The Hexagon Design

A Flexible Sampling Design for Groundwater Monitoring

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September | 2025

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Introduction And Purpose of Study

As one of its responsibilities, the Division of Environmental Assessment and Restoration (DEAR), of the Florida Department of Environmental Protection (FDEP), monitors Florida's freshwater resources. For reporting on water quality condition at statewide and regional scales, DEAR relies on the Status and Trend Monitoring Program which monitors seven fresh-water resources including unconfined and confined aquifers.

Regarding groundwater, DEAR operates two groundwater-quality monitoring networks: (1) the Trend Network and (2) the Status Network (FDEP, 2024). The Trend Network is currently made up of 49 wells and 2 springs across Florida. Data are predominantly used to determine indicator trends at the sites and to determine temporal variability patterns in groundwater quality. The Status Network (SN), to be discussed shortly, was established by DEAR to monitor the entire state, plus six separate regions (zones) of Florida. However, to date, it has had only limited use in monitoring at the sub-region scale. To address this latter concern, DEAR developed an alternate (Hexagon) design, with emphasis on groundwater monitoring. The purposes of this report are to describe how the Hexagon design works, compare its design to that used by the SN, and to discuss potential uses of the Hexagon design by DEAR and other entities interested in the monitoring of their groundwater resources. The Hexagon design is just one of many potential groundwater monitoring designs. The design is useful for monitoring indicator concentrations in a geographical area over time. For networks intending to use fixed-monitoring locations, it can be used to aid in the determination of the placement of monitoring sites.

Status Network

For the SN, DEAR divided the state into six zones. Zones 1-4 correspond to (1) Northwest Florida Water Management District (NWFWMD), (2) the Suwannee River Water Management District (SRWMD), (3) the St. Johns River Water Management District (SJRWMD), and (4) the Southwest Florida Water Management District (SWFWMD). The South Florida Water Management District (SFWMD) is split into western and eastern halves, corresponding to Zones 5 and 6. Figure 1 depicts the state (study area), plus the six zones.

The SN currently uses a sampling design developed by the U.S. Environmental Protection Agency (EPA); the Generalized Random Tessellation Stratified (GRTS) survey (Stevens and Olsen, 2003). The GRTS design allows the user to randomly select sampling sites and to analyze the resulting data in the R statistical platform (R Core Team, 2023). The various R packages provide several benefits to the user. For example, the user can select the local neighborhood variance estimator, which minimizes the estimate of variance. This results in a stronger ability to detect trends if they are present.

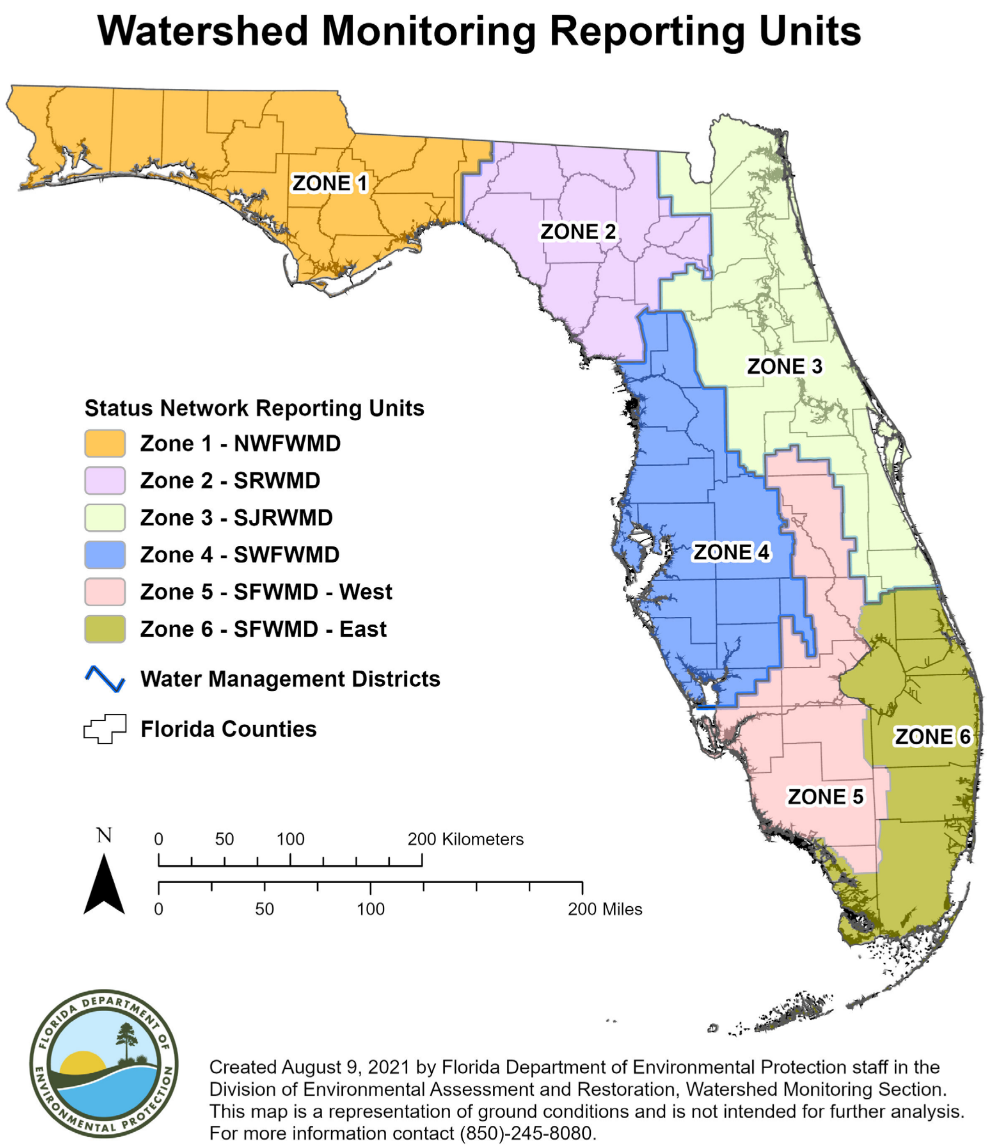

Figure 1. Study Area and Regions (Zones)

The SN is used by DEAR for surface water and groundwater monitoring. Depending on the water resource, the user can address statistical weighting components to be based on: (1) area (e.g. large lakes), (2) lines (e.g. flowing waters), and (3) points (e.g. small lakes and wells). For groundwater monitoring, weighting can be based on either points, or on area. As examples, the user might want to determine the proportion of wells with concentrations of an analyte (e.g. nitrate) exceeding a primary drinking water health standard (e.g. 10.0 mg/L) (Florida Administrative Code 62-550. Alternately the user might want to determine the proportion of area of a water resource that exceeds a threshold.

