Geo 327G Semester Project

GIS Analysis of Ion Concentrations in the Queen City Aquifer

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Objective

The goal of this project was to create various Ion Concentration probability maps of the Queen City Aquifer in Texas. Coupled with other geochemical analysis methods, these probability maps could be used to provide useful insights into the geochemisty of the aquifer.

Methods

To produce ion concentration probability maps I will obtain and manipulate data available on the Texas Water Development Board website. Then I will use a geostatistical interpolation method to predict the concentration of a specific ion across the Queen City Aquifer from 20 years' worth of well concentration data.

Data Collection

The majority of the data required for this project can be obtained from the Texas Water Development Board website.

- http://www.twdb.state.tx.us/groundwater/data/gwdbrpt.asp
    - From here download the "Entire Groundwater Database (mdb)" and also the "GWDB well locations"
- http://www.twdb.state.tx.us/mapping/gisdata.asp
    - Download the "Minor Aquifers Shapefile"

Data Processing

The objective of data processing is to create a shapefile of Queen City Aquifer wells that has millimole ion concentrations.

1. Start ArcGIS and create a new map. Load the "GWDB_well_locations" shapefile into the table of contents.
2. Isolate all of the Queen City Aquifer wells
    a. On the top bar of ArcGIS hit the selection tab and click "select by attribute"
    b. The layer selected is the "GWDB_well_locations". In the box that contains the various fields for the layer, Click "Aquifer_id" and click then "Get Unique Values"

c. Create the query “Aquifer_id” = “QUEEN CITY”. This should look like Figure 1. Hit okay.

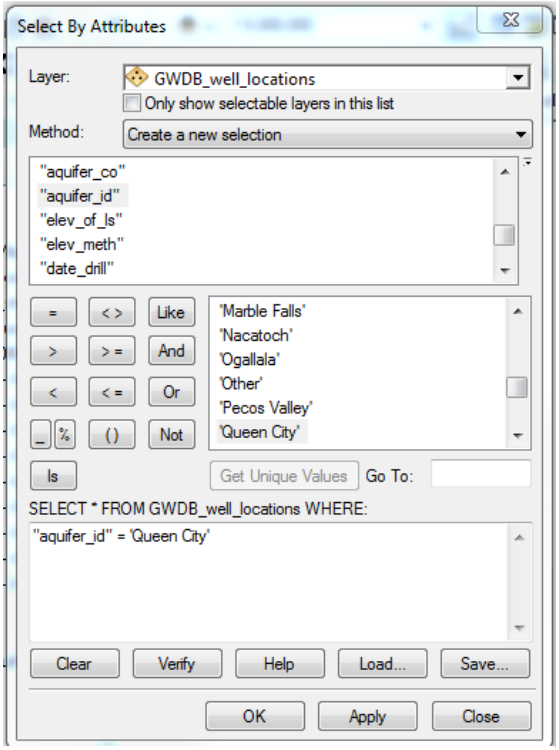

Figure 1

d. To extract the Queen City wells from the “GWDB_well_locations” go to the toolbox > Analysis Tools > Extract > Select.

e. The input feature is the “GWDB_well_locations”. Name the output feature “QC_wells” and save it into your project folder. Hit OK

3. Next obtain the water quality data

a. Open Excel and go to the Data Tab

b. Using the Import from Microsoft Access feature select the “GWDB” Access file that you downloaded. A “Select Table” will pop-up and select “waterqua” from this list. See Figure 2. Click okay and import the data into a table.

