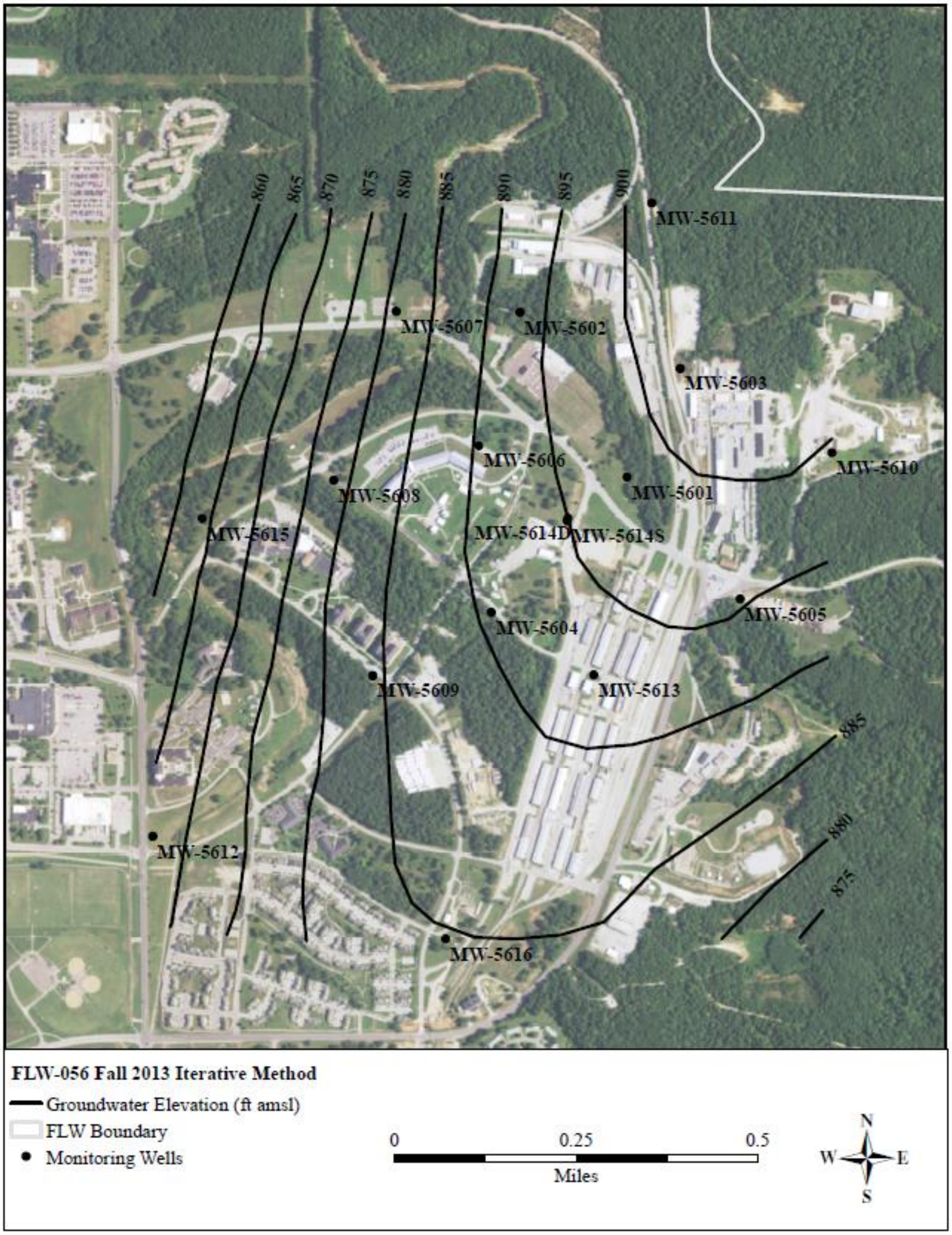
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FLW-056 Fall 2013 Iterative Method
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FLW Boundary
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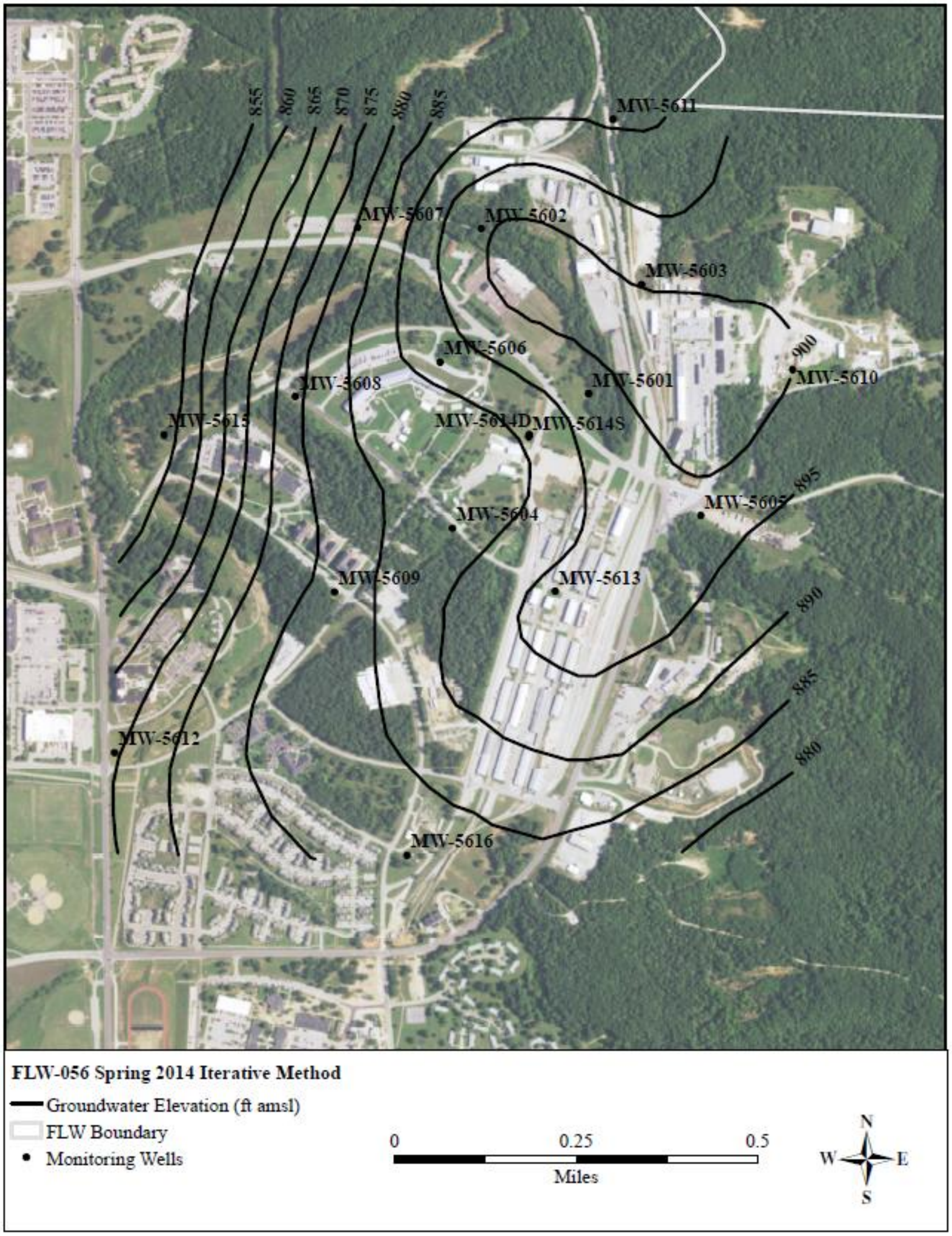
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FLW-056 Spring 2014 Iterative Method
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FLW Boundary