Regarding groundwater quality trends at the statewide and regional scales, for the past two decades, trend analysis investigations conducted by DEAR have been based on two fundamentally different types of design: spatially balanced and (permanently) fixed station. GRTS uses a spatially-balanced design. For each synoptic sampling period (cycle) of the state or of its zones, monitoring sites are randomly selected for sampling from a list of potential wells. Over the course of several sampling cycles, numerous wells are sampled but each is rarely sampled more than once. In a fixed-station design, the same set of wells and springs are sampled on a periodical basis. Over time each site is sampled numerous times but relatively few sites are sampled

Spatially balanced designs have the advantage of generally resulting in an evenly dispersed distribution of sampling sites over the extent of the resource. In addition, the GRTS method generally produces smaller confidence intervals around the estimated central tendency values such as the mean and median. Unfortunately, partially because of an insufficient number of existing wells, spatially balanced designs such as GRTS are rarely used to monitor areas smaller than zones or WMDs for groundwater. At these latter scales, fixed-station designs dominate. Since spatially balanced and fixed-station designs are both being used by various monitoring entities, DEAR needs to be able to efficiently use, and to be able to instruct other entities to use, either design.

Background Network and Its Relationship with the Status Network

Prior to examining the specifics of the SN, a brief discussion of its predecessor, the Background Network (BN), is in order. The BN was authorized by the Florida Water Quality Assurance Act (Florida Statutes, Chapter 403.603) of 1983. The act directed FDEP, with the assistance of additional governmental agencies, to establish and participate in the operation of a statewide groundwater monitoring network. Major participants included the U.S. Geological Survey (USGS), the Florida Department of Health, the WMDs, and several county agencies. The BN used a fixed-station design to document changes in groundwater quality in areas minimally impacted by human land use activities. Its goal was to compare data obtained in areas of the state, suspected of being contaminated, to the BN. The BN became operational in the late 1980s and began monitoring the state in systematic sampling cycles beginning in 1991. The cycles were: 1991-1993 (BN1), 1994-1997 (BN2), and 1997-1999 (BN3). During these cycles, both FDEP and participating agencies sampled network wells. In addition, numerus laboratories were involved in analyzing the water samples.

Beginning in 1996, a major network redesign was initiated. The purpose was to be able to characterize the overall environmental conditions of the state, not only for groundwater, but also for Florida’s surface water resources. The result was the Status Network. It began operations in 2000. As previously mentioned, regarding groundwater resources, the network is designed to monitor unconfined aquifer (UA) and the confined aquifer (CA) resources. The two resources are based on their susceptibility to pollution. Pollutants originating from land surface, can more readily find their way downward to unconfined aquifers. This is because they do not have overlying confining beds that can retard the downward movement of these pollutants. Thus, they are more susceptible, relative to confined aquifers.

Wells in the SN include BN wells, existing public supply, industrial, agricultural, and other types of wells, plus newly installed wells. Annually, DEAR requests well construction and location information from the WMDs, the USGS, and other monitoring agencies for wells that can potentially be incorporated into the SN. As of 2022, the SN includes more than 38,000 wells. The

SN monitors portions of Florida's aquifers that have the potential for supplying potable water or affecting the quality of currently potable water. To reduce laboratory variance, beginning in the mid-1990s, most of the laboratory analyses were conducted by the FDEP Central laboratory.

The first complete statewide sampling cycle of the SN was 2000-2003 (C01). The second cycle was 2004-2008 (C02). A re-design of the SN occurred in 2009. Since then, the SN has been sampled, statewide, in one-year cycles. Each year about 240 SN wells, split equally between the two resources are randomly selected for sampling. Since 2009, each cycle is referred to as C03-C16. Table 1 lists the network, sample cycle name, the years of the cycle, and the cycle number.

Table 1. Background and Status Network Sampling Cycles.

Network	Sample Cycle Name	Year(s)	Sample Cycle Number
Background (BN)	BN1	1991-1993	1
Background (BN)	BN2	1994-1996	2
Background (BN)	BN3	1997-1999	3
Status (SN)	C01	2000-2003	4
Status (SN)	C02	2004-2008	5
Status (SN)	C03	2009	6
Status (SN)	C04	2010	7
Status (SN)	C05	2011	8
Status (SN)	C06	2012	9
Status (SN)	C07	2013	10
Status (SN)	C08	2014	11
Status (SN)	C09	2015	12
Status (SN)	C10	2016	13
Status (SN)	C11	2017	14
Status (SN)	C12	2018	15
Status (SN)	C13	2019	16
Status (SN)	C14	2020	17
Status (SN)	C15	2021	18
Status (SN)	C16	2022	19

Descriptive statistical summaries of the total depths and total casing depths for UA and CA wells are found in Table 2. Data are based only on wells sampled at least once during the 32-year period (1991-2022). Statistics included the 25th, 50th, and 75th percentiles (P_{25}, P_{50}, and P_{75} respectively). Percentiles are referred to as the 1st, 2nd, and 3rd quartiles (Q1, Q2, and Q3). Q2 is also known as the median. An excellent presentation of descriptive statistics is presented by Triola (2018). The median total depth of those UA wells is 52 ft while the median total depth of CA wells is 200 ft.

Table 2. Descriptive statistics of the depths of Sample Unconfined and Confined Aquifer wells.

	n	[2]Q1	[2]Q2 (Median)	[2]Q3
UA Total Depth ([1]ft)	2557	27	52	100
UA Casing Depth (ft)	2557	18	39	77
CA Total Depth (ft)	2365	127	200	308
CA Casing Depth (ft)	2365	80	130	232

[1]one ft = 0.3048 m

[2]Q1, Med, and Q3 = 25th, 50th, and 75th percentiles respectively

Florida's Aquifer Systems, Aquifers, And Confinement

To fully understand the UA and CA monitoring efforts, one needs to be familiar with Florida's three freshwater aquifer systems (Southeastern Geological Society (SEGS) 1986). From deep to shallow, they are: (1) the Floridan aquifer system (FAS), (2) the intermediate aquifer system (IAS) or intermediate confining unit (ICU), and (3) the surficial aquifer system (SAS). The FAS contains the Lower Floridan and the Upper Floridan aquifer. In parts of Florida, the two are separated by the middle confining unit. In most places, the IAS/ICU behaves as an upper confining unit to the FAS. Thus, depending on location, the FAS can be under unconfined or confined conditions. Where present, aquifers within the IAS are generally confined below and above ty relatively impermeable sediments (the ICU). In northwestern Florida, the major aquifer within the SAS is the sand and gravel aquifer. In southeastern Florida, the major aquifer of the SAS is the Biscayne aquifer. The aquifers within the SAS are almost always under unconfined conditions. The areal distribution of Florida's major aquifer systems is depicted in Figure 2.

