STUDENT SUMMER INTERNSHIP TECHNICAL REPORT

Evaluating Spatial Distribution of Contaminants in the Savannah River Site F-Area using ArcGIS Interpolation Methods

DOE-FIU SCIENCE & TECHNOLOGY WORKFORCE DEVELOPMENT PROGRAM

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EXECUTIVE SUMMARY

This research work has been supported by the DOE-FIU Science & Technology Workforce Development Initiative, an innovative program developed by the U.S. Department of Energy's Office of Environmental Management (DOE-EM) and Florida International University's Applied Research Center (FIU-ARC). During the summer of 2023, a DOE Fellow intern, Hannah Aziz, spent 10 weeks doing a summer internship at Savannah River National Laboratory (SRNL) in Aiken, SC under the supervision and guidance of Dr. Hansell Gonzalez-Raymat. The intern's project was initiated on June 3, 2023, and continued through August 12, 2023, with the objective of evaluating the spatial distribution of contaminants using ArcGIS interpolation methods and evaluating sensor-derived data to detect spatial and temporal patterns.

The Savannah River Site (SRS) F-Area is underlain by multiple aquifers, including the upper aquifer, lower aquifer, and Gordon aquifer. Over time, these aquifers have been exposed to contamination including uranium-238, strontium-90, iodine-129, tritium, and much more. Although remediation efforts are underway, areas still exist where there are large contaminant plumes, emphasizing the vital need to understand the spatial extent and movement of these plumes to validate remediation methods or implement new methods. Spatial interpolation is a statistical technique that can be used to visualize the spatial distribution of a contaminant plume given a few select measured points. Inverse Distance weighing (IDW), Natural Neighbor, and Kriging are all powerful interpolation tools that can be accessed through GIS.

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1. INTRODUCTION

Background

The Savannah River Site (SRS) is a 300-square-mile-site, located in Aiken SC, whose focus was the production of basic materials (plutonium and tritium) used in the fabrication of nuclear weapons during the Cold War era. The production of these materials generated different radioactive byproducts that were disposed of in areas within SRS. At the F-Area, approximately 1.8 billion gallons of low-level radioactive waste, originated from the processing of uranium slugs and irradiated fuel in the Chemical Separation Facilities, was disposed of into a series of unlined seepage basins between 1955 – 1988. After entering the basin, some of the wastewater was evaporated, but most seep into the vadose zone.