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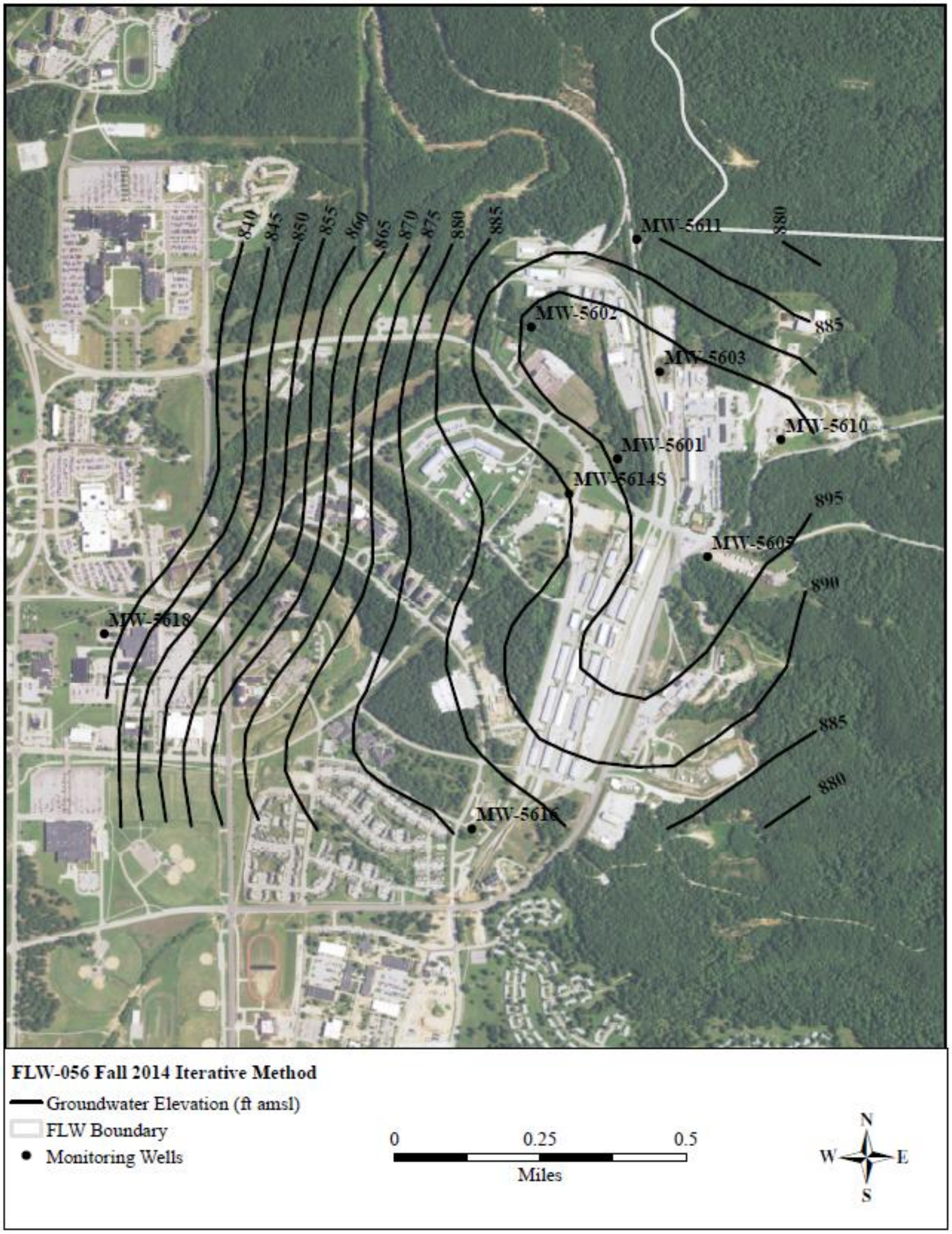
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FLW-056 Fall 2014 Iterative Method
Groundwater Elevation (ft amsl)
FLW Boundary
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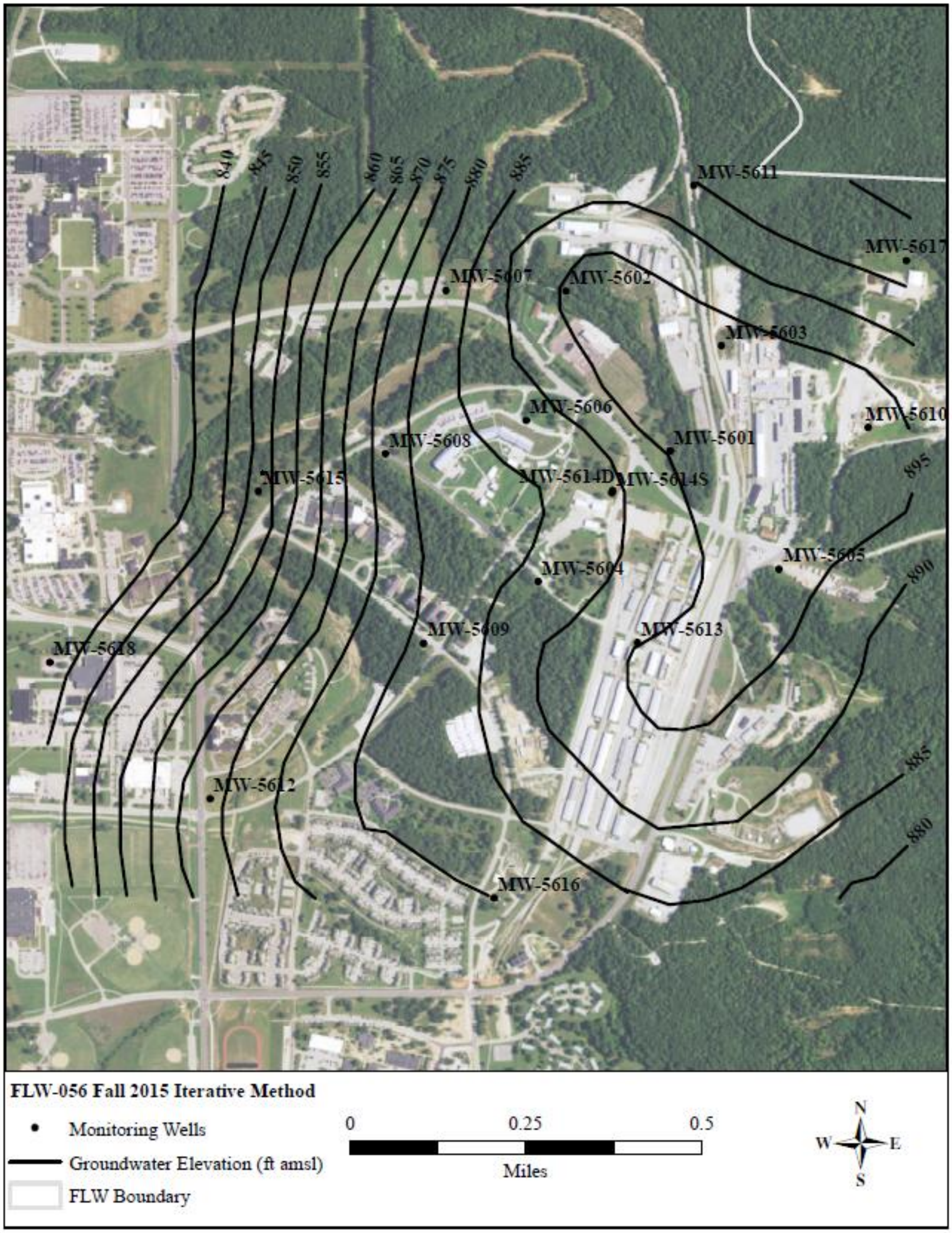
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Groundwater Elevation (ft amsl)
FLW Boundary
