Analysis of Hydrochemical Data Using AquaChem Professional Software

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Introduction

When groundwater flows through rocks their minerals dissolve gradually. The amounts of minerals that dissolve in groundwater are measured as chemical concentrations.

Generally concentrations of chemicals in groundwater reflect residence time or distance of groundwater flow within the subsurface.

Accordingly, groundwater chemistry is considered a manifestation of groundwater flow; therefore, flow systems can be interpreted from the analysis of spatial groundwater chemistry data.

In this lab activity you will use the industry software AquiferTest to analyze groundwater chemistry data and examine groundwater movement.

Objectives - In this lab you will:

- Use AquaChem software to analyze groundwater data
- Integrate hydrochemical data with potentiometric surface data
- Evaluate the plausibility of chemical analysis data using charge balance error calculation
- Determine the ionic strength, activity coefficient, and the activities of major ions of groundwater
- Determine the chemical species in groundwater
- Determine IAP and SI of groundwater with respect to calcite, dolomite, halite, and gypsum
- Use saturation indices, Piper and Schoeller diagrams to interpret groundwater flow

Materials

The data for this lab is in the research paper written by Back and Hanshaw (1970) provided to you. The data is found on page 350 and consist of groundwater samples with the Index numbers 1, 2W, 2S, 3S, and 4S. Also you will find on page 346 a potentiometric surface map on which the data is plotted has also been provided to you. I encourage you to carefully read the entire paper.

You will use the AquaChem software installed on the Biolab computers.

Procedures

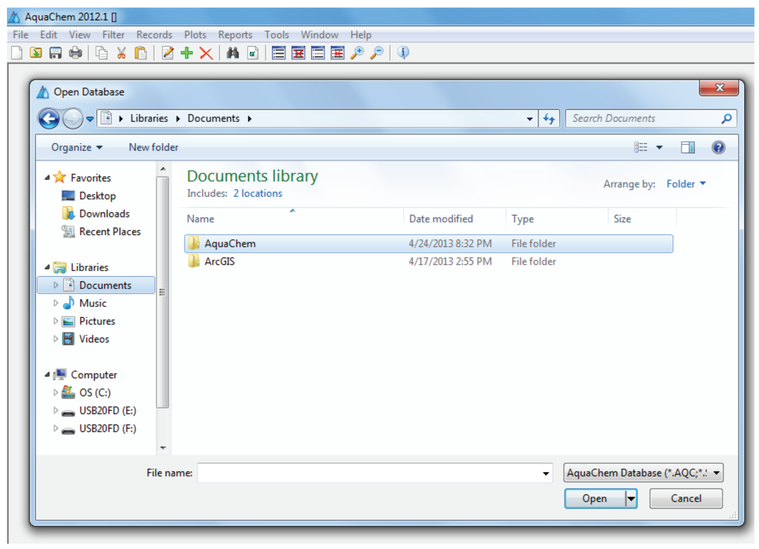
A. Draw flow lines:

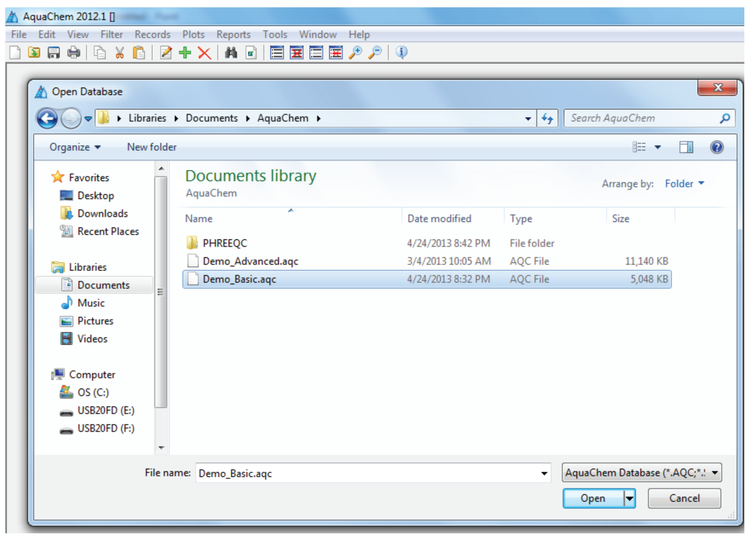
Based on the potentiometric surface map draw a few flow lines and indicate with an arrow the direction of groundwater flow in the vicinity of the selected samples.

B. Entering data in AquaChem

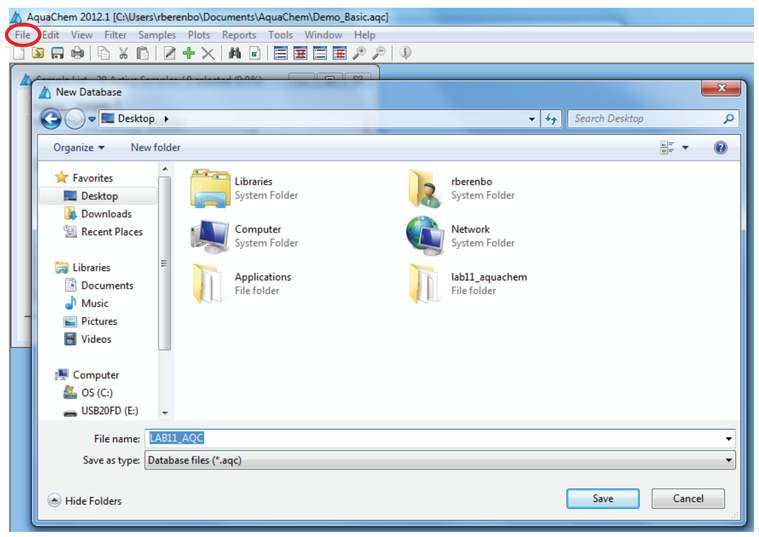
1. Start the program “AquaChem”. AquaChem is started like any window program by clicking on start then ‘All Programs’ to locate the folder containing AquaChem

2. When AquaChem starts click on “documents” in the pop-up window. This will show up the AquaChem folder. Double click on AquaChem folder then select “Demo_basic_aqc”. Click on “open” to open this file. This file you opened is a template.