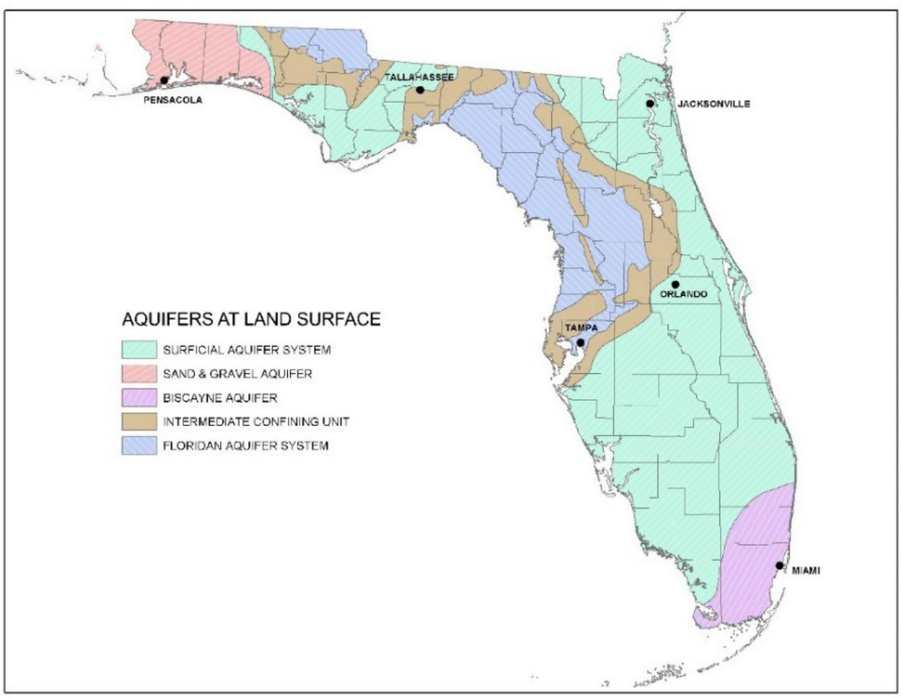

Figure 2. Major aquifer systems and aquifers in Florida. (Modified from Miller (1997) and available at https://fldep.dep.state.fl.us/swapp/Aquifer.asp#.)

The FAS is the most important of the three systems in terms of groundwater extraction. The extent of the FAS across the southeastern United States is in Figure 3. The figure also depicts where: (1) the FAS is under confined conditions and (2) where the FAS is thinly confined or under unconfined conditions. Thinly confined conditions are treated as unconfined.

For detailed discussions regarding the lithologic make up and other aspects of Florida's aquifer systems, several suggested references are Miller (1986), Sprinkle (1989), Scott (2001), Scott, 2016), Berndt et al. (1998), Williams and Kuniansky (2015), and Upchurch et al. (2019). The following abridged version is taken from these references and the SEGS (1986). The FAS is made up of a thick carbonate sequence of rocks. It can be over 2,950 ft (900 m) thick in places. Where it contains freshwater, it is a principal source of water supply. Many of Florida's springs are in areas of the state where the FAS is unconfined or thinly confined (Figure 3). The base of the FAS is the Sub-Floridan confining unit, sometimes referred to as undifferentiated aquifer systems and confining units. These older units contain rocks with significantly lower permeability than the FAS.

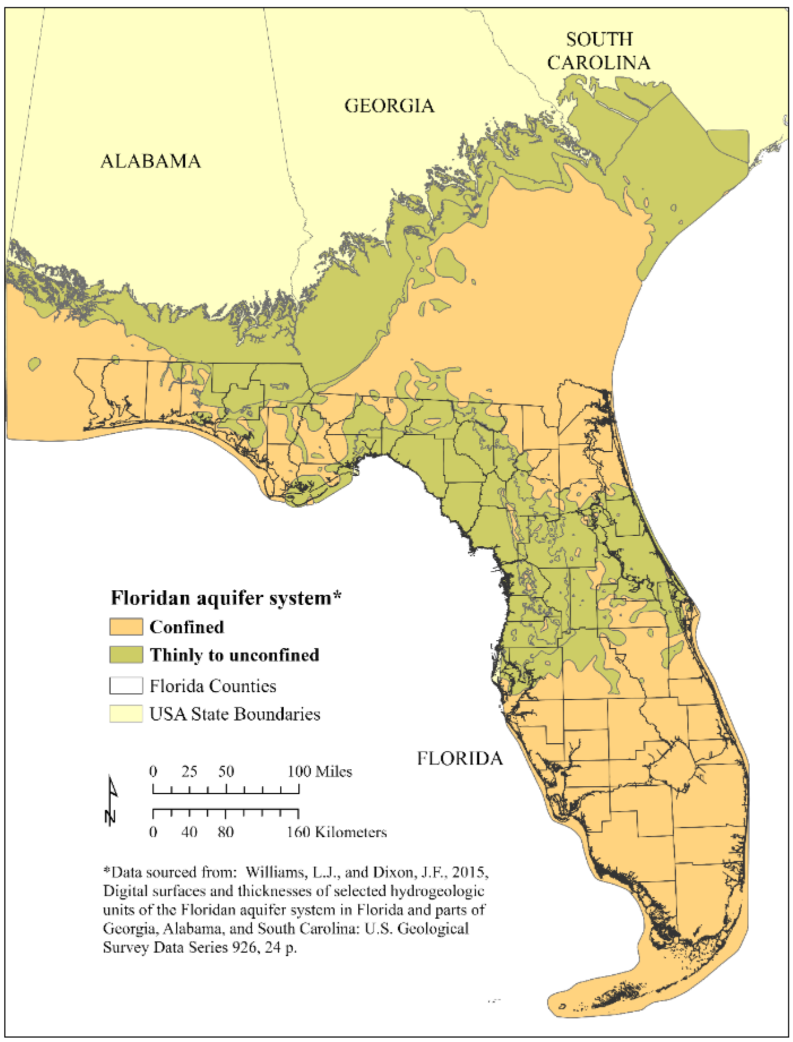

Figure 3. Floridan aquifer system confinement conditions
(Williams and Dixon, 2015).

The IAS and ICU sediments are composed of mostly impermeable sediments. The top of the IAS/ICU occurs at the laterally extensive and vertically persistent lower permeability beds of the unit. The base of the IAS/ICU occurs at the top of the permeable carbonates of the FAS. Beds within the FAS consist of permeable carbonates and siliciclastic sediments, occasionally interbedded with impermeable units. The carbonates and siliciclastic units occasionally exist as regionally limited water-bearing zones (aquifers), where the groundwater is almost always under confined conditions. Where interbedded permeable beds dominate, the term IAS is used. Otherwise, the term ICU prevails.

The SAS is composed mostly of permeable siliciclastic and carbonate sediments, with occasional zones of clayey, less-permeable sediments. In general, sands predominate in northern Florida, while carbonates predominate in the southern portion of the state. The SAS is almost always under unconfined conditions.

Figure 4 is a chart of Florida's hydrostratigraphic units. The figure also displays corresponding formations making up the units.

