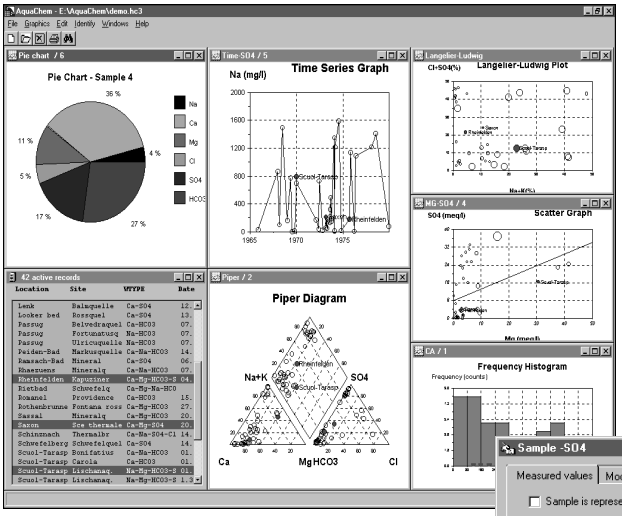
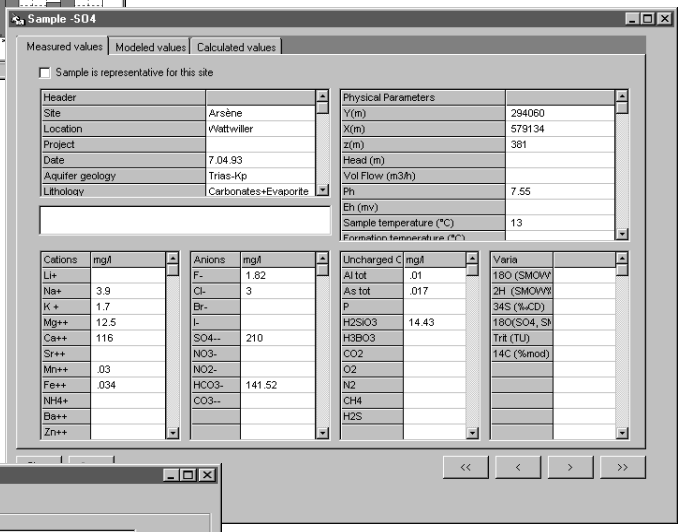
AquaChem for Windows 95/NT

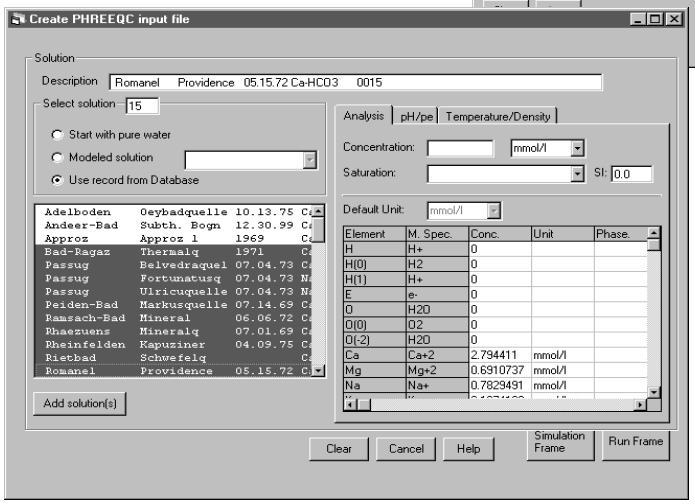
Aqueous Geochemical Analysis, Plotting and Modeling



Comprehensive selection of graphical methods for analyzing, interpreting and plotting data



Convenient data entry forms provide easy access for viewing and editing data



Graphical interface to PHREEQC for geochemical modeling

AquaChem Demo

Introduction

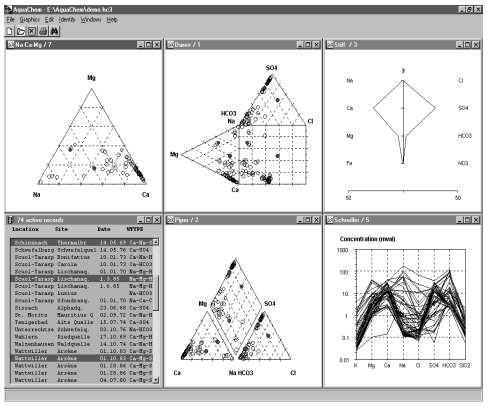
Welcome to the AquaChem Demonstration Guide!

AquaChem is a fully-integrated software package developed specifically for graphical and numerical analysis and modeling of aqueous geochemical data sets. It features a fully customizable database of geochemical parameters and it provides a comprehensive selection of analysis tools and graphical techniques commonly used for interpreting and plotting aqueous geochemical data.

AquaChem's analysis tools cover a wide range of functions and calculations ranging from simple unit transformations, charge balances and sample mixing to more complex functions such as correlation matrices and geothermometer calculations. These powerful analytical capabilities are complemented by a comprehensive selection of commonly used graphical techniques including:

- Piper, Durov, and ternary diagrams,
- Langelier-Ludwig and Schoeller graphs,
- Radial and Stiff plots, and pie charts,
- X-Y Scatter graphs, frequency histograms, and time-series graphs, and
- Geothermometer plots

Each of these graph types provide a unique interpretation of the many complex interactions between the groundwater and aquifer materials.



The key feature among all of these analytical and graphical capabilities is that AquaChem provides an extremely flexible environment to work in. With other geochemical plotting packages many of the graphs and calculations are 'hardwired' into the program and cannot be easily changed or modified to use different sets of parameters. With AquaChem, all of the calculations and graphical options are fully customizable so that you can select from any of the available sample records and parameters to create the figures that you need to properly analyse your data.

In addition, AquaChem features a built-in graphical interface to the popular geochemical modeling program PHREEQC for calculating equilibrium concentrations (or activities) of chemical species in solution and saturation indices of solid phases in equilibrium with a solution.

Once you start using AquaChem, you will see that it is truly one of the most powerful tools available for interpretation, analysis and modeling of simple or complex geochemical data sets.

Quick Start

This chapter presents information on:

- the necessary hardware requirements
- installation, and
- AquaChem basics.

Hardware Requirements

To run AquaChem you will need the following minimum system configuration:

- Windows 95, or Windows NT 3.5.1 or later;
- 486 or Pentium PC;
- 16 Mbytes of RAM (in excess of the operating system requirements);
- 20 Mbytes of free hard disk space;
- a Microsoft compatible mouse, and
- a minimum screen resolution of 800 x 600 (1024 x 768 recommended)

If you are running Windows NT, you must have Microsoft Windows NT Service Pack 2 or greater installed. However, Windows NT Service Pack 3 is strongly recommended.

Installing AquaChem

AquaChem must be installed on your hard disk to run. Please read Section 2.1 to ensure that your system meets the requirements before proceeding with the installation. The executable file **setup.exe** is used to install AquaChem.

The installation procedure outlined here assumes that AquaChem will be installed from drive A: (source drive) to drive C: (destination drive). The default installation directory is C:\Program Files\Whi\AquaChem, but may be modified.