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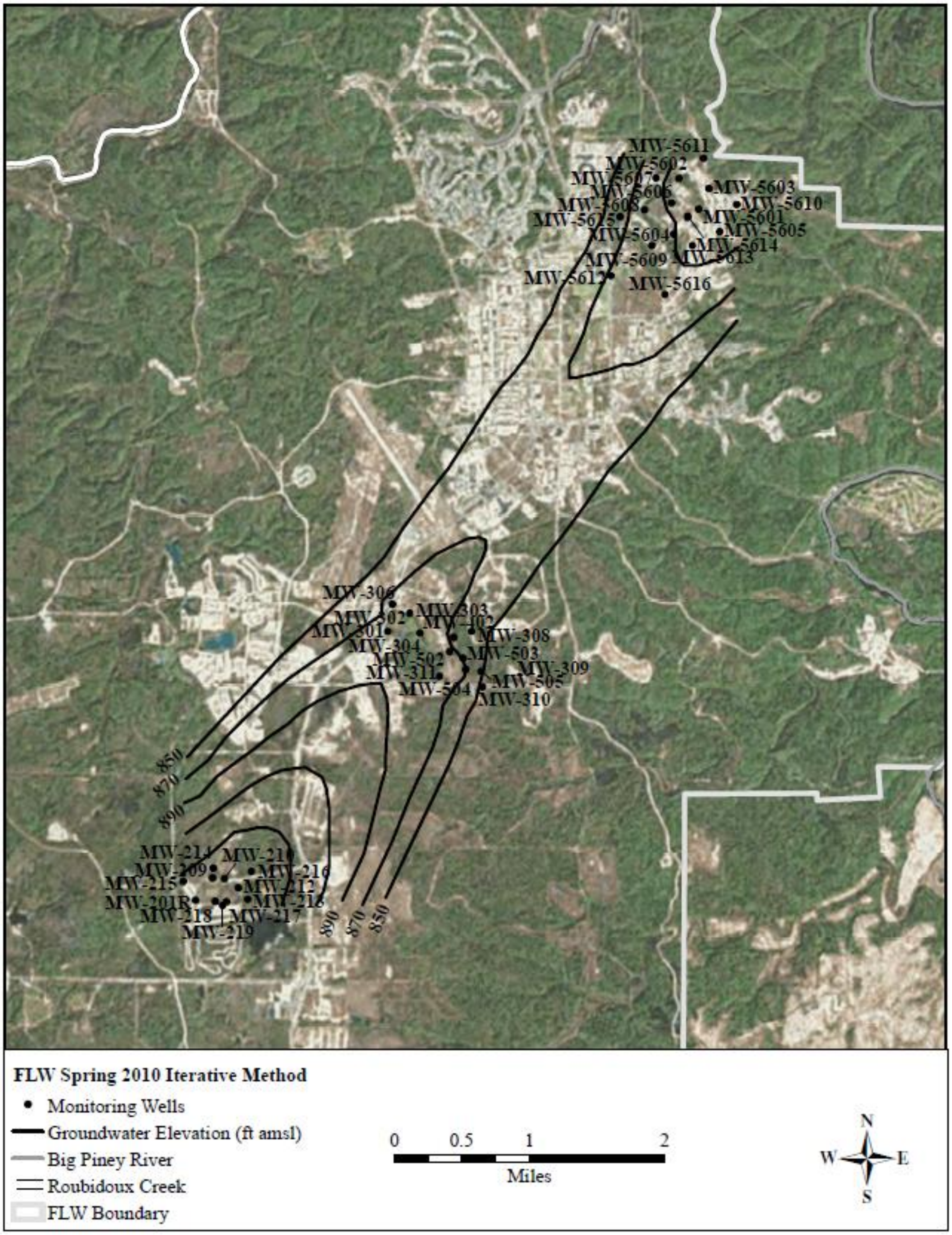
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FLW Spring 2010 Iterative Method
Monitoring Wells
Groundwater Elevation (ft amsl)
Big Piney River
Roubidoux Creek
FLW Boundary
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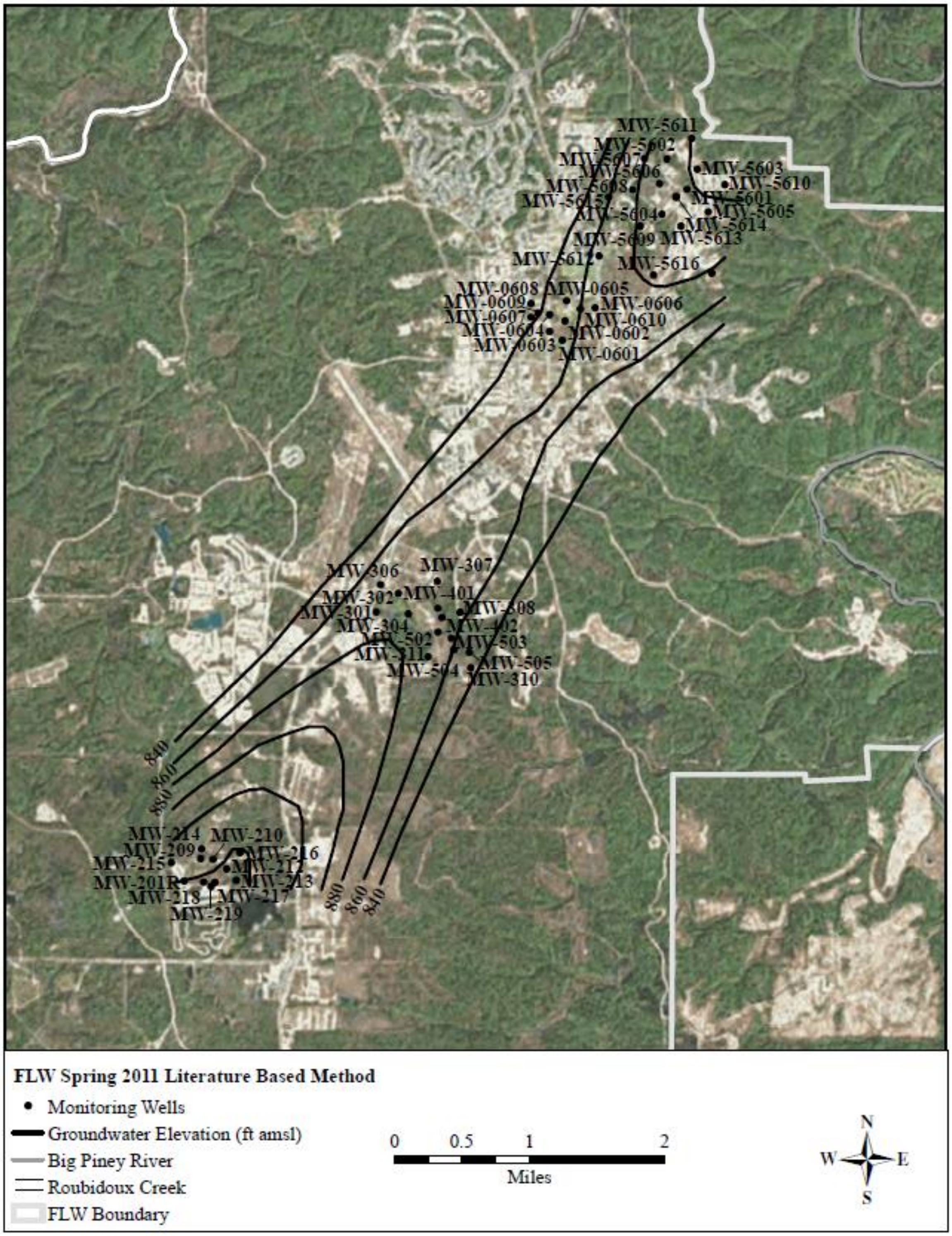
1
2
Miles
N
W
E
S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MW-201R
MW-213
MW-218
MW-217
MW-219