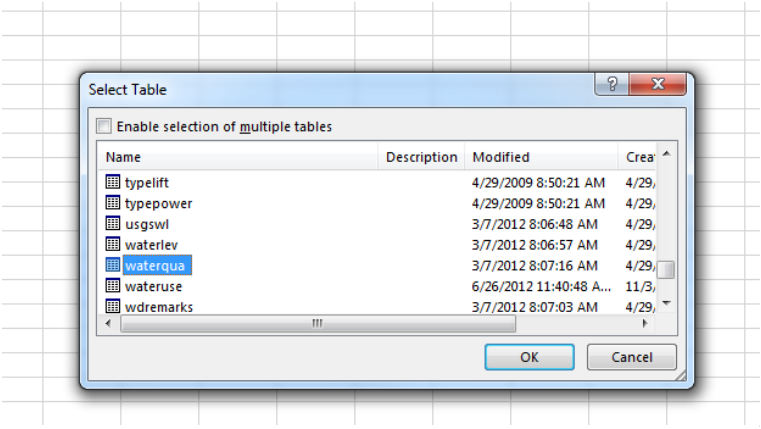

Figure 2

4. Furthermore, manipulate the well quality data so we can get Queen City Aquifer for the past 20 years.
    a. In excel use the “Filter” function and select all the years from 2013-1993
    b. Highlight all the cells and copy and paste them into a new sheet. Name this sheet “20yr”
    c. In this new sheet, highlight all of the cells and use the custom sort feature. Sort by “yydate” and have them ordered largest to smallest.
        i. This will ensure that if there is multiple data for a single well in this time frame the most recent well quality data will be chosen when we join this table to the Isolated Queen city wells in ArcGIS.
5. Next, we use the manipulated well quality data in excel to obtain the Queen City well quality data in this 20 year time span.
    a. In ArcGIS, right click on “QC_Wells” shapefile and go to the Join and Relate section and select join table
    b. You want to join attributes from a table, based on “state_well” field. In the “choose a table to join section” browse to your well quality spreadsheet and select the “20yr” sheet. The Field in the table to base the join on is the state_well_number”. Also we only want to keep matching records. See Figure 3.

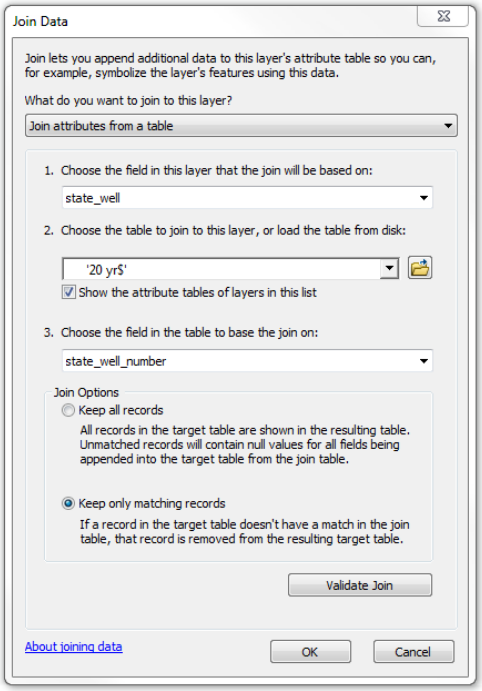

Figure 3

6. Convert the well quality ion concentration data from mg/l of the ions to millimoles.
    a. In ArcGIS, Open “QC_wells” attribute table and select all the data. Then copy and paste this into a new sheet on your existing excel spreadsheet. Name this sheet “20yr_mg”.
    b. Next create a new sheet and name it “mmol” and copy and paste the well numbers from “20yr_mg” plus the desired column headings. Using excel

functions convert mg/l to millimoles. The end result should be that your “mmol” sheet has all of the converted values.

7. Join the “QC_mmol” sheet to QC_Wells
    a. In ArcGIS, right click on “QC_Wells” shapefile and go to the Join and Relate section and select join table
    b. You want to join attributes from a table, based on “state_well” field. In the “choose a table to join section” browse to your well quality spreadsheet and select the “mmol” sheet. The Field in the table to base the join on is the “state_well”. Also we only want to keep matching records.
8. Make this join permanent and create a separate shapefile for the mmol well data.
    a. Right click on “QC_Wells” select “data” then “export data”.
    b. Export all features and use the same coordinate system as the layer.
    c. Under output, browse to your project folder, name it “QC_mmol” and then make sure you save it as a shape file. See figure 4