To install AquaChem on your hard disk, run the setup application, **setup.exe**, found on disk #1 of the installation disks. To do this,

1) Insert the disk into your disk drive.

2) Enter Windows unless you are already in Windows.

3) Run the installation program by clicking **Start** on the Windows taskbar, choosing **Run** and typing **A:\Setup.exe** in the dialogue box. Click [**OK]** to continue with the AquaChem installation.

4) Click [**OK]** to proceed with the installation.

5) Accept the default path or enter your own path for the AquaChem installation. Click the large computer icon to install the AquaChem files to the specified path.

6) After the installation is complete, click **[OK]**.

NOTE: AquaChem has been designed for a screen resolution setting of 1024 x 768 (although full functionality can still be achieved using a screen resolution of 800 x 600). **AquaChem cannot be properly run using a screen resolution setting of 640 x 480.**

Starting AquaChem

To start AquaChem, you must have it installed on your hard disk. If you have not yet installed AquaChem, refer to the installation instructions on the previous page. Otherwise click **Start**, choose **Programs**, and click **AquaChem**.

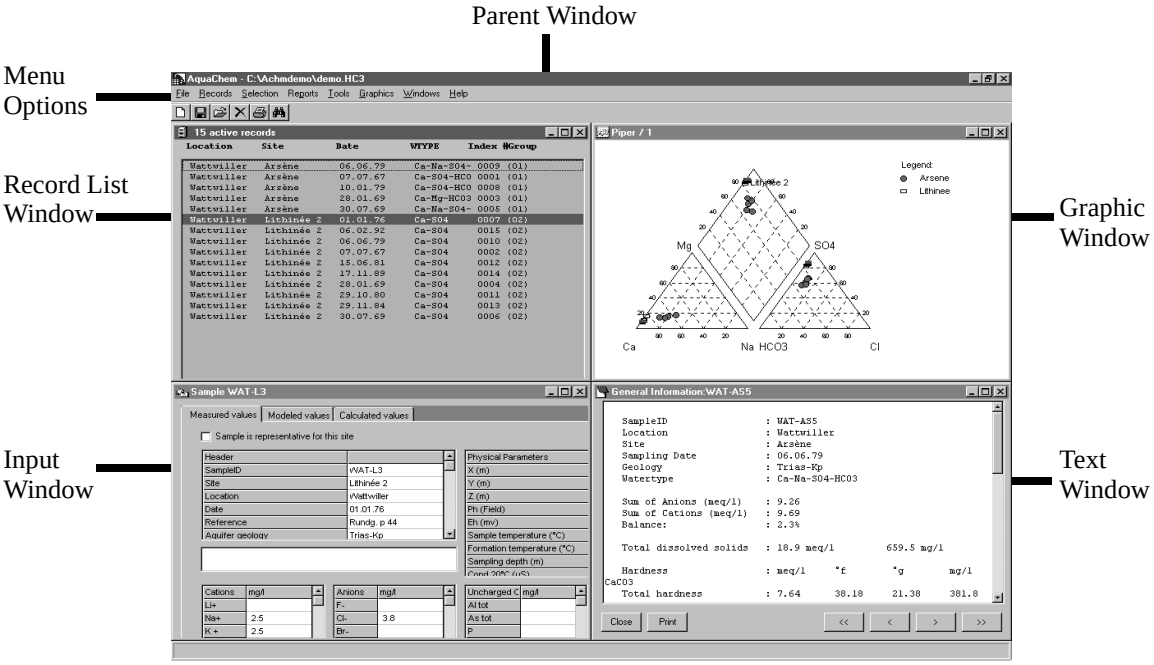
The Open Database dialogue box will be displayed prompting you to choose an existing AquaChem database. Click **[demo3.hc3]** to open the demonstration database.

NOTE: demo3.hc3 should be located in **C:\Program Files\WHI\AquaChem**

Getting Around in AquaChem

The integrated environment in AquaChem consists of five types of windows and menu options as shown in the figure below.

NOTE: Multiple windows may be open at the same time, including multiple windows of the same type. Each type of window has a different set of menu options which appear at the top of the parent window when the window is active. The **Record List** window is considered the **Main Menu**.



Screen Layout

Any of the windows can be minimized to an icon at the bottom of your parent window and reopened as needed. Windows can be arranged on the parent window using the **Windows\Tile Horizontal** or **Tile Vertical** command, which are available from all menus.

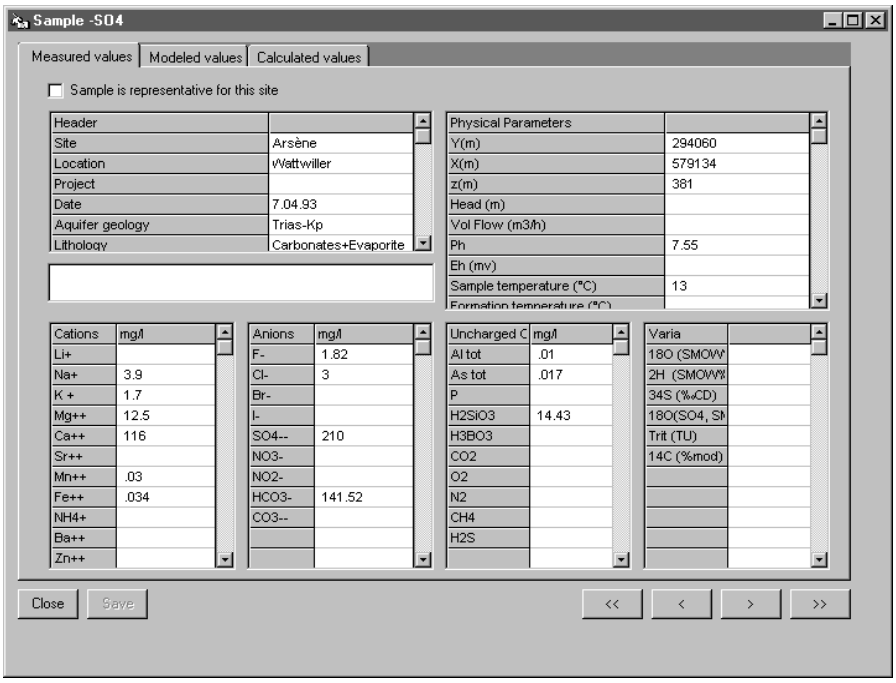
The Record List

The Record List window will always appear when you open an AquaChem database and will remain on-screen as long as the project database is open (i.e the **Record List** cannot be closed unless the project database is closed). The **Record List** contains summarized information about every active record in the database. The column headings displayed in the **Record List** window can be changed by selecting **File\Preferences** from the menu options. To work with a subset of the whole database, you can temporarily omit selected samples by choosing the **Selection\Omit Selected** menu option. Any samples that you omit can be re-displayed by selecting the **Selection\Show All** menu option.