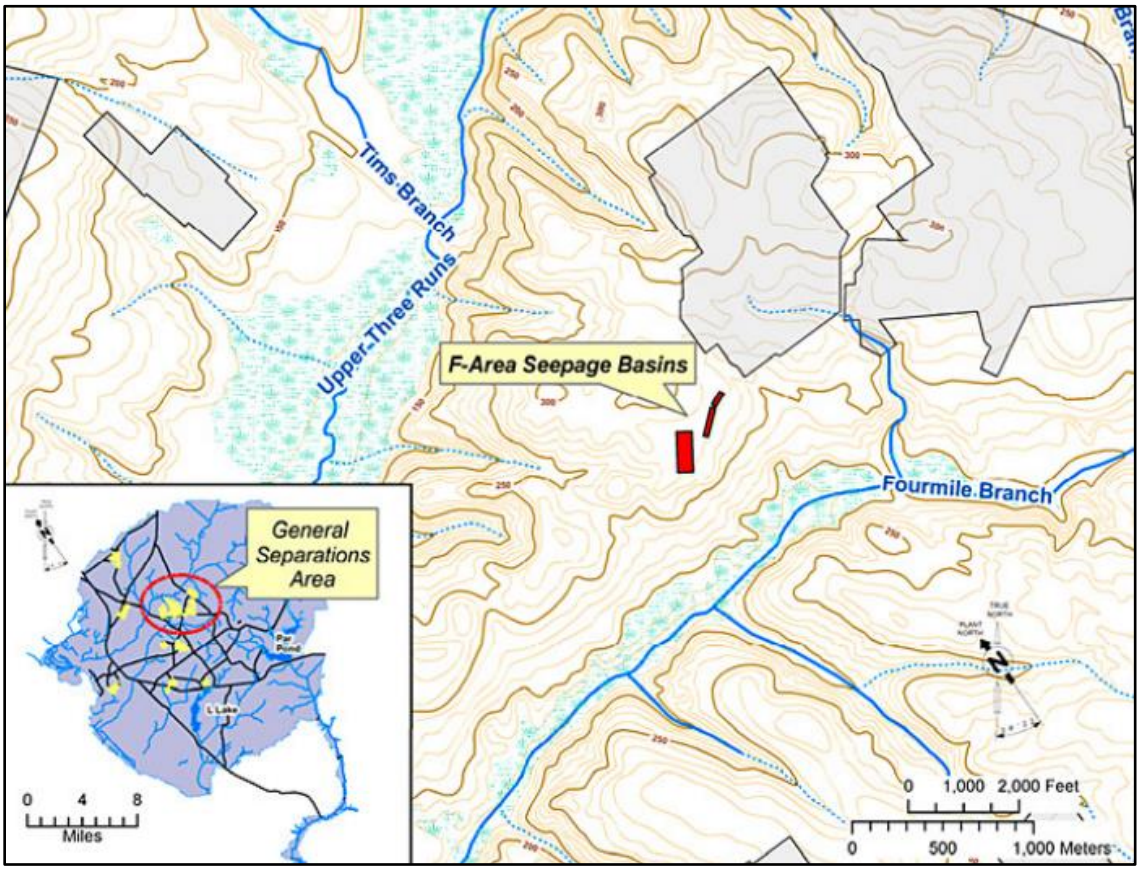

Figure 1. Location of the F-Area **Seepage Basins at the Savannah River Site**. **ITRC (Interstate Technology & Regulatory Council, 2017).**

Over the years, some contaminants migrated from the vadose zone and entered the saturated zone eventually forming a plume with a pH as low as 3.2, and a footprint of about 0.38 square mile (Interstate Technology & Regulatory Council, 2017). The main contaminants of concern in the F-Area include uranium (U) isotopes, iodine-129 (I-129), strontium-90 (Sr-90), tritium, nitrates, and technetium-99 (Tc-99). In the 1990s, remediation started by first installing a protective low permeability clay cap on top of the basin to prevent rainwater infiltration through the source to reduce the mobility of contaminants into the vadose zone and ultimately into the saturated zone.

In 1997, a pump-and-treat system was implemented to extract the contaminants from the groundwater downgradient and reinject the treated water upgrading of the basins. After a few years of operations, the pump-and-treat system was getting diminishing returns, and it was costly to maintain and operated. Therefore, it was replaced in 2004 by a funnel-and-gate system that consisted in the installation of a subsurface barrier wall to redirect the groundwater flow to the gates where base injections are performed periodically to increase the groundwater pH to enhance the attenuation of cationic contaminants such as uranium isotopes and strontium-90.

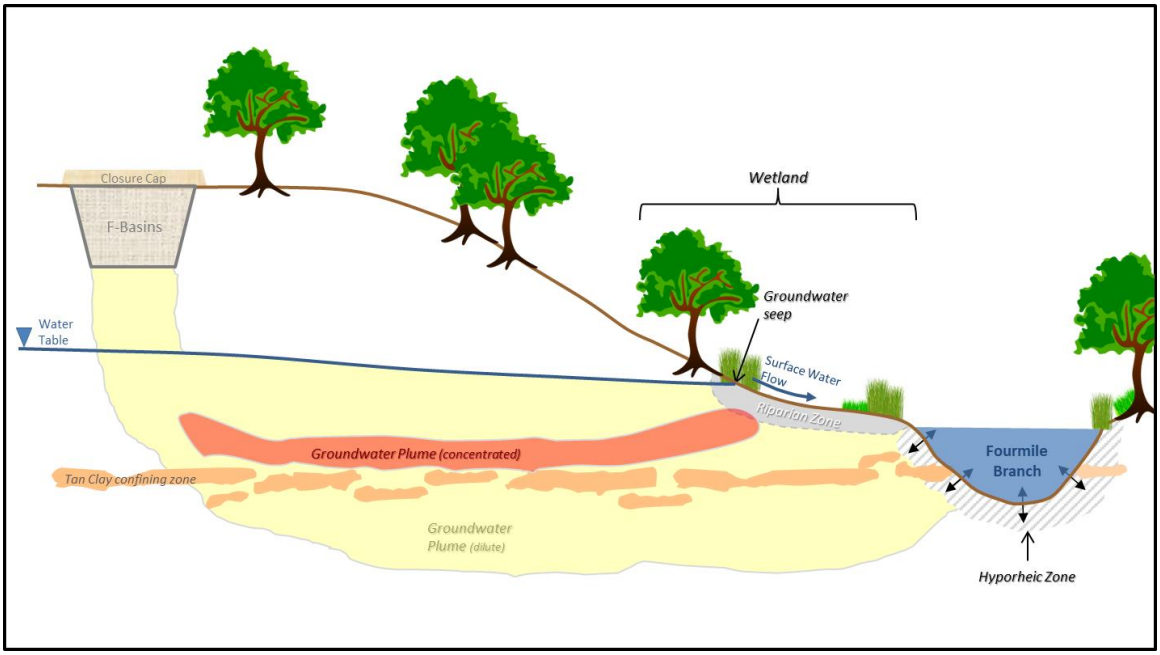

Figure 2. Conceptual model of F-Area **groundwater plume. ITRC (Interstate Technology & Regulatory Council 2017).**

The current methods used to remediate the F-Area are now being monitored to confirm that the remediation strategies remain effective over a long period of time. The main objective of this project was to create contaminant contour maps using ArcGIS spatial interpolation methods and compare the statistical tools to determine which method can produce the most accurate map. The spatial interpolation methods that will be tested are: Inverse Distance Weighing (IDW), Natural Neighbor, and Kriging tool. For the testing, historical U datasets from the monitoring well network at the F-Area Seepage Basins will be used and the results will be compared to decide which tool works best for evaluating the spatial distribution of contaminants in groundwater. If the testing shows positive results, then the best tool can be selected to analyze how the plume for different contaminants evolve with time.