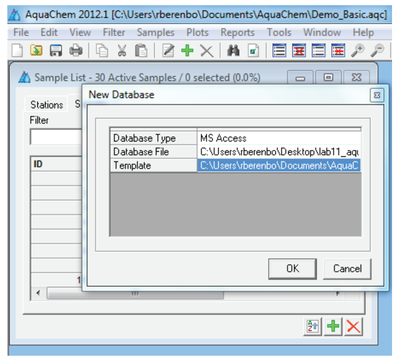




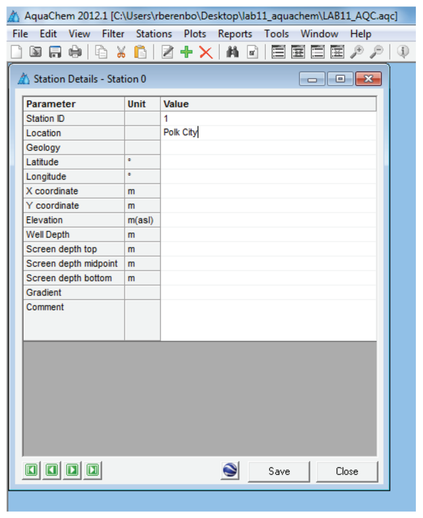
3. Create a new file for your work. Click on ‘file’ in the left top corner then click new. This will show up the following dialog box. Type the name for saving your work and select a folder where you want to save your work.



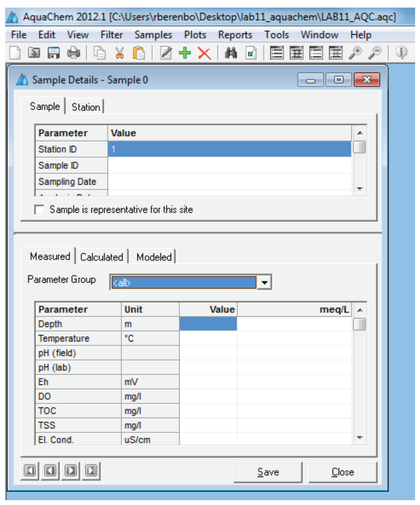
4. A dialog window shows up asking you to select a template. Click on the right corner of the template to show up another dialog window. Click on document > AquaChem then select Template_Basic.TPL. Click OK



5. To enter your data (5 samples): Click on the plus sign to add attribute data for your hydrochem data



6. Save your attribute data, close the dialog window and click on samples to add your chemical data. Click the plus sign again to add your data



Data Analysis

A. Graphical Plotting

Use the plots menu on the main menu bar to plot your data on Piper and Schoeller diagrams

Distinctively label each sample on the diagrams. Explore a way to do this or get help from your instructor

B. Analytical Accuracy and Thermodynamic Calculations

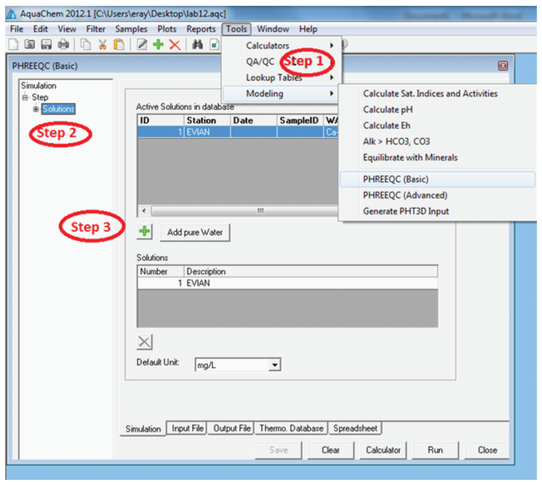
Perform calculation of ionic strength, activity, activity coefficient, speciation, and saturation indices using Phreeqc integrated with Aquachem

In AquaChem, go to file then select preferences, select set up phreeqc database, executable etc in the dialog window.

Next, click on the tools menu > Modeling > PHREEQC (Basic)

In the Opened PHREEQC window, click to highlight solutions as shown in step 2 then select Active Solution in database

In step 3 add the sample as solution then finally run PHREEQC.



To Be Turned-In

(i) Potentiometric surface map with your flowpaths drawn with arrows indicating groundwater flow direction in the vicinity of the selected wells

(ii) For each of the groundwater samples, report in a table format their charge balance error, ionic strength, activity coefficient, and activities of the major ions.

(iii) For each of the groundwater samples, please report in a table format their IAP and SI. Comment on the saturation state of the minerals (calcite, dolomite, halite, and gypsum) for each of the groundwaters

(iv) Discuss and draw conclusions about groundwater flow from one sample location to another location based on your interpretations the values of saturation indices, plots of the chemical data on Piper and Schoeller diagram. Indicate this direction on the map (potentiometric surface map) provided. Does the flow direction indicated by the potentiometric surface agree with what you have delineated using groundwater chemistry?

References

Back, W., Hanshaw, B.B., 1970. Comparison of chemical hydrogeology of the carbonate Peninsulas of Florida and Yucatan. Journal of Hydrology, vol.10, 330 - 368.