The Input Window

Records can be created, edited, or viewed in the **Input** window (see the figure below). To display this window for a record in your database, double click the sample in the **Record List** or select **Records\Edit** from the **Main Menu**. You can view the **Input** window for other records by selecting the **Record\Previous** or **Record\Next** menu option. This can also be done by clicking on the push buttons at the bottom of the text window or by using the **<F8>** and **<F9>** keys.

To enter or edit a parameter in the **Input** window, click in the cell of the parameter that you want to edit, then type the new value and press **<Enter>** to accept this value. Use the up and down arrow keys to navigate through the list of parameters. Any value that you enter in the active cell will replace the existing value and will be saved to the database as soon as you advance to the next record (or click the **[Save]** button). The values in the **Calculated values** tab are automatically calculated by AquaChem and cannot be edited.



The Text Window

The text windows provide reported information on a selected sample(s) from the database. The reports can be accessed by highlighting a sample in the **Record List** and selecting one of the reports from the **Reports** menu option. The three text reports available are: 1) **General,** 2) **Isotopes**, and 3) **Drinking Water Regulations**. Text reports for other samples can be viewed by selecting the **Record\Previous** or **Record\Next** menu option. This can also be done by clicking on the push buttons at the bottom of the text window or by using the **<F8>** and **<F9>** keys. The text reports can be edited, printed, written to a text file, or copied and pasted to another Windows application.

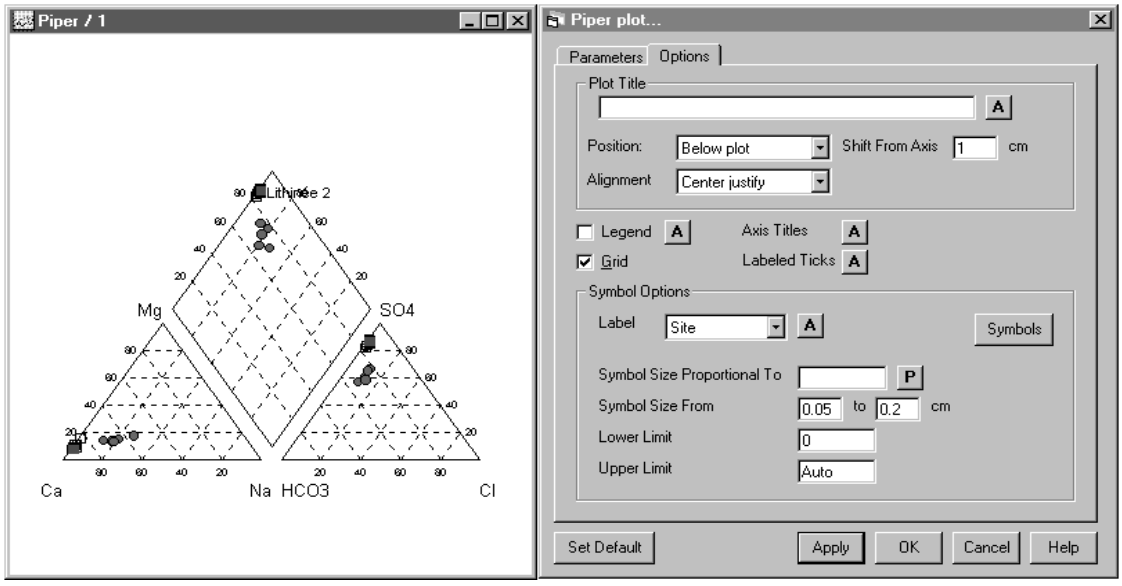
The Graphics Window

AquaChem provides you with a selection of thirteen different plotting techniques commonly used for analyzing and interpreting aqueous geochemical data sets. Follow the steps listed below to create a graph of the sample records in your demo database.

REMINDER: The **Record List** window must be selected to access the **Graphics** menu option.

1) Select **Graphics\New** from the **Main Menu**.
2) Choose the appropriate graph from the list. (a popup window will appear)
3) Fill in the desired parameters in the popup window.
4) Click [**Apply]** or [**OK]**. (The graph window will appear)

It is important to remember that the data plotted on the graphs are directly linked to the database. Any changes to the data are immediately reflected in each of the open graphs (you can have more than one graph open at any time). Changing the number of records in the **Record List** automatically updates all graphs, and clicking a data point on a graph selects the corresponding record in the **Record List** (it also highlights the corresponding data points in the other open graphs).



The AquaChem Database

The data for each AquaChem project is stored in an AquaChem database file that has a ".HC3" file extension. The data structure for each record in the database (i.e. the selected geochemical parameters and the order that they appear) is stored in a maskfile that has a ".MSK" file extension.

Although it is easy to setup your own customized data structure, it is likely that you will be able to utilize the data structure of the demonstration database (DEMO.MSK) since it contains parameters that are commonly used in aqueous geochemical analyses and investigations.

The AquaChem database contains ten distinct parameter groups. Nine of these parameter groups consist of parameters that need to assigned by the user:

- **Header Info**
- **Physical Data**
- **Cations**
- **Anions**
- **Uncharged Compounds**
- **Variable**
- **PHREEQC Description**
- **PHREEQC Minerals**
- **PHREEQC Activities**

The other parameter group is the **Calculated Parameters** (sum cations, sum of anions, ion balance, hardness, alkalinity, etc.) which are automatically calculated by AquaChem based on the values of specific parameter fields.

Data can be entered into the .HC3 database file by either;

(i) importing a tab-delimited ASCII text file;

(ii) using the **Input** window, or

(iii) using the **Spreadsheet** window.

Once the data is entered into the AquaChem database, it may be conveniently viewed and modified using either the **Input** window or the **Spreadsheet** window. The **Input** window is typically used to view/edit all of the parameter measurements from a single record, while the **Spreadsheet** window is used to compare measured parameter values from multiple records.

Data Classes

There are three classes of data available in AquaChem: assigned text parameters, assigned numeric parameters, and calculated parameters. The Header Info data group contains descriptive text information, while all the other parameter groups contain numeric information for the measured and calculated parameter values. These data classes are described in the following sections.

Text Parameters

The following fields provide a text description of each sample record in the database:

Name	Length	Description
Site	30	Name of the borehole or spring
Location	30	Location of the sampling site
Date	8	Sampling date, format is "DD.MM.YY" "D.M.YY" is also accepted
SampleID	15	Identification tag associated with each individual sample
Geology	15	Name of the aquifer formation e.g. Jura-u for upper Jurassic
Lithology	20	Aquifer lithology e.g. sandstone, granite etc...
Reference	30	Either the laboratory sample label or the reference if the analysis is copied from literature
Zone	20	Zone can help in identifying samples from the same area
WType	20	Water type is automatically calculated according to the composition of the major elements
Comment	40	Additional remarks
Project	10	Name of the project

New text fields can be easily added to an existing database by selecting **File/Preferences/ Data Structure**.

Numeric Parameter

The numeric parameters are subdivided into the following groups:

- physical parameters (e.g. x-y-z coordinates, temperature, pH, etc.),
- cations (e.g. Ca, Na, K, Mg, etc.),
- anions (e.g. Cl, Fl, SO4, F, HCO3),
- uncharged chemical components (e.g. SiO2, gas concentrations, B, P etc.)
- variable parameters (e.g. isotopes, bacteria), and
- modeled parameters (e.g. saturation indices, activities).