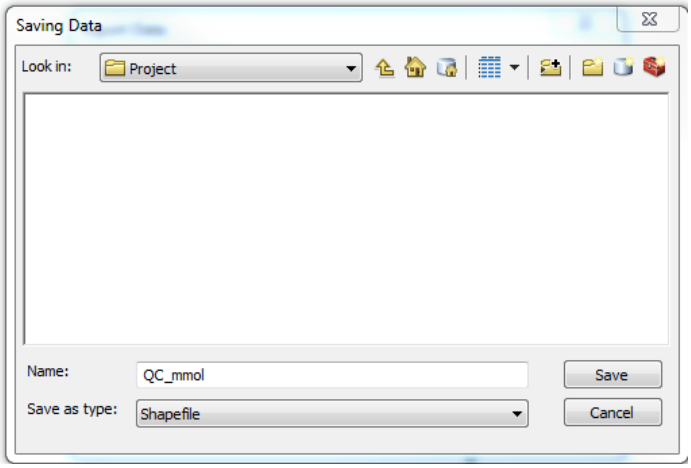

Figure 4

9. Extract the Queen City Aquifer shapefile from the “New_minor_aquifers” shapefile
    a. Place the “New_minor_aquifers_dd” shapefile onto the table of contents
    b. On the top bar of ArcGIS hit the selection tab and click “select by attribute”
    c. Choose the “New_minor_aquifers_dd” layer
    d. In the box that contains the various fields for the layer, Click “AQU_NAME” and click then “Get Unique Values”

e. Create the query “AQU_NAME” = “QUEEN CITY”. This should look like Figure 5. Hit okay

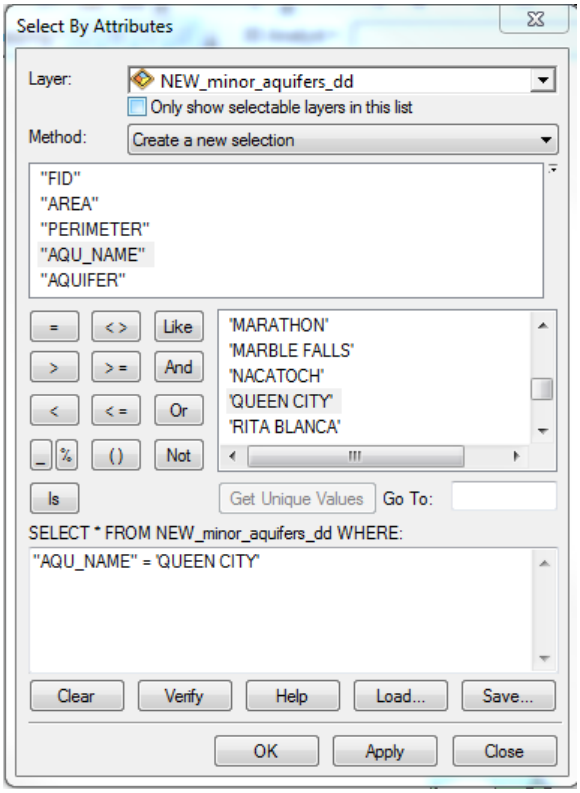

Figure 5

f. Next go to the toolbox > Analysis Tools > Extract > Select.
g. The input feature is the “New_minor_aquifers_dd”. Name the output feature “QC_aquifer” and save it into your project folder. Hit OK

ArcGIS Processing

Once we have our data all sorted, we can now start to construct our probability maps of ion concentrations. We will utilize the Kriging method in the Geostatistical Analyst Extension. Kriging an

interpolation method that is based statistically. So before we start kriging you must check if your data set has a few important characteristics:

1. Is the data in a Gaussian distribution?
    a. Kriging predictions are best if the data are Gaussian, and Gaussian distribution is needed to produce confidence intervals for prediction and probability mapping.
    b. Within the Explore data feature of the geostatistical analyst, you may use the Histogram feature to check the data's distribution. If it is not we will have to use a transformation method during Kriging to make our data Gaussian.
2. Are there any trends in the data?
    a. If trends exists, the mean data value will not be the same everywhere, violating one of the assumptions of data stationarity of the kriging model.
    b. Within the Explore data feature of the geostatistical analyst, the Trend Analysis tool can be used to determine if there are any trends.
    c. It is important to note any trends as we can try and remove them through the kriging process.
3. Are there any spatial autocorrelation and directional influences in the data?
    a. The Semivariogram feature, within the explore data section of the Geostatistical Analyst, is a graph that displays the distance between the location of points versus the difference of their values squared.
        i. Points that are close together should have a small difference squared values indicating that these points have similar values. It is expected however that as points get further away their difference of their values squared should start to vary more.
    b. So an assumption for geostatistics is that any two locations that have a similar distance and direction from each other should also have similar values for their differences of their values squared.
        i. Directional relationships are important. If in one direction, values change more rapidly or slowly compared to another direction there is an anisotropy. We must note this and take account of it when Kriging.

With this in mind, and after going through all of the ion concentration data, I found that each ion did not have a Gaussian distribution, contained trends, and had anisotropies associated with them. As a consequence, the kriging method explained here for the Chloride concentration can be applied to all of the other ions.

1. Go into the Geostatistical Analysts and select the Geostatistical Wizard.
2. Select the "Kriging/CoKriging" method.
3. The Source Dataset is the "QC_mmol" shapefile and select the data field corresponding to the chloride concentration. See figure 6. Then click next.

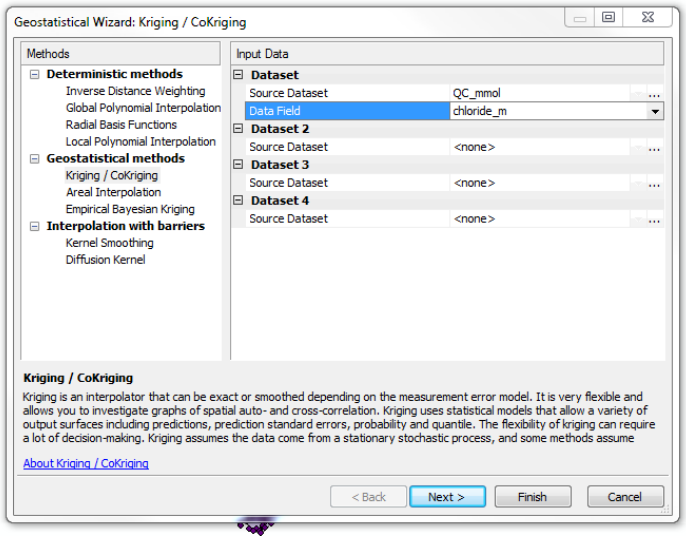

Figure 6

4. We will use simple kriging with a transformation type of “Normal Score”. Also we want to decluster the data before this transformation and remove second order trends. Kriging Step 2 of 8 should look like figure 7.