2. RESEARCH DESCRIPTION

Spatial Interpolation

Spatial interpolation is the process of using a set of point data to create surface data (Wu and Hung, 2016). This was used as a method to predict the spatial distribution of contaminants in the F-Area and see the evolution over time. The main types of interpolation used in this project were either geostatistical or non-geostatistical. The slight difference between the two is that geostatistical methods utilize the statistical properties of measured points, while non-geostatistical methods create surfaces from similarities within the dataset, including distance or direction (*How Natural Neighbor Works—ArcGIS Pro | Documentation*). The types of interpolation that were analyzed and discussed in this report include Natural Neighbor, Inverse Distance Weighing (IDW), and Kriging. The interpolation was done using ArcGIS Pro. It should be noted that determining a "best" method for interpolation is difficult and can be affected by several factors including the distribution of data points, parameters, and location of the interpolation. This project involved the use of 2D visualization and historical maps to try and determine which interpolation is best suited for this dataset.

Study Area and Tools

The historical U-238 data that was used in this study was obtained from the monitoring well network at the SRS F-Area. To perform the spatial interpolation, the suite of tools such as IDW, Natural Neighbor, and Kriging were accessed using the ArcGIS software.

The first step was to preprocesses U-238 data to only include the main wells of the F-Area around the seepage basins running down to Fourmile Branch. The data was also filtered to only include sample data from July – September 2020, the upper aquifer wells, and any wells without contaminant data from the third quarter. In addition, a refence contour plume map, found in the Annual Corrective Action Report (Figure 3), was used to compare results and determine which interpolation method resulted in the most accurate map.