This order cannot be changed.

Although you may add new parameters to the database, you should not change the spelling of existing parameter names since many of them are used by AquaChem to automatically calculate hardness, alkalinity, ion balance, etc. For example, the name for silicon is always SiO_2, whether you enter your data as SiO_2, H_2SiO_3, or Si. The aqueous species is specified by the formula weight and the charge of the ions, not by its name.

Calculated Parameters

AquaChem automatically performs a number of calculations commonly used in aqueous geochemical data analyses and interpretations. These calculations are described in the following table. In order for AquaChem to properly perform these calculations, the corresponding database parameters must be included in the database with the default naming convention supplied with AquaChem.

Name	Required Parameters	Description
Sum Cations	major cations	sum of major cations in milliequivalents
Sum Anions	major anions	sum of major anions in milliequivalents
Molality	major ions	molal sum of all elements
Charge Balance	major ions	charge balance between major anions and cations
Total hardness mmol/l	Ca, Mg	Ca+Mg in mmol
Total hardness, ° f	Ca, Mg	Ca+Mg in French degrees
Total hardness, ° g	Ca, Mg	Ca+Mg in German degrees
Alkalinity, mmol	HCO_3^-	HCO_3^- in mmol/L
Alkalinity ° f	HCO_3^-	HCO_3^- in French degrees[1]
Alkalinity ° g	HCO_3^-	HCO_3^- in German degrees[2]
SAR	Na, Ca, Mg	sodium adsorption ratio
Adjusted SAR	Na, Ca, Mg, HCO_3^-	adjusted Sodium adsorption ratio
TDS	major ions	sum of chemical elements
z(^{18}O)*	^{18}O	estimated infiltration height based on ^{18}O conc.
z(^{2}H)*	^{2}H	estimated infiltration height based on ^{2}H conc.
T(^{18}O)*	^{18}O	estimated average annual temperature of recharge area based on ^{18}O concentration
T(^{2}H)*	^{2}H	estimated average annual temperature of recharge area based on ^{2}H concentration
H_H_2Ol Jg	temperature	enthalpy of liquid water
H_H_2Ov Jg	temperature	enthalpy of steam

[1] 1.0 German degree = 17.8 mg $CaCO_3$/L

[2] 1.0 French degree = 10 mg $CaCO_3$/L

* Needs the coefficients of the equations which describe the altitude and temperature isotope relation.

Tutorial

This concludes the basic description of the data structure and interface layout for AquaChem. The following sections provide a tutorial to guide you through some of the key features and applications of AquaChem for analyzing, interpreting and plotting aqueous geochemical data.

Introduction

This exercise is a step-by-step example of some of AquaChem's key features and analysis capabilities. You will use AquaChem to query the database, calculate various hydrochemical properties, and create a variety of common aqueous geochemical graphs. The example study seeks to characterize water samples from two mineral springs that are fed by the Muschelkalk aquifer located in Alsace, France. The water from the Lithinee mineral spring is used for mineral water, while the water from the Arsene site is a mixture of ascending mineral water and surficial water

Terms and Notation

The following terms and notations will be used:

type	Type in the given word or value
select	Click the left mouse button where indicated
↦	Press the **<Tab>** key
↵	Press the **<Enter>** key
☞	Click the left mouse button where indicated
☞☞	Double-click the left mouse button where indicated

The **bold faced type** indicates menu or window items to click, or values to type.

[...] denotes a button to click.

...\...\... denotes a menu selection.

The **Main Menu** is displayed when the Records List window is active.

The **Graphics Menu** is available when a graph window is active.

The **Input Menu** is available when the Input window is active.

Starting AquaChem

To start AquaChem, you must have the demo program installed on your hard disk. If you have not yet installed AquaChem, go to page 3 for installation instructions. Otherwise, click **Start-Programs-WHI Software-AquaChem**.

type	**demo.hc3**	(in the Open Database dialog box)
☞	**[Open]**	

A **Record List** window will appear with some summary information for the records from the sample database. The displayed summary information can be customized by selecting **File/Preferences** from the **Main Menu** and adding or subtracting items from the **Record List Columns** frame. The available parameters are listed in the box on the left-hand side of the frame. To remove an item, double-click on the target item and press the **<Backspace>**

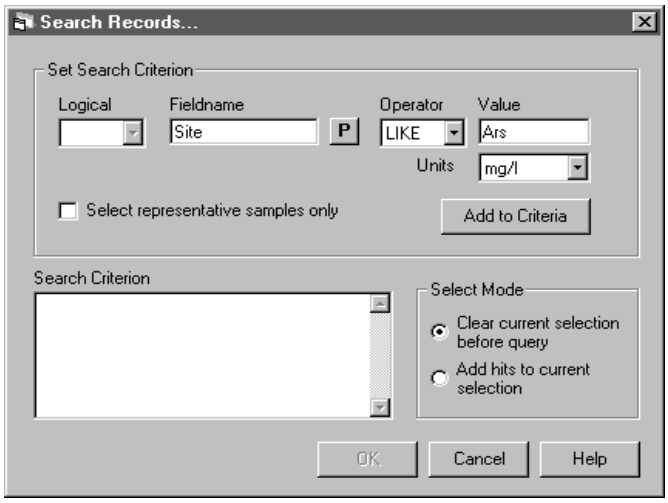
key. To add an item, double-click the open field and select the desired parameter from the list of available parameters. Alternatively, press the **[P]** button to load the **Parameters** window and then drag the desired parameter from into the target Record List Columns field.

To see how your new selections look, press the **[Apply]** button at the bottom of the window.

Once you have a **Record List** that you like, click the **[Save]** button to return to the **Main Menu**.

Querying the Database

From the **Main Menu**, select **Records\Search**. The Search Records dialog box will appear.



In this example you will search the database for all records from the Arsene site.

In many instances you will not remember the exact name of the parameter that you want to search for, so AquaChem provides a parameter list of all available parameters for the open database. To activate and display the Parameters window:

☞ **[P]** (under Set Search Criterion)

Now click and drag '**Site'** from the **Parameter List** window into **Fieldname** text box. The parameter '**Site'** should now appear in the **Fieldname** text box.

Click the arrow button under **Operator**, and choose '**LIKE'** from the drop down menu.

type **Ar** (in the **Value** text box)

☞ **[Add to Criteria]**

'Site = Ar' should now appear in the **Search Criterion** text field.

☞ ⊙ **Clear current selection before query**

☞ **[OK]**

All of the Arsene samples should now be selected in the **Record List**.

NOTE: Since the demo database contains only 28 records you could have manually selected these records from the **Record List**. However, with larger project databases, the search tool is a very convenient method of identifying records of interest.

Defining Symbol Groups

In the demo database there are two distinct groups of data; one group belonging to samples from the Lithinee site and the other group belonging to samples from the Arsene site. In order to easily identify the data points from these two groups on a plot, it is necessary to assign a specific symbol to each group. Each symbol group has a defined number, symbol shape and color for easily identifying the associated sample records in the **Record List** and on a graph.