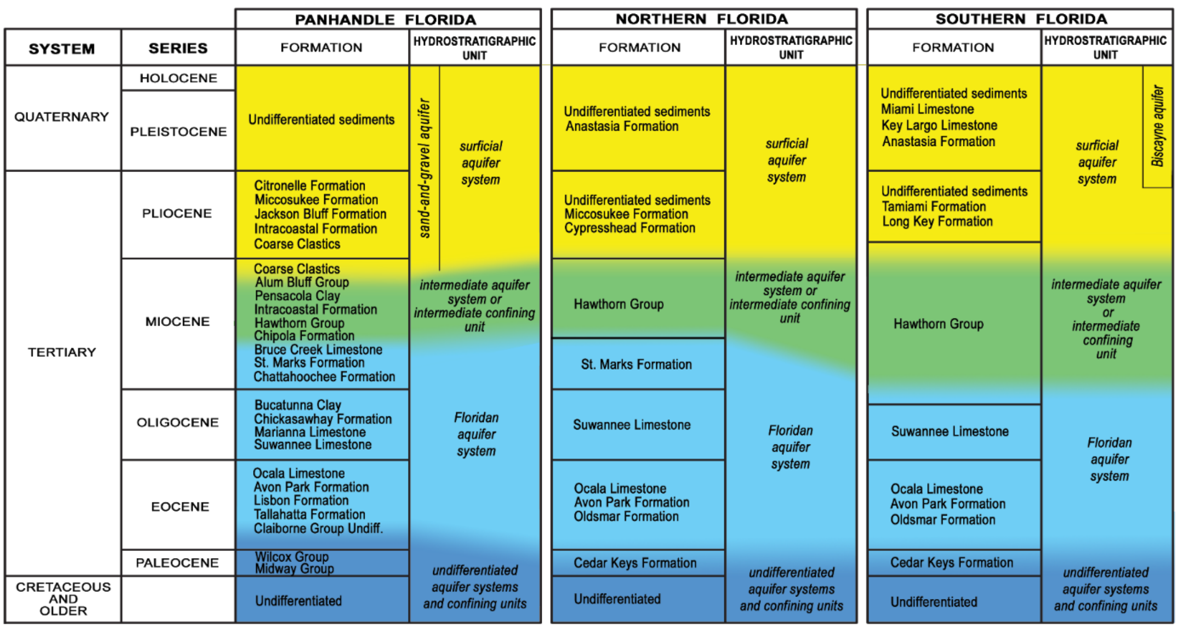

Figure 4. Florida hydrostratigraphic nomenclature chart.
(Modified from SEGS (1986); Upchurch et al. (2019); and Scott (2016).

Materials And Methods

Data Sources, Quality Assurance, And R Scripts

Data were obtained from FDEP's Oracle-based Generalized Water Information System. All sample collection and all field and laboratory analyses were conducted in accordance with Chapter 62-160, F.A.C. Data analyses were conducted with open-source statistical packages in the R programing language (R Core Team, 2023).

Statistical Methods

The distributions of most indicators used in this investigation are positively skewed. They have numerous positive outliers. Some indicator concentrations are often below the corresponding method detection limit. For these reasons, nonparametric statistical methods were often used. Most statistical analyses were conducted in the R programming language platform (R Core Team, 2023). Occasionally, the mean and median values were calculated using Excel® spreadsheets.

Comparison of Monitoring Designs

Introduction

Recall, one purpose of this investigation is to compare two fundamentally different types of monitoring (spatially- and fixed-station) designs and to introduce the reader to the Hexagon design of monitoring, especially for groundwater. As mentioned previously, at geographical areas smaller than WMD, groundwater monitoring networks, almost always, have fixed-station designs. The Hexagon design can be adopted for use at many geographical scales and can be used with both spatially-balanced and fixed-station sampling.

The Hexagon Design

There are several probability-based designs that are often used for environmental monitoring (Gilbert, 1987). The Hexagon uses a simple random sample design, whereas the GRTS design uses a stratified random sample design where each zone represents a stratum. Triola (2018) stated that in a simple random sample, each member (unit) of the population has an equal probability of being selected. Gilbert (1987, p. 24) made a slight change to the definition; a simple random sample assures that each population unit has the same chance of being selected for measurement. For the Hexagon design, imagine a map of equally sized hexagons that is overlain on a map of the area of interest. Regarding groundwater, either wells or hexagons are considered sampling units. The rationale for using hexagons of a pre-determined size will be discussed later.

If wells are randomly selected, the geographic coordinates of each sampled well are assigned to the corresponding hexagon. Since wells are randomly sampled, the corresponding hexagons are also randomly sampled. If more than one well is sampled in a hexagon during a sampling cycle, the mean and/or median value of all samples in the hexagon are used to represent the multiple-sampled hexagon. A disadvantage of the design is that the sample variance, based on the number of sampled hexagons, is greater than that using the number of sampled wells. In addition, the local neighborhood variance estimator, available through the GRITS design, is not available in the Hexagon design.

If hexagons are to be selected, a list of all hexagons containing at least one well must be generated, and a pre-determined number of hexagons must be determined. Hexagons are then randomly selected for sampling. For hexagons with multiple wells, a secondary, random selection process is needed to select only one well in the corresponding hexagon.

Groundwater and Fixed-Station Networks Concerns

Regarding DEAR water-quality monitoring projects, for any design, to obtain a water sample, samplers encounter at least two initial steps prior to sampling. First, samplers must obtain permission from the landowner to collect a sample at the site and, second, samplers must determine if the site can be accessed and in a timely manner. Each step has related labor costs. For spatially-balanced-sampling designs, the labor costs are incurred, repeatedly, during each sampling cycle. Regarding the fixed-station design, the major labor costs of the two steps occur during the establishment of the network. Once established, these two costs are eliminated. Occasional exceptions occur when replacement sites, or “fill-in” sites are added.

Groundwater networks often face an additional potential initial cost; well installation. The GRTS spatially-balanced-sampling design generally assures the distribution of sampled sites represent the distribution of the actual water resource. For example, GRTS assures the distribution of small lakes (sampled as points) mimic the areal distribution of small lakes over a geographic region. Unfortunately, regarding groundwater monitoring, the distribution of existing wells does not necessarily represent the distribution of the underlying aquifers. Regarding confined aquifers, if one were to drill a well deep enough anywhere in Florida, groundwater under confined conditions will eventually be encountered. Regarding unconfined aquifers, almost anywhere in Florida, the uppermost aquifer is under unconfined conditions. Thus, the extent of Florida’s UA and CA resources are closely related to the extent of the area being monitored.