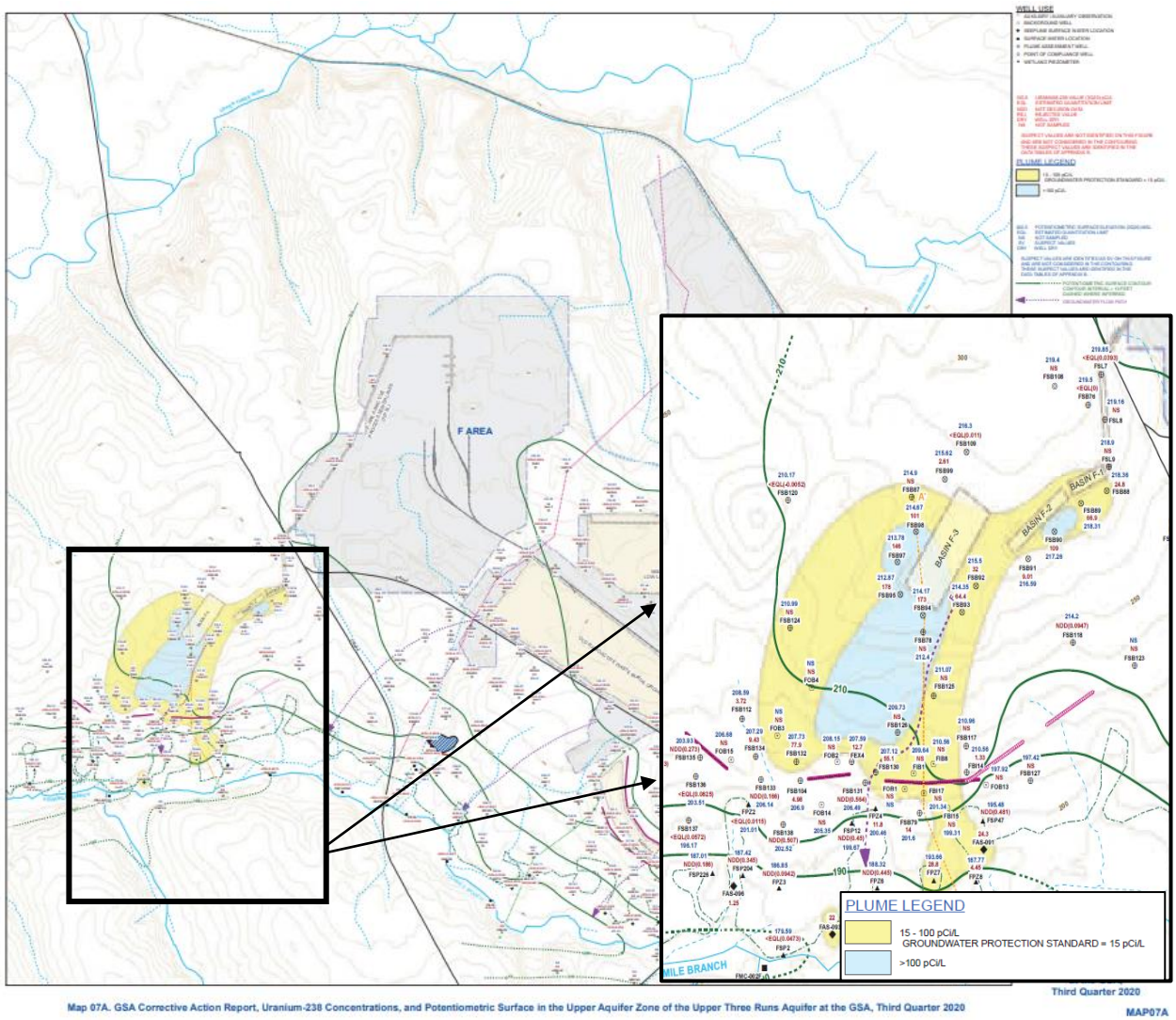

Figure 3. SRS corrective action map reference contour map of Uranium-238. Contour mapping was done manually.

Methods

Once the 2020 U-238 dataset was preprocessed, it was added into ArcGIS. Adding the data into ArcGIS required the user to specify the coordinates needed for the X and Y field. The data therefore needed to be spatial or include location coordinates, otherwise spatial interpolation would not have been possible. Thus, the historical data included UTM_East, and UTM_North coordinates. Once the data points were added to ArcGIS, the interpolation was carried out, starting with the IDW method. Completing the interpolation only required the input of the 2020 U-238 dataset and specification of the contaminant results as the Z field. For the scope of this project, default values were maintained for the other parameters, which is further explained in the Results section of this report. For each interpolation, a filter was placed based on the drinking water standards of U-238. Therefore, any location in which U-238 concentration was less than 15 pCi/L would show no color in the interpolated map. Anything between 15 pCi/L-100 pCi/L, and above 100 pCi/L was considered contaminated or highly contaminated.

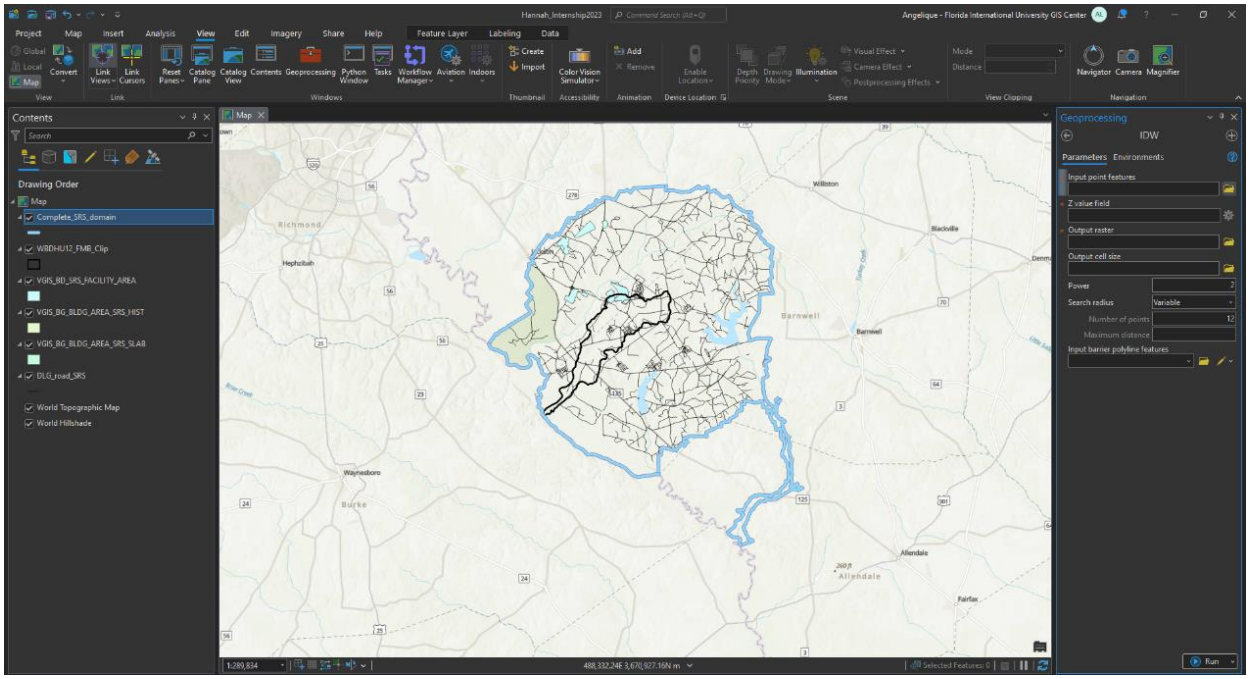

Figure 4. ArcGIS Pro interface with IDW panel. Parameters such as power and search radius were left with the default values.