To assign the Arsene records to a symbol group,

NOTE: All of the samples from the Arsene site should still be selected (highlighted) in the Record List. If you have inadvertently caused the records to become unselected, please repeat the Querying section.

☞ **Selection/Assign Symbol**

An **Assign Symbol** dialogue box will appear displaying a list of available symbol groups. By default, each record is initially assigned to the Default symbol group. The number in brackets beside each Group will be displayed in the **Record List** to show which group the record belongs to.

☞ **Group 1 (01)**

☞ **Assign**

☞ **Close**

Notice that the Arsene records now have a '(01)' displayed under the **Group** column heading. This indicates that these Arsene records are assigned to Group 01.

Now from the **Main Menu**, select **Selection/Invert**.

All of the Wattwiller samples from the Lithinee site should now be selected.

To assign the Lithinee records to a symbol group,

☞ **Selection/Assign Symbol**

An **Assign Symbol** dialogue box will appear displaying a list of available symbol groups.

☞ **Group 2 (02)**

☞ **Assign**

☞ **Close**

Notice that the Lithinee records now have a '(02)' displayed under the **Group** column heading.

Analyzing the Data

General Report

To create a general summary report of the chemical properties of sample 0004:

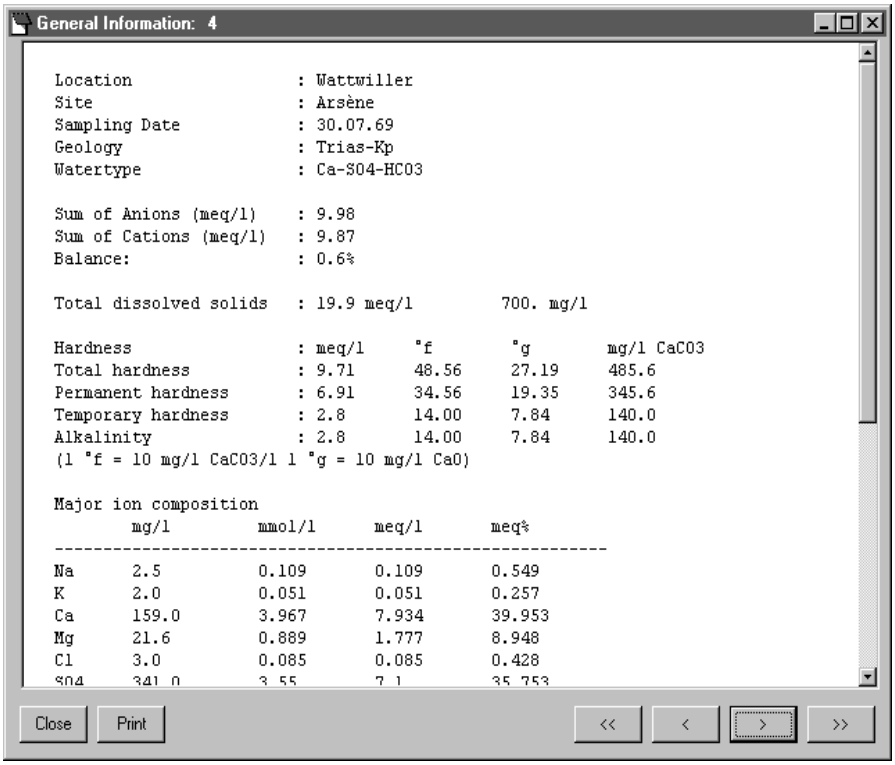
Select the record with the index number 0004.

From the **Main Menu**, select **Reports\General**.

The General Information report window will be displayed as shown in the following figure.

To view the General Information report for other samples, select **Records\Previous** and **Records\Next** from the active menu bar or click the push buttons on the bottom right-hand side of the text window.

The General Information report can be printed, saved to a text file or copied and pasted into a spreadsheet or report document for formatting.



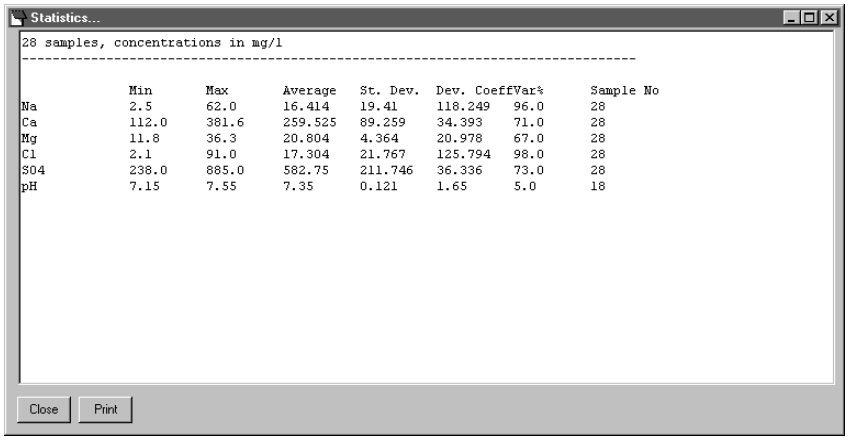
Calculating a Statistical Report

To view a statistical analysis of the Wattwiller samples:

From the **Main Menu**, select **Tools\Statistics**. A Statistics dialogue box will display the default settings for the parameters that will be used for the statistical analysis.

☞ **[OK]** (to accept the default settings)

The minimum, maximum, arithmetic mean, standard deviation, as well as other values of interest will be calculated for the default parameters.



	Min	Max	Average	St. Dev.	Dev. Coeff	Var%	Sample No
Na	2.5	62.0	16.414	19.41	118.249	96.0	28
Ca	112.0	381.6	259.525	89.259	34.393	71.0	28
Mg	11.8	36.3	20.804	4.364	20.978	67.0	28
Cl	2.1	91.0	17.304	21.767	125.794	98.0	28
SO4	238.0	885.0	582.75	211.746	36.336	73.0	28
pH	7.15	7.55	7.35	0.121	1.65	5.0	18

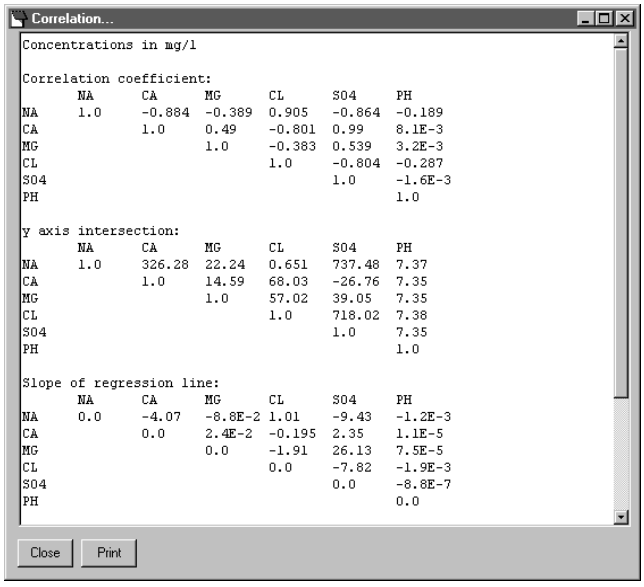
Calculating a Correlation Matrix

To calculate a correlation matrix for the major ions:

From the **Main Menu**, select **Tools\Correlation matrix.**

☞ **[OK]** (to accept the default settings)

A correlation matrix will be plotted for the default parameters as shown in the figure below.