Figure 5 displays the distribution of the currently used UA and CA hexagons for which at least one well has been sampled since 1991. The figure shows that over most of Florida, the distribution of sampled hexagon is good. Nevertheless, even after sampling over 9,000 individual wells since the early 1990s, there are many hexagons which have never been sampled. If groundwater samples are needed in the unsampled hexagons, the only way to obtain a sample is to: (1) continue searching for existing wells or (2) install new wells. Often, well installation is cost prohibitive. In addition, if the monitoring entity does install a monitoring well, it will probably want to sample the well multiple times during the life of the well. Thus, the entity is more likely to use a fixed-station design, rather than a spatially-balanced design.

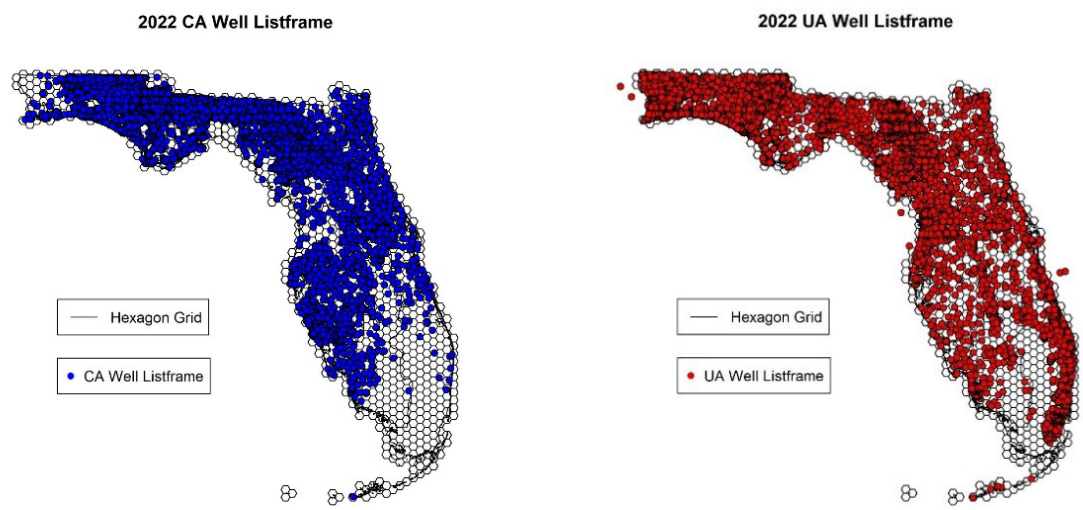

Figure 5. Hexagons with at least one sampled CA or one sampled UA well since 1991. Note, wells in several hexagons for the UA are incorrectly located.

Autocorrelation and Hexagons

All environmental monitoring networks need to be able to address: (1) serial and (2) spatial autocorrelation (AC) (Helsel and Hirsch, 2002). The presence of either type of AC is, in part, analogous to obtaining a duplicate sample and treating the duplicate as an independent sample. AC can potentially, and adversely, affect trend analysis test results by incorrectly lowering the p-value (Yue et al., 2002; Dale and Fortin, 2002).

Note, the Hexagon design only addresses spatial AC. Serial AC can be addressed during the data analyses. For detecting the presence of serial AC, see Gilbert (1987), Helsel and Hirsch (2002), Pankratz, (1983) and Box and Jenkins (1970). For addressing serial AC if present, see Hirsch and Slack (1984), Helsel and Franse (2006), and Millard and Neerchal (2001).

Regarding spatial AC, imagine that two wells are located very close to each other (e.g. 10 ft). Both wells are identically constructed. If one were to obtain a water sample from each well for, say, chloride (Cl), one would expect Cl concentrations from each sample to have concentrations very similar to each other. Over time, if the wells are periodically sampled at the same times, one would expect the variability in Cl concentrations from the corresponding well samples to be small, and the correlation in chloride concentrations to be high. Now, suppose the two wells were located 300 ft from each other. One expects the variability in the concentrations between each corresponding pair of Cl samples to be greater than if the two wells were only 10 ft apart and the corresponding correlation to decrease. If the distances between the two wells continues to increase, it is reasonable to assume that a certain distance is reached, concentrations in the two wells have no relationship with each other. That is, concentrations become independent of each other and the correlation in chloride becomes insignificant. This distance at which concentrations become independent is referred to as the range (Bras and Rodriguez-Iturbe, 1985). Ideally, for any groundwater monitoring network, wells are located at distances equal to or greater than the range. If not, autocorrelated samples can be the result. One can think of autocorrelated samples as being duplicates of each other. Since AC can potentially affect the results of trend tests, the effects of AC should be eliminated, or at least minimized.

To find the range, a structural analysis exercise is often performed (Bras and Rodrigues-Iturbe, 1985). When it is used, the analysis is informally referred to as "Kriging". The name is from Daniel Krige (Krige, 1951) who invented the procedure. To understand how to conduct such an analysis, semivariance is often of interest. In geostatistics, semivariance is simply half of the variance of the differences between all possible points spaced a constant distance apart. For a formal mathematical definition of semivariance, see Bras and Rodreguez-Iturbe. Figure 6 is an example of a semivariogram (ESRI, 2024), where semivariance is plotted on the y-axis and distance is on the x-axis. In the figure, semivariance levels off at the range, about 2.122 x 10^5 meters.

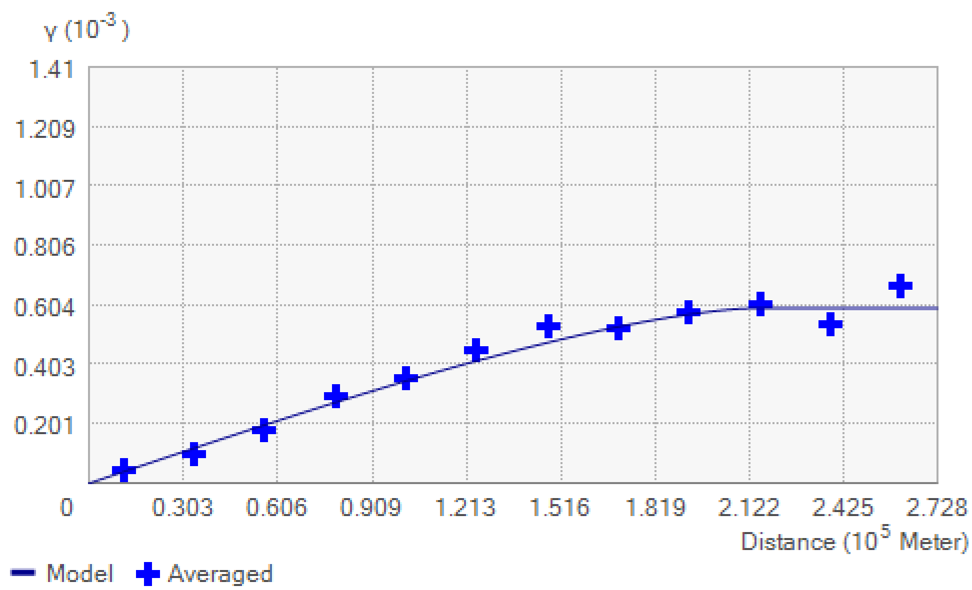

Figure 6. Example Variogram (ESRI, 2024) Comparing Semivariance to Distance.