IDW is frequently used in soil studies (Abdulmanov et al., 2021). IDW basically uses distances to draw a pattern between points. The measured point holds a weight, and as the location from that point increases, the weight of that point decreases. IDW assumes that each measured point has a local influence that decreases with increasing distance (Abdulmanov et al., 2021). IDW uses the following equation to determine interpolation values.

$$Z = \sum_{i=1}^{n} \frac{1}{(d_i)^p} Z_i \div \sum_{i=1}^{n} \frac{1}{(d_i)^p}$$

The next method tested was Natural Neighbor. For Natural Neighbor the process of interpolating again only required the input file (which is the U-238 data added), and the Z-field which, as before, were the contaminant concentrations. Again, default parameters were used, and when the interpolation was done the only thing to be changed was the plume legend and the symbology to indicate only concentrations larger than the drinking water standard, as mentioned above. The Natural Neighbor technique is done using geometric relationships, and the number of neighbors is determined by constructing natural neighbor circles (two points are natural neighbors if they lie on the same natural neighbor circle). The weights depend on the area around each of the data points (Voronoi polygons) (Sibson, 1981).

The last interpolation method tested was geostatistical Kriging. Kriging interpolation encompasses a wide range of different interpolations that are quite advanced, and powerful. There is universal kriging, ordinary kriging, simple kriging, Empirical Bayesian kriging, and many more. Each type can be used under different circumstances based on the results desired, the data available, the information available about the data (i.e., metadata), whether the data is univariate or multivariate, etc. In ArcGIS geostatistical Kriging must be done through the geostatistical wizard.

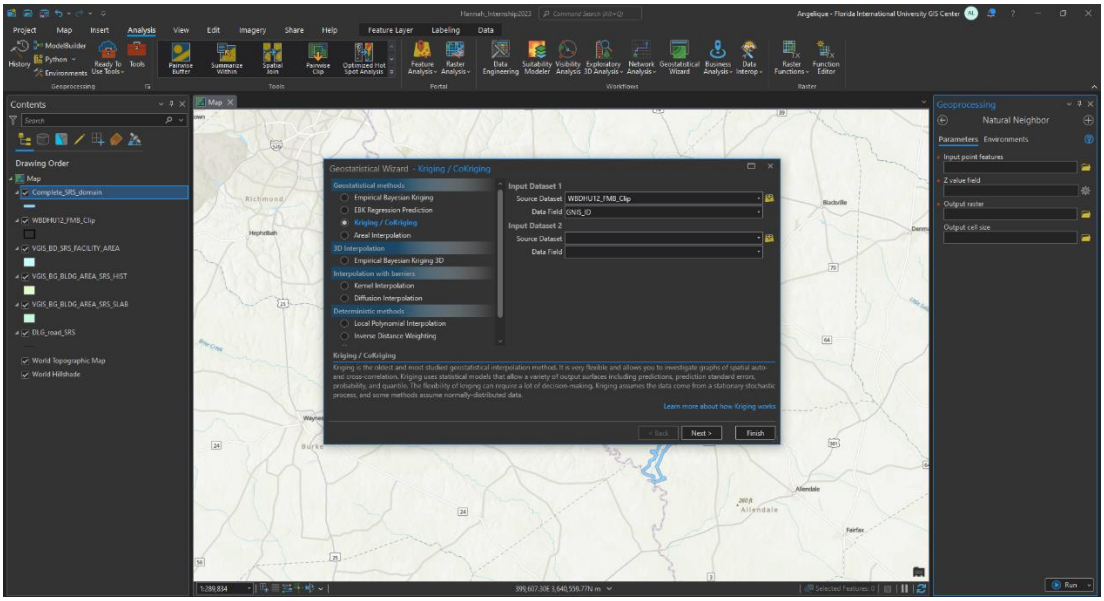

Figure 5. Geostatistical wizard interface where the Kriging interpolation may be accessed.

The Kriging interpolation used for this project was predictive simple Kriging. Typically, ordinary Kriging is done when the mean of the sample set is unknown; however, in the case of ArcGIS, simple kriging is possible because the mean of the sample set can be calculated. ArcGIS will for the most part fill in all parameters, but there is more user input required. The user can change the distribution of the sample set, the type of semi-variogram used, the number of neighbors considered, and parameters of the semi-variogram. Semi-variogram and covariance are mathematical forms of autocorrelation (Abdulmanov et al., 2021). This input can help to create a more precise interpolation, but more knowledge is needed on the effect of each parameter. For Kriging and many interpolation methods, the dataset itself is incredibly important. The distribution, uniformity, and density of the data can all affect the interpolation output, and in the case of Kriging, the semi-variogram/covariance model. With the complexity of the Kriging interpolation, it is important to use the cross-validating function which provides the mean error, root-mean square, and root-mean square error value which was used to validate the interpolation alongside the visual comparison against the corrective action map.