Correlation coefficient:

	NA	CA	MG	CL	SO4	PH
NA	1.0	-0.884	-0.389	0.905	-0.864	-0.189
CA		1.0	0.49	-0.801	0.99	8.1E-3
MG			1.0	-0.383	0.539	3.2E-3
CL				1.0	-0.804	-0.287
SO4					1.0	-1.6E-3
PH						1.0

y axis intersection:

	NA	CA	MG	CL	SO4	PH
NA	1.0	326.28	22.24	0.651	737.48	7.37
CA		1.0	14.59	68.03	-26.76	7.35
MG			1.0	57.02	39.05	7.35
CL				1.0	718.02	7.38
SO4					1.0	7.35
PH						1.0

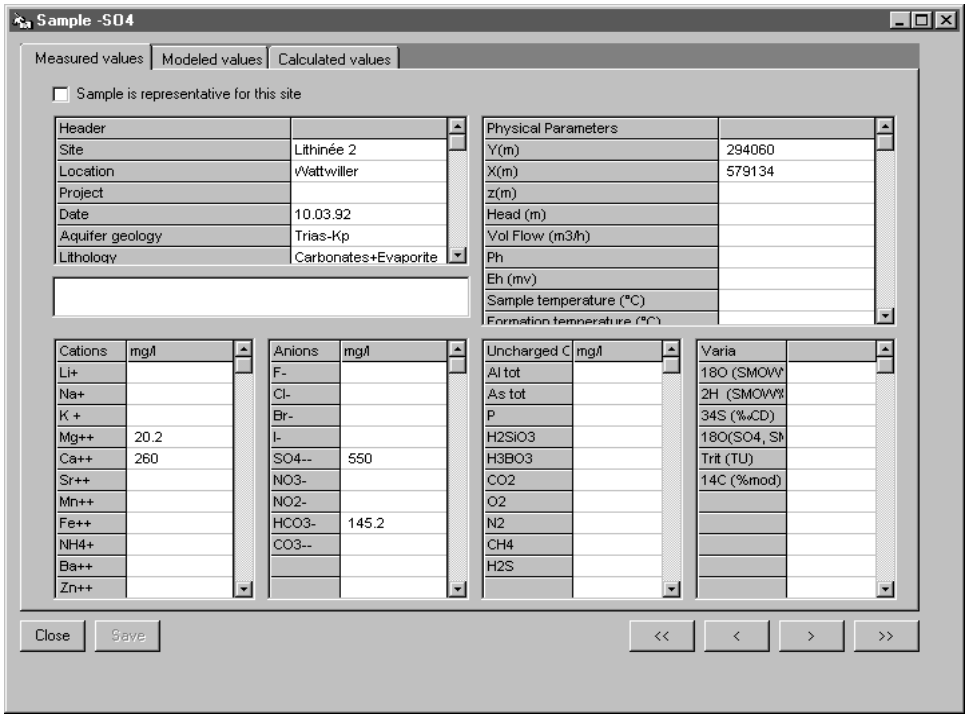
Slope of regression line:

	NA	CA	MG	CL	SO4	PH
NA	0.0	-4.07	-8.8E-2	1.01	-9.43	-1.2E-3
CA		0.0	2.4E-2	-0.195	2.35	1.1E-5
MG			0.0	-1.91	26.13	7.5E-5
CL				0.0	-7.82	-1.9E-3
SO4					0.0	-8.8E-7
PH						0.0

Please close all report windows before proceeding to the next section of the tutorial (click the 'X' in the top right-hand corner of the Text Windows).

Editing the Data

In this example you will not be able to save any modifications to the database since this is only a demo version of the software. However, the **Input** window is fully operational and is generally used to view/edit all of the measured data for a single sample record. To activate the **Input** window simply double-click on any record in the **Record List** (or right-click on a record and select **Edit**). The **Input** window should appear as shown in the following figure.



To change the displayed concentration units select **Unit/meq/L** from the top menu bar. All of the measured values for the Cations, Anions and Uncharged compounds will be immediately updated to reflect the new concentration units.

In some instances you may not have information on one of the major ions. AquaChem allows you to calculate the concentration of the missing ion based on a valence balance. To see how this works you must first delete the Na value for the open record.

Click in the **Na+** field under the Cations parameter group calculate the concentration of Na by selecting **Calculate/Missing/Na** from the top menu bar of the AquaChem parent window. The calculated value should be quite close to the original value. Similarly, you can also calculate the missing concentrations of any of the major ions.

Close the **Input** window by clicking the 'X' short cut button in the top right corner.

Graphing the Data

AquaChem allows you to create 13 different types of graph commonly used for aqueous geochemical data analysis and interpretation. The following sections of the tutorial will describe how you can easily create, customize and display multiple graph types.

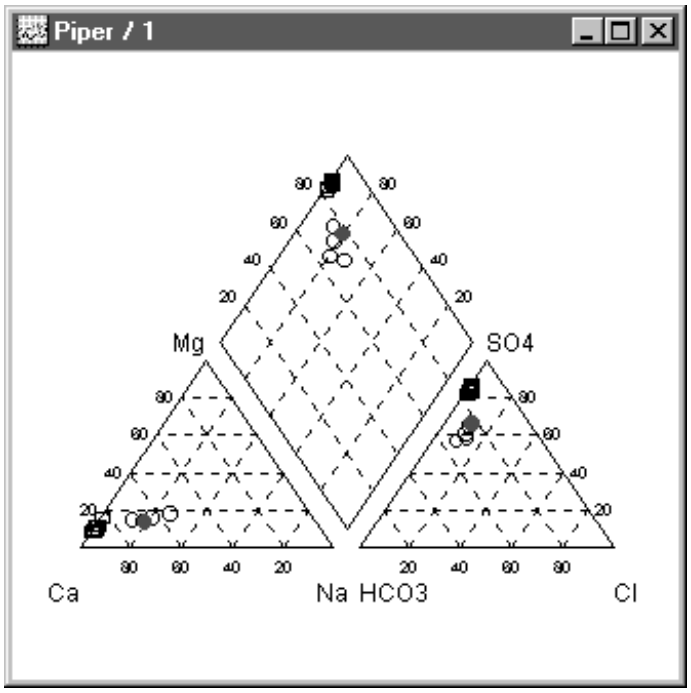
Piper Plot

Piper graphs provide an overview of the chemical composition of the samples. You will usually find it useful to start your analysis with a Piper graph.

From the **Main Menu**, select **Graphics\New\Piper**.