Many of the concepts used to develop the current Hexagon design are based on the work of Boniol (2002) and Boniol and Toth (1999). To address spatial AC, Boniol conducted a Kriging exercise using the conservative chemical chloride to determine the distance at which spatial AC is reduced sufficiently within the St. Johns River WMD (SJRWMD) (Figure 1). Chloride was used because it is neither involved in major precipitation or dissolution reactions under conditions found within the Floridan aquifer system (FAS) (Boniol and Toth, 1999). Boniol determined the range to be 50,000 ft (15,240 m). Using a geographical information system (GIS) tool, Boniol overlaid a hexagon grid over a map of the district. Each hexagon had a diameter of 50,000 ft (15,240 m). The SJRWMD staff then used the hexagons to aid in the placement monitoring wells in a districtwide network.

Copeland and Woeber (2021) built on the work of Boniol (2002) but did not conduct a Kriging exercise. They used an ArcGIS script tool for creating Thiessen hexagons that was obtained from the Center for Research in Water Resources, University of Texas at Austin (Whiteaker, 2015). Copeland and Woeber (2021) used all Background Network wells, tapping the FAS, that were sampled across Florida for chloride during the period (1991-1997). Distances between each pair of wells were determined and the distances were grouped into three categories: (a) <50,000 ft, (b) 50,000 - 100,000 ft, and (c) greater than 100,000 ft. Within each distance category, for each well (w) pair, chloride concentrations were compared. For example, in the <50,000 ft category, comparisons were observed; w1 to w2, w1 to w3, …wn; w2 to w3, w2 to w4, …w2 to wn; and so on. The process was repeated for the 50,000 to 100,00 ft category, and then for the >100,00 ft category. Within each distance category, Pearson correlations (Triola, 2018) in the chloride concentrations between wells pairs were determined. It was found that correlations were significantly reduced or statistically eliminated in the latter two distance categories. The same exercise was repeated for Background Network wells, but for the period 2005-2011. Again, it was observed that correlations were reduced significantly or statistically eliminated at distances >50,000 ft. This was their basis for using 50,000 ft. hexagons for the Hexagon design for use at both regional and statewide scales. However, in the future, groundwater monitoring networks are established using the Hexagon design at different area scales than zonal or state, the determination of corresponding ranges will need to be completed.

The hexagon diameters used in the investigation were designed for the FAS. However, wells in the study also include those tapping the IAS and the SAS. Although separate Kriging, or analogous exercises, were not performed for the IAS and SAS, a series of tests comparing the results of the GRTS to the Hexagon design were performed. The results, to be discussed later, indicate that the GRTS and Hexagon design produced comparable statewide and zonal results. This fact supports the idea that the 50,000 foot-diameter hexagons adequately address spatial AC at the state and regional scales for all three of Florida's aquifer systems.

A total of 1173 hexagons were used to cover the entire state. During 19 sampling cycles of the BN/SN, the number of sampled hexagons per cycle ranged from 97 to 384. One can think of the state in three dimensions, where the hexagons represent area (two dimensions), and sampling cycles are stacked on top of each other in time (a third dimension). Spatially, each hexagon represents an independent cell. In the time dimension, analytical procedures were used to assure serial independence.

Comparison of GRTS And Hexagon Designs' Results

Having established the Hexagon method of analyzing data, a question arises. How does the Hexagon design compare to the GRTS method?

Using the Status Network data, comparisons of Hexagon-generated means (and medians) were compared to GRTS-generated means and medians. The GRTS design generates central tendencies for each zone based on a series of unequal weighting factors. It estimates statewide means/medians by using weights based on the size of each reporting unit; zone or stratum. Weighting is essentially based on number of wells per zone (points). However, it can also generate statewide mean/median estimates based on the area of each zone. The Hexagon design uses the equal-area weighting of hexagons to generate zonal and statewide means. To compare GRTS to Hexagon results, requires the areas of each zone. A. Woeber (FDEP), personal communications, supplied the areas (Table 3) to the author. The area units are hectares.

Table 3. Areas of Florida and Each Water Management District.

Region	Area (Hectares)	Proportion of Area of Florida
Zone 1	2,892,895	0.1982
Zone 2	1,957,948	0.1342
Zone 3	3,037,845	0.2082
Zone 4	2,532,564	0.1735
Zone 5	2,091,404	0.1433
Zone 6	2,081,725	0.1426
State	14,594,381	1.0000

To compare the results of the two designs, a brief discussion of confidence intervals (CIs) is needed. Triola (2018) defined a CI as a range of values that are likely to contain the true value of a population parameter. Suppose a random sample is collected, and for the sample, the confidence interval of the central tendency (mean or median) is set at 95%. For an infinite number of future randoms samples, the true value of the mean (or median) will fall within the CI, 95% of the time. Using this logic, the objective of this investigation is to determine if 95% of sample mean (or median) values produced by the Hexagon design fall within the 95% CIs of the corresponding means/medians generated by a GRTS method. Data collected during 2021 were used. Since the two sets of data used were identical, it is assumed that at least 95% of the Hexagon means (and medians) will, indeed, fall within the CIs of GRTS means. However, if differences are observed, it indicates the weighting factors and/or spatial AC influenced the results. If no differences are observed, it indicates that the two methods' weighting factors produce results that do not differ significantly. It also supports the concept that the 50,000-foot hexagons effectively address spatial AC within the SAS and/or the IAS.

The GRTS method is a stratified random sample (Stevens and Olsen, 2003). For a simple random sample, Triola (2018) stated that the equation used to estimate the grand mean of the various aggregated strata means is the weighted mean formula:

$$wt(\bar{x}) = \Sigma(wt \cdot x)/\Sigma(wt)$$

where, x = stratum mean, wt = weight, and $wt(\bar{x})$ = weighted strata mean (or grand mean). It can be generated using the "stat" package in R (CRAN, 2023).

The weighted median formula is more complex. For a discussion, see Cormen et al., (2001). It can be generated using the "weighted.median" command the "spatstat" package in R. The GRTS method calculates both the statewide weighted mean and weighted median for each indicator for each sampling cycle. As previously mentioned, the weights of both central tendencies can be based on either area or, for groundwater, the number of well in each strata (zone). For the statewide exercise weights are based on the areal proportion of each zone, relative to the area of Florida.

Twelve indicators were selected for analysis for the year 2021 (Table 4) for analyses, using both UA and CA resources. The 12 indicators were selected to represent subsets of nutrient, rock, saline, and field indicators.