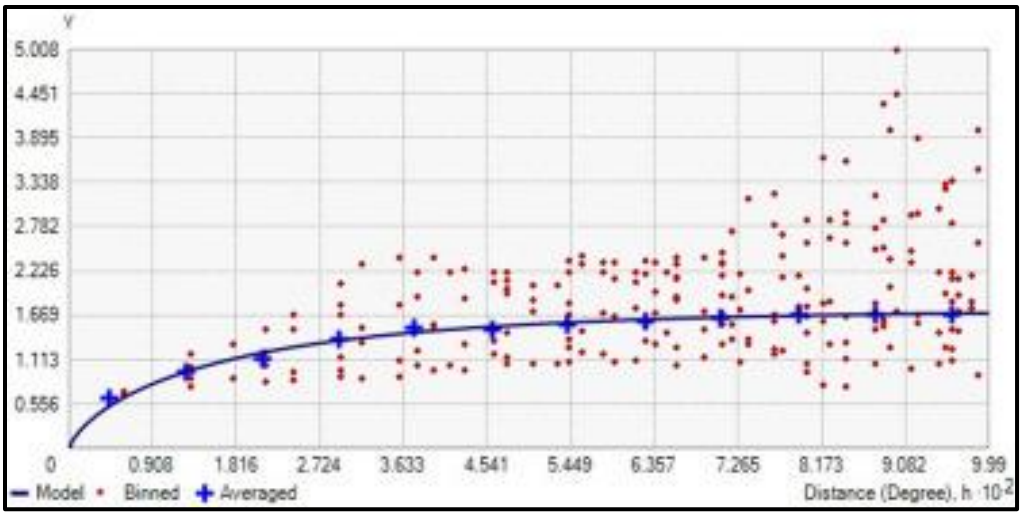

Figure 6. Example of semi-variogram from ArcGIS (Abdulmanov, 2021).

Once the interpolation for Kriging was completed and cross-validated, then all 3-interpolation methods were complete.

Visual analysis by comparing interpolation maps to the corrective action map helped determine the interpolation method that worked best for the spatial distribution of contaminants, and to continue testing the interpolation method it was applied to the 2016, and 2012 U-238 data. By applying the interpolation method to the previous years, the plume evolution can be understood.

3. RESULTS AND ANALYSIS

After completing the three interpolations of the spatial distribution of U-238 contaminants within F-Area, the results clearly revealed which interpolation method was the best. Below are the images of the original corrective action map, alongside the results of each interpolation map.

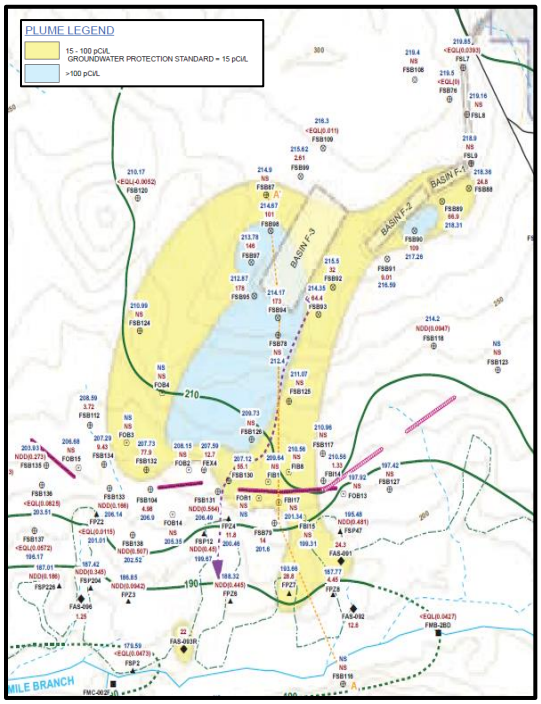

Figure 7. Corrective action map with U-238 data from 3rd quarter 2020.