☞ **[OK]** (to accept the default settings)

This plot clearly indicates that there are two distinct groups of data. The circles on the plot represent the Arsene samples (Group 01), and the squares on the plot represent the Lithinee records (Group 02). The location of these groups corresponds to the water type classification of the records in each group. Notice that the mineral water samples from the Lithinee site are all located in the Ca-SO_4 sector, whereas the surficial water samples from the Arsene site are located throughout the Ca-Na-SO4, Ca-SO4-HCO3, and the Ca-Mg-HCO3 sectors.



Notice that if you click on a sample point in the graph, the corresponding record will be selected in the Record List. In addition, you can also place a label beside each of the selected sample points.

To open the graphic options dialogue box you must right-click on the open graph window (in this case, right-click on the Piper plot). A **Piper plot** graphic options dialogue box will then

appear. Notice that each graphic options dialogue box has a **[Set Defaults]** button that allows you to save the appearance settings for each of the graph types.

☞ **Options** tab

The **Options** tab allows you to modify the appearance of the graph by adding a title, changing the fonts, adding a legend, or removing the grid. It also provides options for customizing the appearance of the graph symbols.

To label the symbols,

☞ **Label** (in the Symbol Options frame)

☞ **Site** (from the list of available symbol labels)

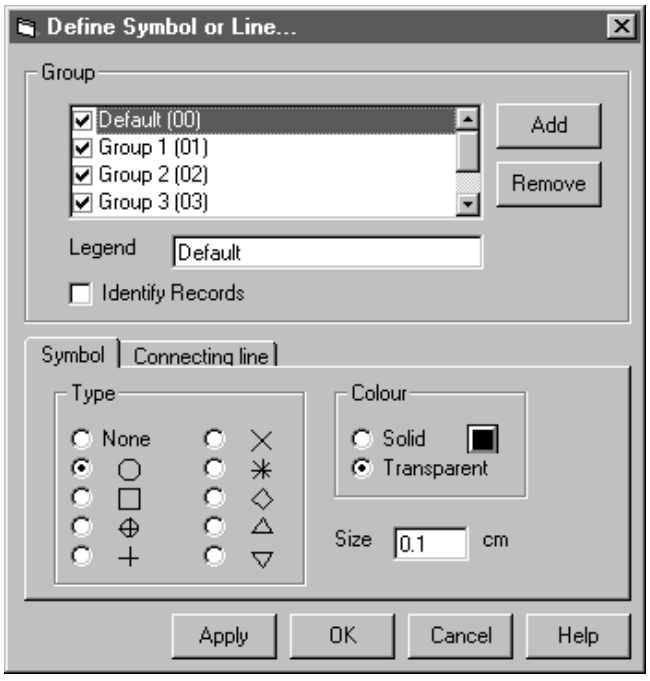
☞ **[Apply]** to accept this change

Now all of the highlighted symbols on the Piper plot will have labels.

To change the name, shape and color of the symbols,

☞ **[Symbols]**

A **Define Symbol or Line** dialogue box will appear as shown below.



The list of available Groups is shown in the list box with a checkbox to indicate which ones are active. Initially there are six available groups and all are active. These groups can be removed or new groups can be added to the list. The names of the groups will be displayed in the legend of each plot. These names can be easily changed by clicking on the group name and entering a new name in the **Legend** text box.

Select **Group 01 (01)** and change the name to Arsene (press **<Enter>** to accept the change).

Select **Group 02 (02)** and change the name to Lithinee (press **<Enter>** to accept the change).

The symbol shape for each group is indicated in the **Symbol** tab in the bottom half of the dialogue box. The symbol shape associated with each group can be easily changed to any of the symbol shapes provided. For this example you will not adjust the symbol shapes.

☞ **[OK]** (to accept the remaining symbol settings)

You are now returned to the Piper plot graphic options dialogue box.

To display a symbols legend with the Piper plot,

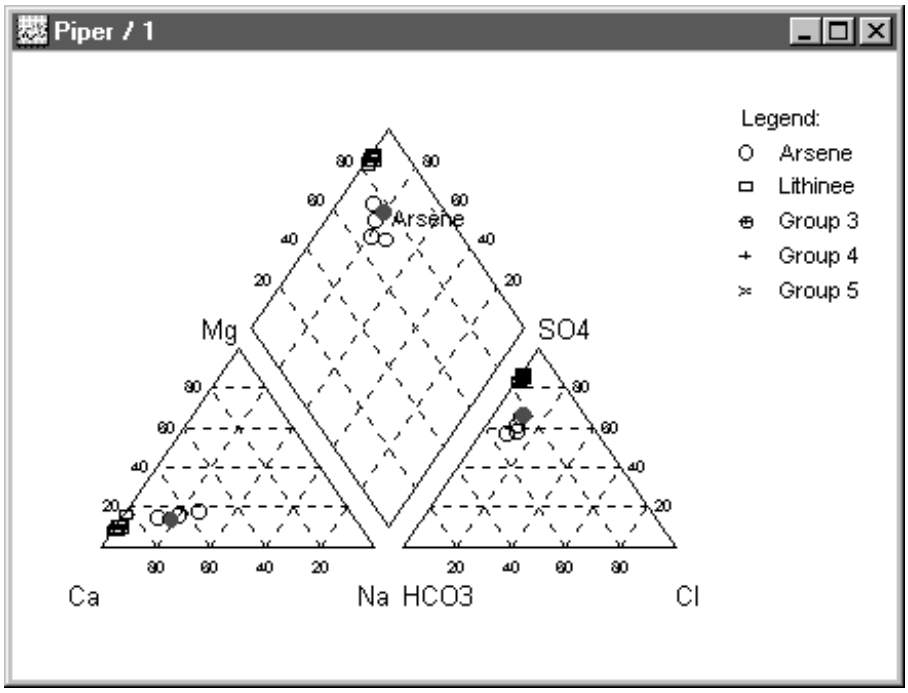
☞ **Legend** (to activate the checkbox)

☞ **[Apply]** (to apply these changes to the Piper plot)

☞ **[Set Defaults]** (to save the Piper plot settings)

☞ **[OK]**

The legend will be plotted along the right-hand side of the Piper plot graphics window. Stretch the window to the right to display the entire legend (as shown in the following figure).



Notice that all of the groups are listed in the legend because all of the groups are initially set to active. If you assign a record(s) to these groups then the graph will be automatically updated to reflect the appropriate symbol shape. Alternatively, you can remove these groups from the legend by deactivating them (select **Edit/Symbol or Line** from the **Graphics** window menu bar).