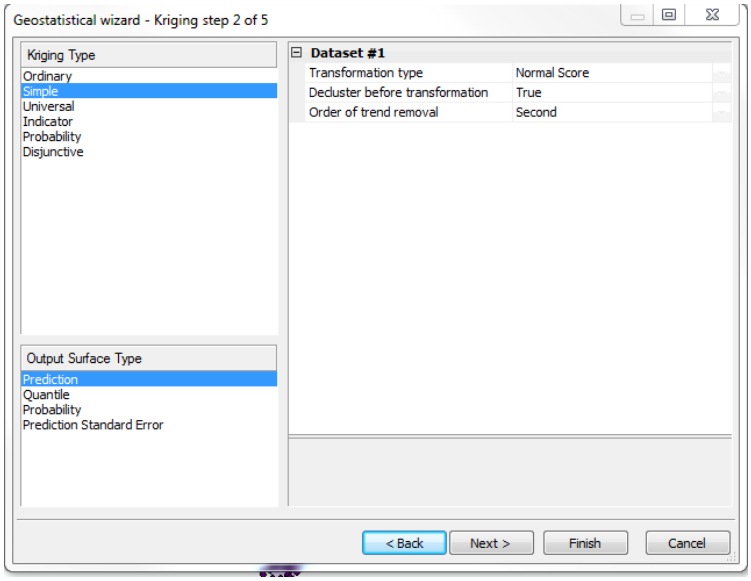

Figure 7

5. In step 3 of 8, we leave all of the default setting except that we will set “Advanced mode” to true. Then in the advanced properties we will only change the sector type to 4 Sectors. After these changes your window should look like figure 8. Click next

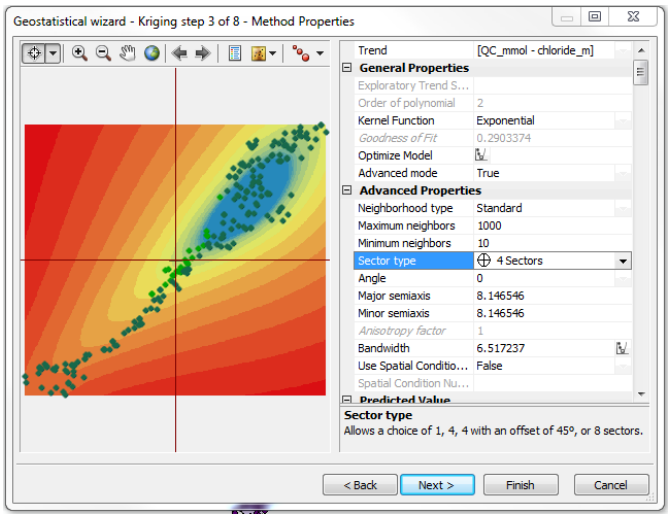

Figure 8

6. Step 4 of 8 involves declustering the data. We will use the polygonal method and our clip layer will be “QC_aquifer”. It should appear similar to figure 9.

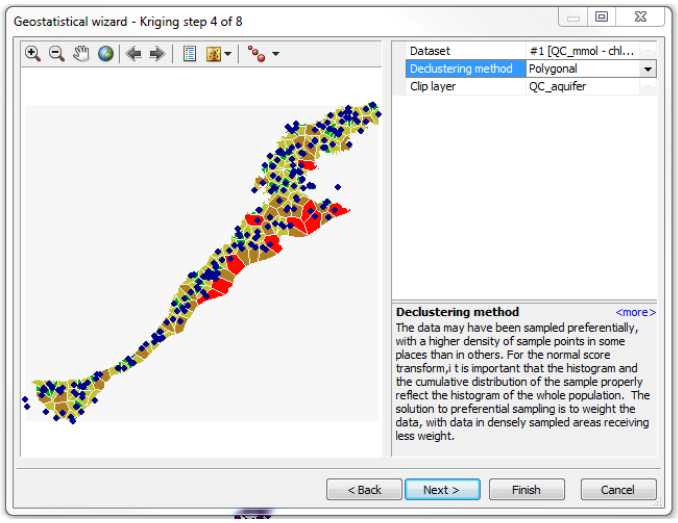

Figure 9

7. Step 5 of 8 involves normalizing the data set to a Gaussian distribution. No fields were touched here. The data appears to have been successfully adapted to the Gaussian distribution.
8. Step 6 of 8 involves Semivariograms. The important thing to note here is if there is any anisotropies in our data. Within the Covariance map we can see that the data changes rapidly in the N-S direction but really slow in the E-W. This is an anisotropy so to take

account of this we may turn the “Anisotropy” field under Model#1 to “true”. It should look simil8ar to figure 10.