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FLW Spring 2011 Literature Based Method
Monitoring Wells
Groundwater Elevation (ft amsl)
Big Piney River
Roubidoux Creek
FLW Boundary
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Miles
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E
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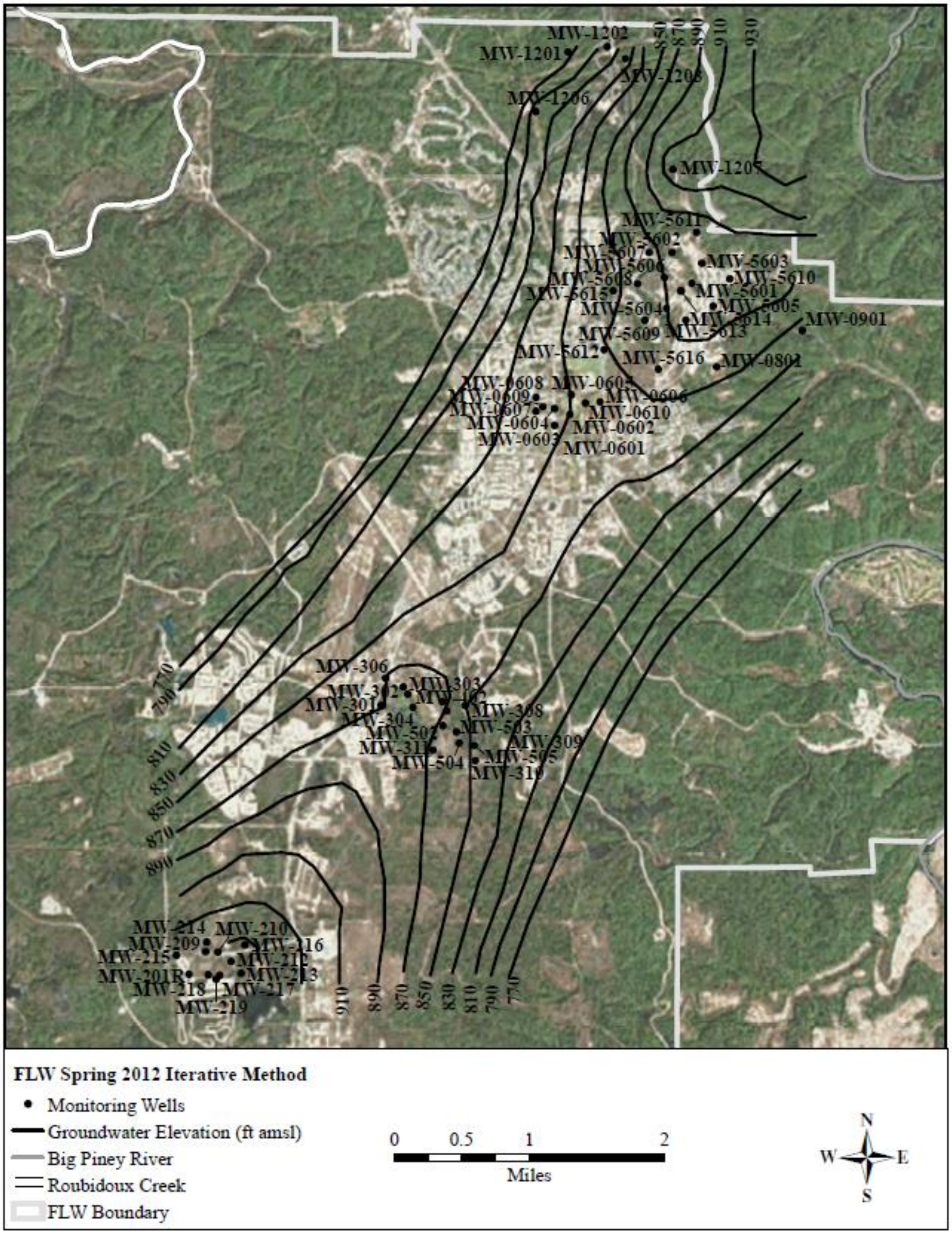
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Monitoring Wells