Results regarding weighted statewide means are displayed in Table 4a, while results of medians are in Table 4b. The indicator is in column 1. Columns 3 and 4 list the statewide UA GRTS-generated and the Hexagon-generated central tendencies. Columns 2 and 5 contain the lower and upper 95% confidence bounds of the GRTS-generated central tendencies for the UA resource. Columns 7 and 8 list the statewide central tendencies for the CA resource. Columns 6 and 9 contain the lower and upper 95% confidence bounds of the GRTS-generated central tendencies for the CA resource. A total of 48 comparisons were made using the 2021 data (12 UA means, 12 UA medians, 12 UA means, and 12 CA medians). Of the 48 comparisons, all (100%) of the Hexagon-generated means (Table5a) and medians (Table 4b) fell within the CIs of the GRTS-generated central tendencies at the statewide scale.

Table 4a. Comparison of 2021 Unconfined and Confined Statewide Means from the GRTS and Hexagon Methods based on area, for 12 Selected Indicators.

Analyte	UA[1] LCB[3] GRTS Mean	UA GRTS Mean	UA Hexagon Mean	UA UCB[4] GRTS Mean	CA[2] LCB GRTS Mean	CA GRTS Mean	CA Hexagon Mean	CA UCB GRTS Mean
NH3	0.224	0.489	0.409	0.753	0.212	0.242	0.247	0.271
Ca	61.517	72.832	74.369	84.148	73.219	83.56	79.516	93.902
Cl	142.171	342.408	344.707	542.645	217.805	413.863	344.817	609.921
Mg	11.681	25.443	27.214	39.205	29.455	40.761	38.585	52.067
NOx	0.214	0.918	0.905	1.622	0.082	0.154	0.225	0.226
DO	1.466	1.88	1.853	2.293	0.666	0.897	0.764	1.128
pH	5.991	6.12	6.236	6.249	7.15	7.261	7.281	7.372
P	0.073	0.142	118	0.212	0.041	0.069	0.088	0.096
K	2.657	6.518	7.169	10.38	5.148	8.387	7.578	11.626
Na	73.734	181.856	187.17	289.978	119.271	223.056	186.649	326.841
SO4	29.607	68.155	60.629	86.704	80.096	106.855	91.921	133.615
Temp	23.918	24.224	24.194	24.529	23.426	23.619	23.612	23.812

[1] = Unconfined Aquifer with sample sizes: GRTS 117, Hexagon 109. [2] = Confined Aquifer with sample sizes: GRTS 120, Hexagon 103). [3]LCB = Lower confidence bound. [4]UCB = Upper confidence bound.

Table 4b. Comparison of 2021 Unconfined and Confined Statewide Medians from the GRTS and Hexagon Methods based on area, for 12 Selected Indicators.

Analyte	UA[1] LCB[3] GRTS Median	UA GRTS Median	UA Hex Median	UA UCB[4] GRTS Median	CA[2] LCB GRTS Median	CA GRTS Median	CA Hex Median	CA UCB GRTS Median
NH3	0.038	0.061	0.07	0.1	0.109	0.2	0.205	0.251
Ca	32.256	59.415	64.7	74.116	53.035	62.247	62.1	69.868
Cl	10.602	14.2647	12	19.517	12.76	18.13	19	20.565
Mg	2.272	3.349	3.77	3.986	11.23	13.667	13.5	18.922
NOx	0.05	0.05	0.05	0.05	0.004	0.05	0.05	0.05
DO	0.282	0.467	0.48	0.628	0.148	0.178	0.18	0.237
pH	6.347	6.615	6.69	6.766	7.232	7.272	7.27	7.323
P	0.032	0.041	0.037	0.053	0.013	0.019	0.019	0.024
K	0.945	1.194	1.2	1.785	1.161	1.504	2	2.856
Na	6.228	9.478	7.5	12.584	10.006	11.93	14	15.743
SO4	4.175	7.142	6.6	10.412	6.446	11.406	13	16.833
Temp	23.552	24.985	24	24.603	23.212	23.463	23.8	23.947

[1] = Unconfined Aquifer with sample sizes: GRTS 117, Hexagon 109. [2] = Confined Aquifer with sample sizes: GRTS 120, Hexagon 103). [3]LCB = Lower confidence bound. [4]UCB = Upper confidence bound.

To compare zonal results, comparisons were again made using the 2021 central tendencies. Table 5 lists the number of sampled wells and sampled hexagons for each of the six zones. However, because of the relatively large number of zonal comparisons, only six indicators were used. They are listed in Tables 6a and b. Table 6a displays the results for the UA and the CA for the zonal means. Whereas Table 6b displays the results for the UA and the CA for the zonal medians. The indicators are listed in Column 1 of both tables. The number of comparisons, the number of successes, and the percentage of successes for the UA are found in columns 2-4 for both tables. The number of successes, and the percentage of successes for the CA indicators are found in columns 5-6 of both tables. Using Temp as example in the UA, the six means (one per zone) generated by the Hexagon design, were compared to the 95% confidence bound of the corresponding GRTS-generated means. For each zone, if the Hexagon-generated central tendency fell within the lower and upper confidence bounds of the GRTS-generated central tendency, it was considered a success. In the UA, all six zonal comparisons of means for Temp were successful. Including all six selected analytes, 35 of the 36 comparisons of means were successful.

Including both means and medians, for 2021 in the UA resource, a total of 72 comparisons were made. Of these 71 central tendencies of the Hexagon were within the GRTS generated CIs (98.61%). For the CA resource for means and medians, again 72 comparisons were made. Success was achieved 68 times (94.44%). The grand total was 139 successes of 144 comparisons (96.53%).

Table 5. Number of sampled wells and sampled hexagons per zone in 2021.

Zone	Unconfined Aquifer Wells	Unconfined Aquifer Hexagons	Confined Aquifer Wells	Confined Aquifer Hexagons
Zone 1	20	14	20	18
Zone 2	20	19	20	16
Zone 3	19	17	20	20
Zone 4	19	19	20	19
Zone 5	20	20	20	17
Zone 6	19	15	20	13

Table 6a. Comparison of Zonal Means from the Hexagon and GRTS Methods based on area, for 2021 Selected Indicators. (N = number of zones, Success = number of successful comparisons in the six zones)

Indicator	N	UA Mean Success	UA Mean % Success	CA Mean Success	CA Mean % Success
NH3	6	6	100	6	100
NOx	6	6	100	5	83.33
DO	6	6	100	6	100
pH	6	5	83.33	5	83.33
TP	6	6	100	6	100
Temp	6	6	100	6	100
Total	36	35	97.22	34	94.44

Table 6b. Comparison of Zonal Medians from the Hexagon and GRTS Methods based on area, for 2021 Selected Indicators. (N = number of zones, Success = number of successful comparisons in the six zones)

Indicator	N	UA Median Success	UA Median % Success	CA Median Success	CA Median % Success
NH3	6	6	100	6	100
NOx	6	6	100	5	83.33
DO	6	6	100	6	100
pH	6	6	100	6	100
TP	6	6	100	5	83.33
Temp	6	6	100	6	100
Total	36	36	100	34	94.44

What if the GRTS weighting was changed to the number of wells per stratum and the statewide central tendencies were then compared to the Hexagon statewide central tendencies, based on area? We would expect a difference. Results are found in Table 7. The type (area to area compared to number of wells to area) is listed in column 1. The number of comparisons, the number of successes, and the success rate are found in columns 2-4. Comparing the results of GRTS design, based on area, to the results of the Hexagon design, based on area (row 2), indicates the two designs produce comparable results. All 24 (100.00%) of the Hexagon-generated means fell within the 95% confidence intervals of the GRTS-generated means, when the weighting factor of both designs were based area. However, when the results of the Hexagon design, based on area, were compared to the results of the GRTS design, based on the number of wells, differences were observed. Only 7 of 24 (29.17%) of the Hexagon-generated means fell within the GRTS-generated confidence intervals. Then a comparison was made between the two percentages. Using the two-sided proportions test (Triola, 2018), the resulting p-value is 0.646×10^{-7}.