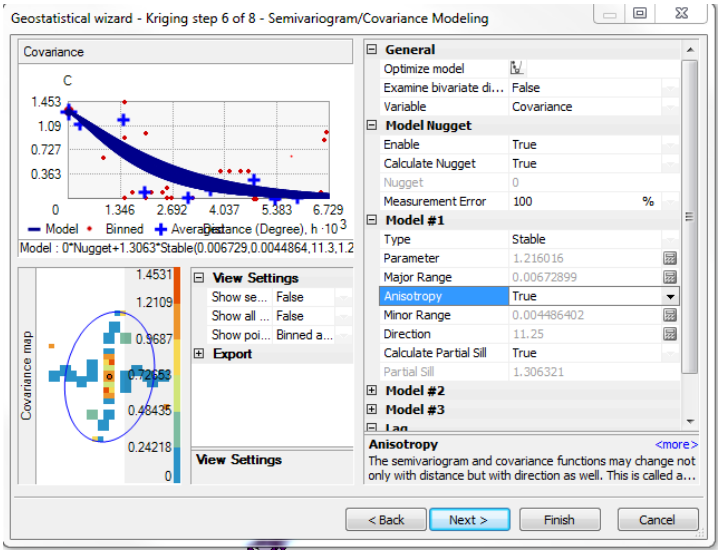

Figure 10

9. Step 7 of 8 involves the Searching Neighborhood. I did not change anything in this section.
10. Step 8 of 8 displays the cross validation plot and the prediction errors. Ideally we want the mean close to zero, the Root Mean Square error and Standard error to be minimized, and the Root Mean Standardized error close to one. As we can see in Figure

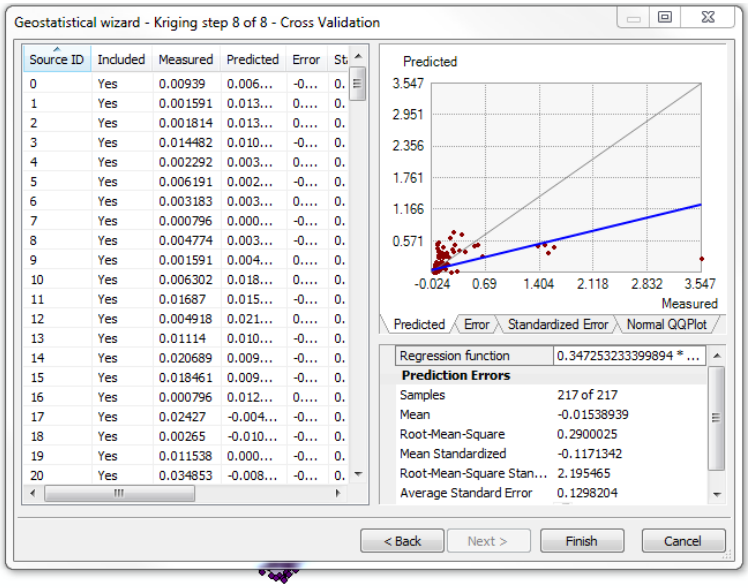

Figure 11

11, our result coincides well with these values except for the Root Mean Square Standardized error. Click finish.

With the kriging done we now have a probability map for a large Area. To be more useful we want the probability map to be fit to just the shape of the aquifer. The steps are as follows:

1. Right click on the CL- prediction map and go to data, then export to vector.
2. Keep the input as “Cl-“, change the contour type to “Filled Contour”, and change the contour quality to “Presentation”. In the output section select your project folder and name it “Cl_contour”. This should look similar to figure 12. Click OK.