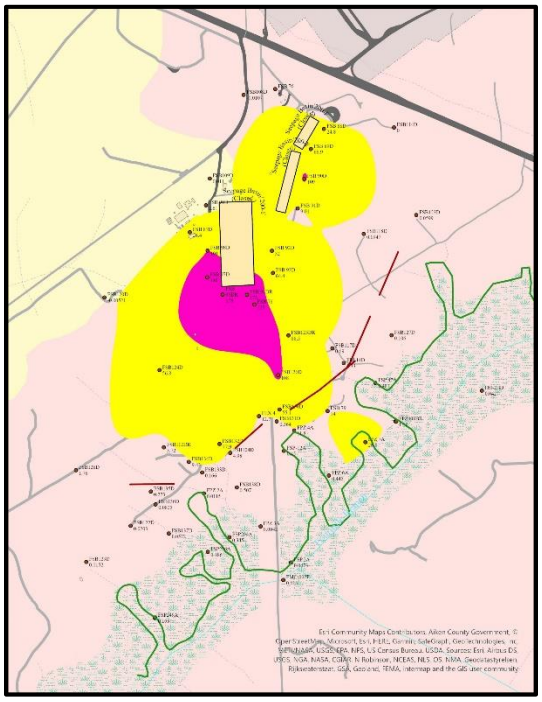

Figure 8. Natural Neighbor interpolation with U-238 data from 3rd quarter 2020.

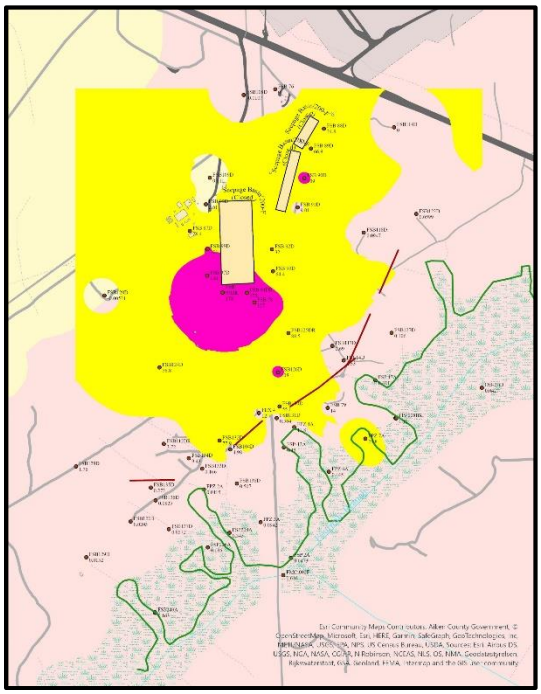

Figure 10. IDW interpolation with U-238 data from 3rd quarter 2020.

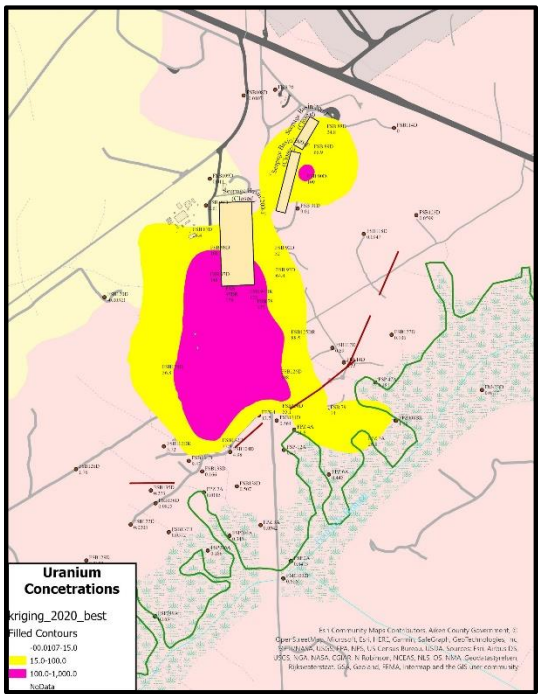

Figure 9. Kriging interpolation with U-238 data from 3rd quarter 2020.

From all the maps, the interpolation that yielded the results most like the reference map was the geostatistical Kriging technique. All interpolation methods used the exact same wells and data from the upper aquifer. Using the reference map as a comparison is also valid since it used the same well and data. Despite all interpolation methods using the same data, there is a clear difference between each map. The differences between the results can be explained through the mathematical functions that are used to do the interpolation, and what exactly is being used to create predictions. As previously mentioned, IDW uses distance from measured points, and Natural Neighbor uses area relative to the measured points to see what points are within the radius around those measured points. Kriging on the other hand, uses the semi-variogram/covariance model to predict values. Ranking from worst interpolation to best will start at IDW.

IDW struggles to form a consistent interpolation of the general area sampled. Looking closely at the map, their "contaminant" predicted over the seepage basins, which makes little sense because the water flows down from the top of the seepage basins to Fourmile Branch. So, although there can be contaminant under the basin itself there would be no way for it to flow upwards. IDW uses a power function to give measured points their weight, and the more the user increases the power in ArcGIS the more weight each point has. For the scope of this project, the spatial distribution IDW was not the best fit, if the farther you get from a measured point the smaller the influence on the area. However, it should be noted that with every interpolation method there were challenges. The contaminant seen over the seepage basin is the result of IDW using a perimeter to contain the interpolation within a certain border. This can be solved by simply creating a boundary within ArcGIS; however, areas of high concentration are still indicating lower than expected, so the interpolation is not the best.