Groundwater Elevation (ft amsl)
Big Piney River
Roubidoux Creek
FLW Boundary
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Miles
N
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770
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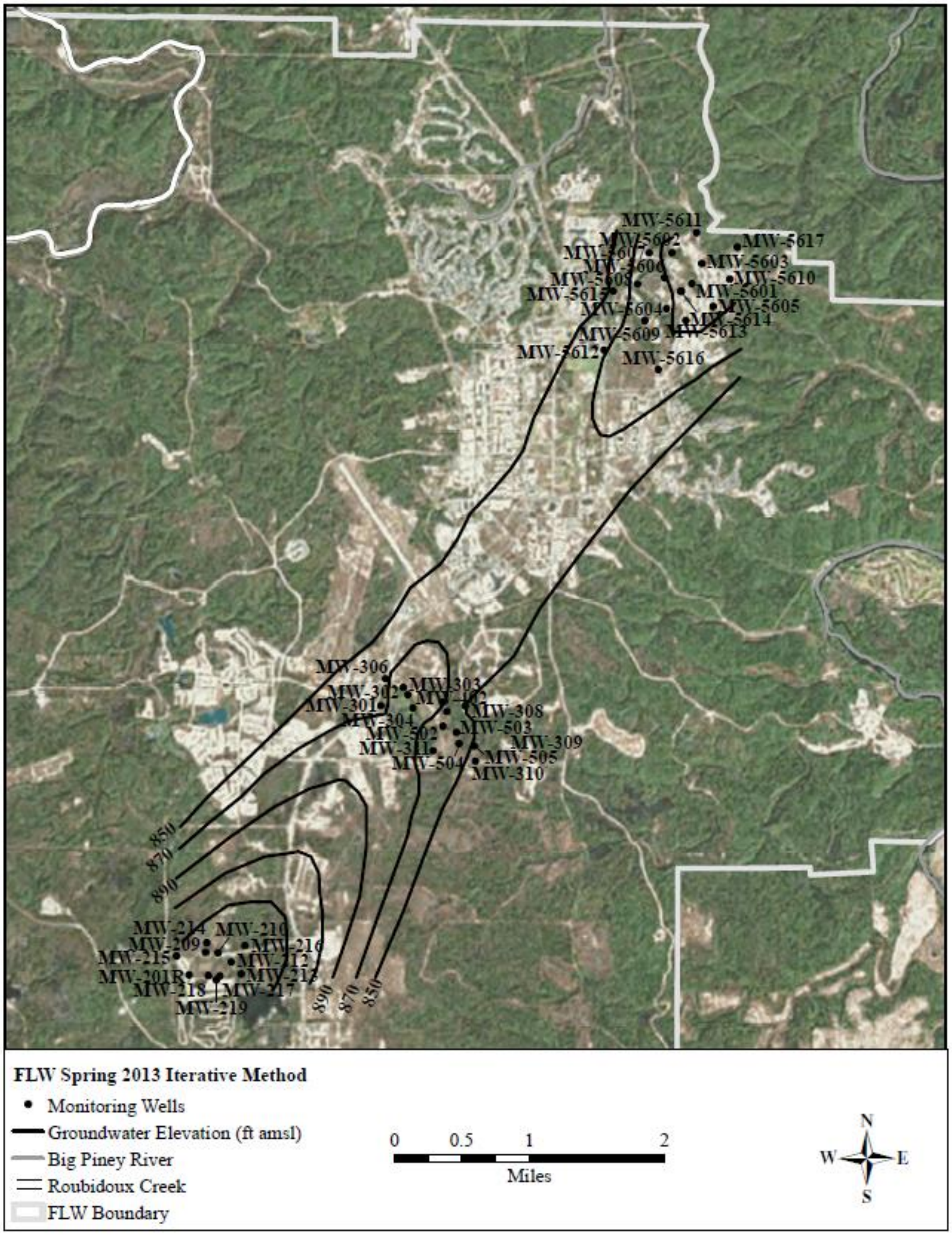
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MW-219
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FLW Spring 2013 Iterative Method
Monitoring Wells