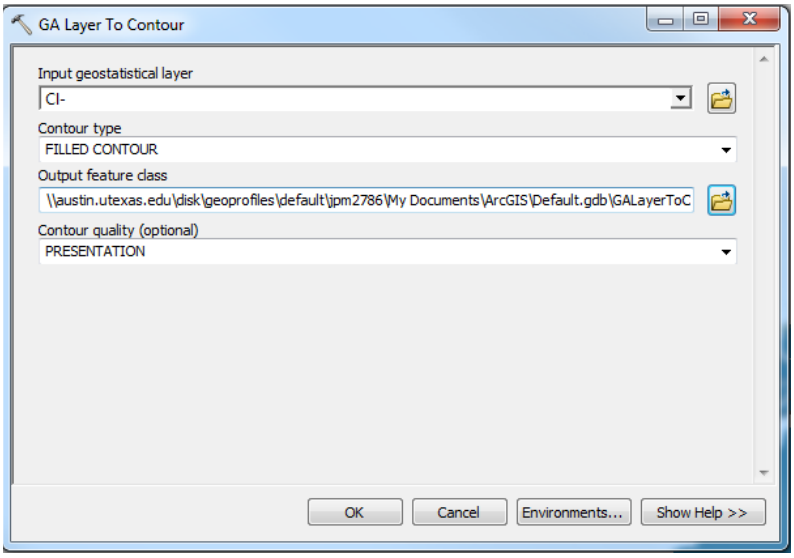

Figure 12

3. Next, go into the toolbox, and select clip, within the Extract feature of the Analysis Tools. Select “Cl_contour” as your input feature. Select “QC_aquifer” as your clip feature. In the output feature class select your project folder and name it “CL_prob_clip”. See Figure 13.
4. The last step is to set the symbology of this clipped probability map. To do this, right click on the “Cl_prob_clip” in the table of contents. Select properties and click on the symbology tab. Click the “import” box in the right hand corner of this window. Within the Import symbology window we want to import from another layer in the map, which

in this case would be the “Cl_contour” shape file. Click ok. The keep the default settings in the “Import Symbology Matching Dialog” window and click OK.

5. Your final product should look like figure 14.

To complete the rest of the probability maps replicate all of the steps explained in the ArcGIS

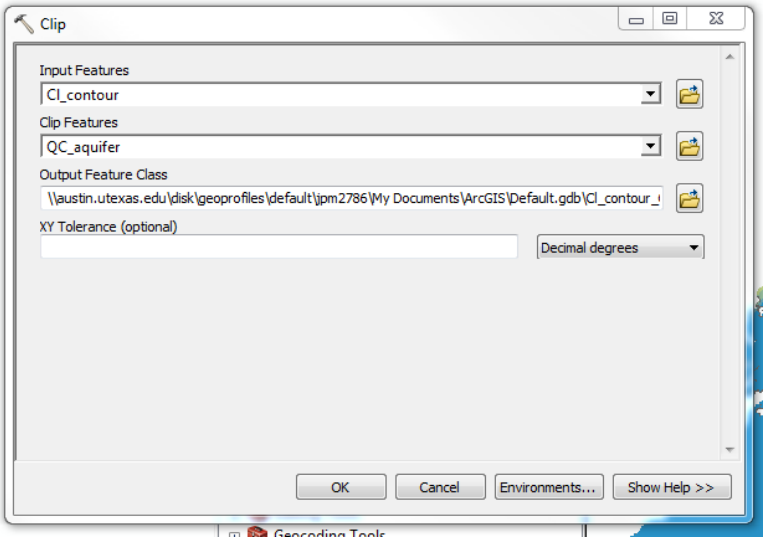

Figure 13

processing section over again. However there is one important difference. When you go to Krig, the Source Data set remains the “QC_mmol” shapefile but the Data field selection will be changed to the desired ion.