Natural Neighbor interpolation was a bit better than IDW. It has a better formation around the F-Area, and the high contaminant concentration appears to be spreading down to the wetland area. Natural Neighbor is a great tool for interpolating; however, it works best with large dense data sets. In this case, the contaminant data was sparse, and there were not many sample points available. Applying weight based on area is not the best method to interpolating this dataset.

Lastly, Kriging was used in the geostatistical wizard. The plume developed from this interpolation method was the most similar to what is seen in the reference map, and there are points to highlight. The Kriging tool was able to identify contaminant concentration underneath basins F-1 and F-2. There was also a C-shape forming near the bottom of the plume. This could be a result of the barrier wall installation, since water is now funneled through the gates and is no longer flowing directly down, it also gets pushed towards the west. The Kriging tool did a great job; however, more is needed to understand the semi-variogram function, and the parameters that are used in modeling the plume. Kriging is another interpolation tool that was limited due to the smaller, random dataset used. Nonetheless, in the case of contaminant distribution, Kriging is successful. In Croatia, Kriging is used for mapping soil contamination (e.g., Castrignano and Romić, 2007, Sollitto Et Al., 2010). Kriging is an advanced statistical tool, and the figures below depict its use to interpolate theU-238 distribution in 2012 and 2016, both in the upper aquifer using the same wells if available.

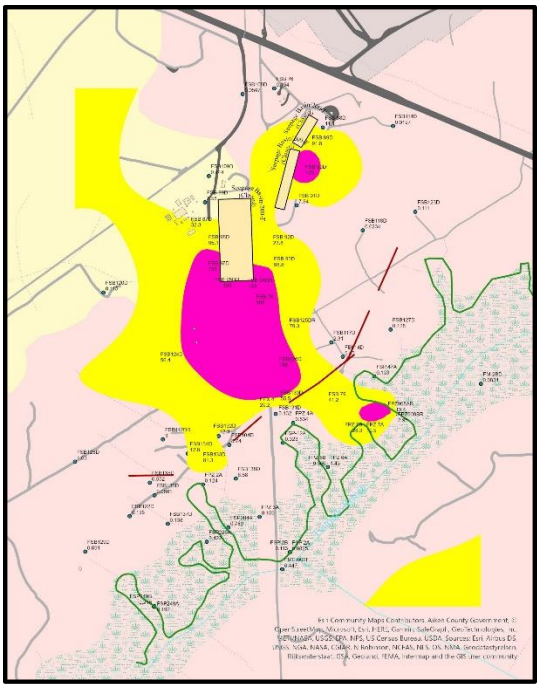

Figure 11. 3rd quarter 2016 U-238 plume created using ArcGIS Kriging interpolation.

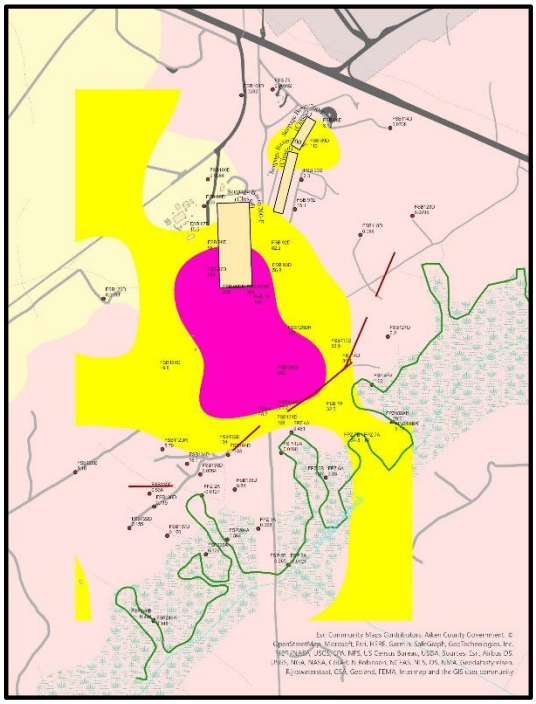

Figure 12. 3rd quarter 2012 U-238 plume created using ArcGIS Kriging interpolation.

These maps show evolution of the plume over the last 8 years, but unfortunately Kriging does also need a perimeter to perform the interpolation which can distort the interpolation itself.

4. CONCLUSION

The results indicate the power of interpolation methods. ArcGIS is a commercial tool, and the interpolation tools are easily accessible. Each interpolation function will work best based on the data provided, and the parameters adjusted. For the case of contaminant spatial distribution in the F-Area, simple Kriging was the best tool. It provided the most accurate interpolation. There are still challenges and more understanding needed of the semi-variogram/covariance model used to create the Kriging interpolation. In the future it may be worth it to understand the model and look toward more advanced forms of interpolation, including machine learning (ML) models that have been recently developed and have shown promising results.

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