Conducting statewide trend analyses using the number of wells per stratum as weights will produce different results than analyses using areas per stratum as weights. Either method is valid. However, the two methods represent different perspectives of monitoring. If, in the future, DEAR wants to conduct statewide trend analyses, based on area, it has two options. The easiest way is to simply use the GRTS design and the area of each stratum (Table 3) as weights. However, an alternative is the Hexagon design.

Table 7. Comparison of Statewide Central Tendencies for Select Indicators

Comparison of UA and CA Resources	Number of Comparisons	Comparisons within 95% CI	Percent within 95% CI
Compare GRTS Central Tendencies (Weight by Area) to Hexagon Central Tendencies (Weight by Area)	24	24	100
Compare GRTS Central Tendencies (Weight by Well) to Hexagon Central Tendencies (Weight by Area)	24	7	29.17

Conclusions

An overall general comparison of the two designs was conducted. Emphasizing groundwater monitoring, the conclusions are as follows:

1. The GRTS design calculates zonal means (and medians) based on a series of unequal weighting factors and a tessellation procedure which addresses spatial AC issues. As currently used, the method estimates statewide central tendencies using weights based on the number of wells (points) in each zone. If needed, it can use the area of each zone as a weighting factor. The Hexagon design calculates both zonal and statewide means (and medians) based on equally weighted areal hexagons. It addresses spatial AC by using hexagons of a predetermined diameter. To determine the appropriate hexagon diameter requires an upfront structural analysis exercise to determine the range at which spatial AC is significantly reduced or becomes insignificant.

2. The GRTS design is a stratified random sampling design. The user can select the local neighborhood variance estimator option to reduce variance. The Hexagon design uses a simple random sample design. The estimate of population variance using the Hexagon design will be greater than using a stratified random sample (Thompson, 2002). The Hexagon design does not have the advantage of reducing variance using the local neighborhood variance estimator.

3. The GRTS design is a spatially balanced design. The upfront costs needed to obtain access to landowner property and determine if the site can be accessed in a timely manner, over the long term, can be extensive. The Hexagon design is easily adaptable for both spatially balanced and fixed-station designs. For fixed-station designs, the upfront costs are only encountered during the network installation process, and during periodic replacement-well efforts. However, well installation costs can be high.

Potential Uses of the Hexagon Design with Fixed Stations

An example at the springshed scale is presented to demonstrate how the Hexagon design can be useful to DEAR whenever it needs to monitor groundwater quality using fixed-stations. The Hexagon design is useful when the primary interest is to determine changes over time over a geographical area.

Establishment of a Spring Basin Network

FDEP has the authority to declare a spring, or other waterbody, to be impaired (Chapter 62-303, Florida Administrative Code). If so, DEAR has the responsibility to lead the efforts to restore it. This may be accomplished through a Basin Management Action Plan (BMAP) or a Total Maximum Daily Load (TMDL) (Chapter 62-304, Florida Administrative Code). The BMAP represents the "blueprint" for restoring the water quality of the basin. The TMDL is a tool for providing a target load for pollution reduction.

DEAR works with other governmental agencies and the public to enact a BMAP restoration plan, which includes a monitoring plan. If the Hexagon design is to be used, one of the first steps is to determine the range at which spatial AC becomes insignificant. This can be accomplished by a kriging (Bras and Rodrigez-Iturbe, 1985). Note, the range only represents the minimum distance at which spatial AC becomes independent. Using hexagon diameters larger than the range will result in fewer hexagons over the area of interest but potentially increases confidence intervals of the results. Once the hexagon diameter is determined, overlay a hexagon map on the area of interest. The hexagons represent primary areas for the establishment of network wells.

Note, as is often the case, point sources of pollution will be of interest and there is often an interest in establishing one or more wells around the pollution source. The use of these point-source wells in the Hexagon design is not discouraged. For the sake of accounting, label these wells (e.g. point source wells). Data from the point source wells can be used during trend analysis. Examples will be presented shortly.

Regarding the analysis of the point source wells in the Hexagon design, the data analyst can: (1) opt to treat each set of point source wells as separate, mini monitoring networks or (2) include each point source well as any other well in the Hexagon design. That is, calculate the corresponding hexagon mean (or median) using data from all wells in the hexagon. It is a case-dependent decision.

In designing a groundwater network a decision will need to be made regarding the use of existing wells, and the installation of new wells for the network. A goal should be to fill in as many hexagons as practical with at least one monitoring well. Decisions regarding the use of existing wells are often based on the well construction information, such as its total depth, depth of casing, or casing material. Each may ultimately disqualify the well for use in the network. Decisions regarding well installation are often based on economic decisions.

Gap Analysis

Suppose an existing fixed-station network has been in operation for a time and the operators of the network recognize gaps in the distribution of wells. They decide additional wells are needed. If it has not already been completed, conduct an exercise to determine the range. Produce a corresponding hexagon map and overlay the map on a map of the area of interest. If hexagons are missing wells, they represent priority areas for additional wells. The range determination exercise is a one-time effort. Thus, the hexagons are useful for the lifetime of the network.

The Alachua County Environmental Pollution Department (ACEPD) (2023) used the Hexagon design in a gap analysis of their groundwater quality monitoring network. Using chloride data generated by the Status Network over several years, ACEPD conducted a structural analysis exercise to determine the appropriate range (14,373 ft (4,380 m)). To their managers, ACEPD recommended the use of hexagons with a 30,000 ft diameter to assist them in gap analysis. They also prioritized areas of the county for the addition of wells to the network and based this decision on aquifer confinement. Seven hexagons were identified as having high priority for the addition of wells to their network.

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Acknowledgements

The author would like to acknowledge many individuals for supplying numerous types of assistance. Without them, this project could not have been completed. From the Watershed Monitoring Section, the author would like to thank Jay Silvanima, Stephanie Sunderman-Barnes, and the rest of the staff at the Watershed Monitoring Section of DEAR.