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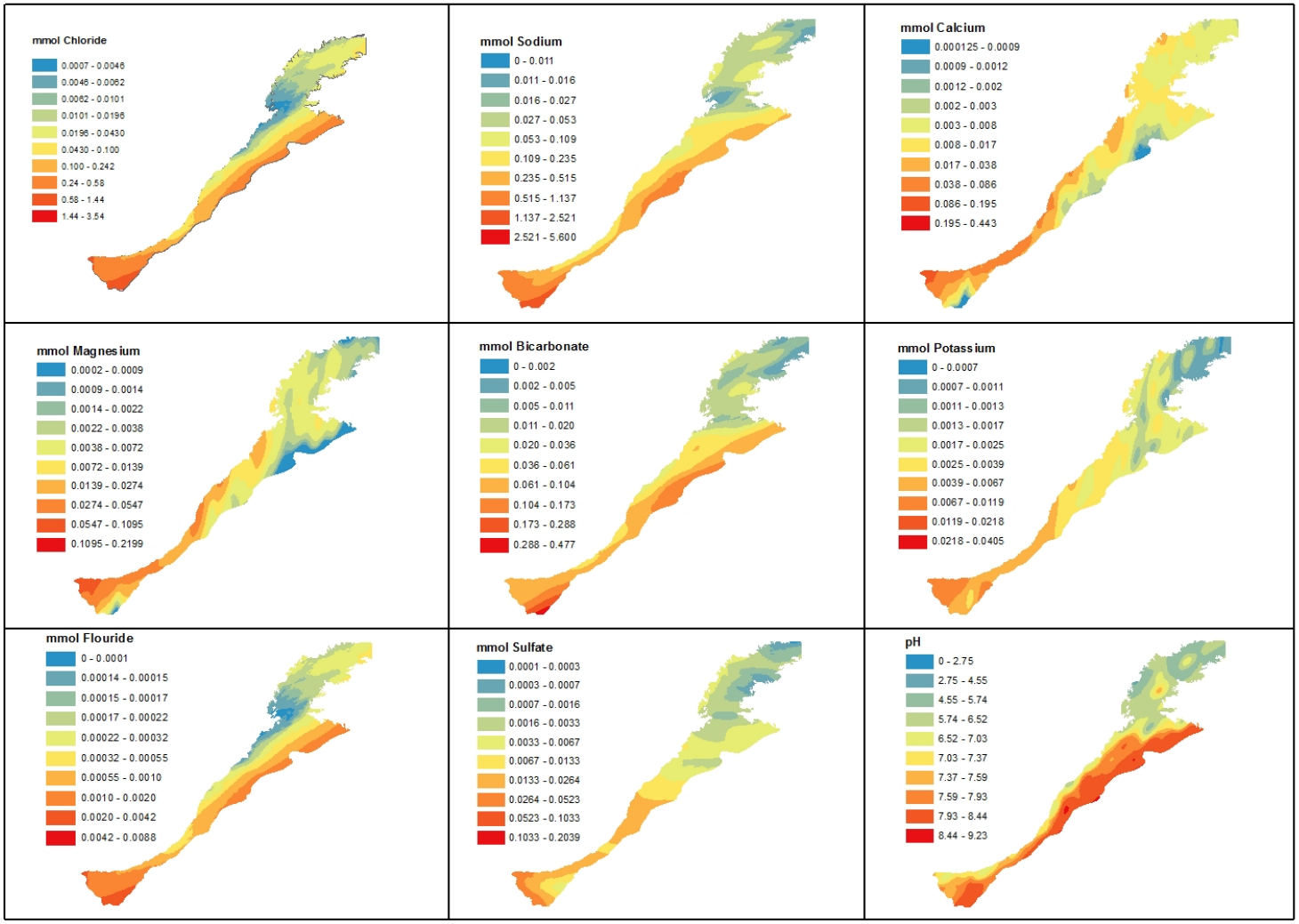
Ion Concentration Map of the Queen City Aquifer, TX



Conclusion

Using the geostatistical interpolation method of Kriging for ion concentration maps can give you a broad sense of the geochemical reactions that may be taking place. For instance, you could compare the Sodium and Chloride concentrations and see if they coincide. This would indicate a 1:1 ratio between these ions which we would expect. However, a thing to note about these maps, is that they were done with a 20 year span of data. Surely, ion concentrations will vary by location over this time scale. Therefore making any assumptions made from these have a high amount of uncertainty. Additionally, much of the Kriging that was done did came close but did not fit the error parameters discussed perfectly. Consequently, this increases the uncertainty of any assumptions made.