Groundwater Elevation (ft amsl)
Big Piney River
Roubidoux Creek
FLW Boundary
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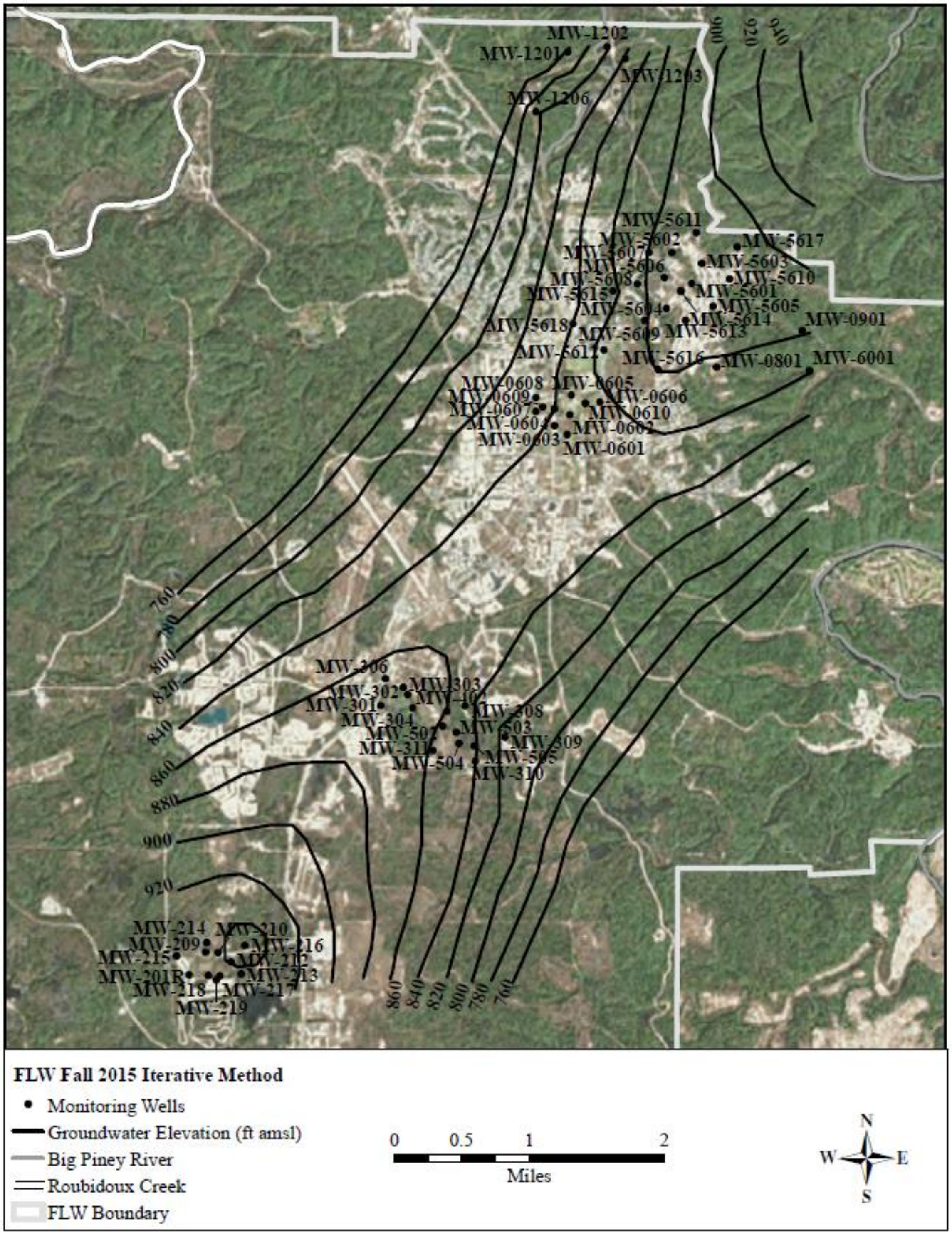
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FLW Fall 2015 Iterative Method
Monitoring Wells
Groundwater Elevation (ft amsl)
Big Piney River
Roubidoux Creek
FLW Boundary
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Miles
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VITA

Rachel Mae Uetrecht was born in Rolla, Missouri to Daniel Uetrecht and Connie Ziegler. Rachel earned her B.S. in Environmental Engineering with a minor in Sustainability in May 2016. In December 2017 she received her M.S. in Geological Engineering from Missouri University of Science and Technology. During her time at Missouri S&T, she was an active member of the Water Environment Federation, Missouri Stream Team, Missouri Water Environment Association, American Society of Civil Engineers, and French Club.

Rachel worked as a research and development intern at American Peat Technology in Aitkin, Minnesota during the summers of 2014 and 2015. She is registered as an Engineer Intern in the State of Missouri and intends to pursue her Professional Engineering license. An extended abstract of Rachel's work has been accepted for the ASCE-EWRI Hydraulic Measurements & Experimental Methods conference