Schoeller Graph

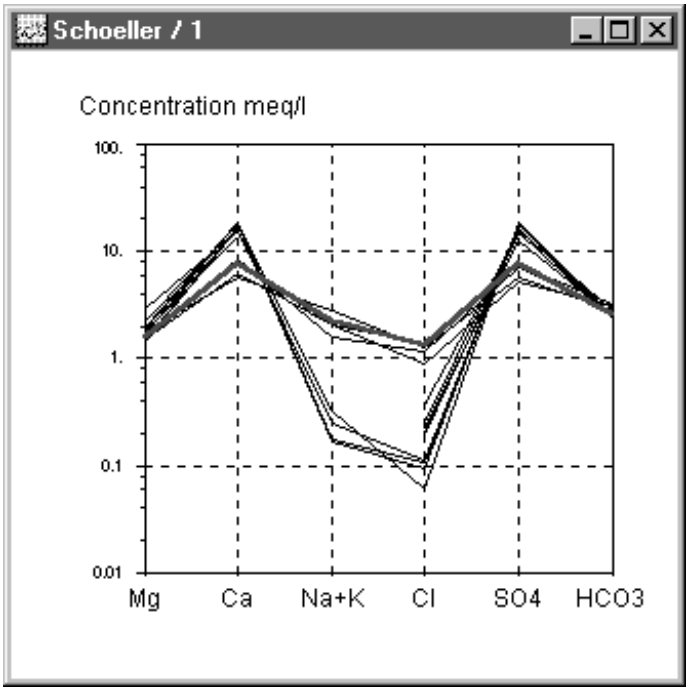
Next you will plot a Schoeller graph to evaluate the concentrations of the major ions for each record in the database.

From the **Main Menu**, select **Graphics\New\Schoeller**.

A **Schoeller plot** graphic options dialogue box will

☞ **[Apply]** (to accept the default settings)

A Schoeller graph will appear as shown in the figure below. This graph provides a comparison of the log of the concentrations of the major ions for each sample record in the database.



The highlighted line on the graph corresponds to the selected record in the **Record List**. To see the legend and the symbols, select the **Options** tab in the **Schoeller plot** graphic options dialogue box.

☞ **Legend**

☞ **Symbols**

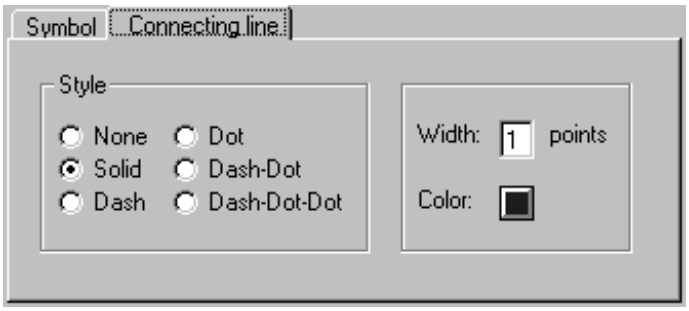
☞ **[Apply]**

To modify the line settings,

☞ **[Symbols]**

The **Define Symbol or Line** dialogue box will appear.

Select the **Connecting Line** tab to access the line appearance options as shown in the following figure.



☞ **Arsene (01)** (in the list of groups)

☞ **Dash**

☞ 

A color selection dialogue box will appear. Choose one of the blue shades.

☞ **[OK]**

☞ **[OK]**

The Schoeller graph should now appear with a legend on the right-hand side and blue lines representing the Arsene sample records.

Now you should have both a Piper plot and a Schoeller graph displayed on your screen. Notice that if you select a record in the **Record List**, this record is highlighted on both the Piper plot and the Schoeller graph. In addition, any changes that are made to the sample data will be immediately reflected on both of these plots.

Scatter Plots

To see a direct relationship between only two of the parameters in the sample records it is common to plot an X-Y Scatter graph of the data.

From the **Main Menu**, select **Graphics\New\Scatter**.

A **Scatter plot** graphic options dialogue box will appear with the default settings for plotting an X-Y Scatter graph for Na vs. Cl. You will need to change these default settings.

☞ **[P]** (to load the **Parameter List**)

Then double-click in the **X-Parameter** text box to select Na.

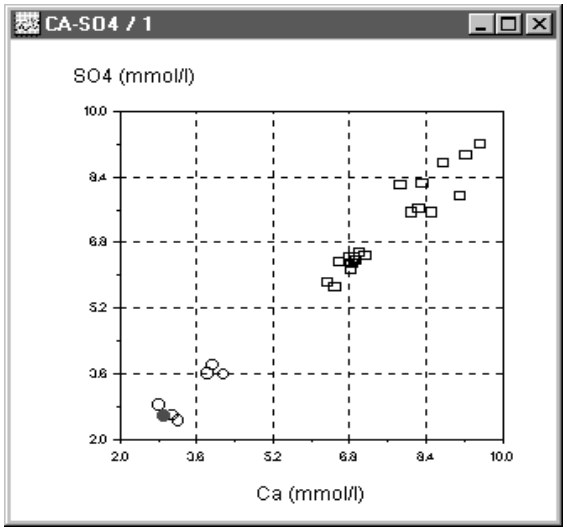
Now search the **Parameter List** for Ca and drag it into the **X-Parameter** text box.

Then double-click on the **Y-Parameter** text box to select Cl.

Now search the **Parameter List** for SO4 and drag it into the **Y-Parameter** text box.

☞ **[Apply]** (to accept the new settings)

A scatter graph will appear as shown in the figure below.

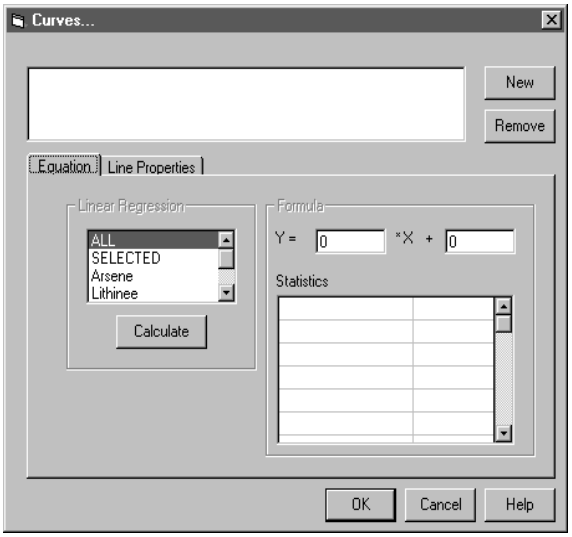


This graph shows an excellent correlation between the concentration of Ca and SO4 in the samples taken from both sites. To determine the exact relationship between these two parameters you can also perform a regression analysis on the data as follows:

Select the **Options** tab in the **Scatter plot** graphic options dialogue box.

☞ **[Lines]**

A dialogue box will appear as show below.



This dialogue box allows you to perform a regression analysis on either; (i) all of the data in the **Record List**; (ii) only on selected records; or (iii) only on selected groups of records

To create a line through all of the records in the demo database,

☞ **[New]**

A line will be created and will be labelled **Line 1**. To perform a regression analysis on **ALL** of the samples,

☞ **[Calculate]**

The equation of the line will then be calculated and displayed along with general statistics on all of the samples.

☞ **[OK]**

The line that you just calculated will be plotted on the X-Y Scatter graph.

However, this is not the only relationship that you can show on this graph (or any graph for that matter). AquaChem also allows you to easily plot the symbol sizes relative to the concentration of any parameter in the database.

Now search the **Parameter List** for '**TDS**' and drag it into the **Symbols Size Proportional To:** text box. The symbol sizes for both the Arsene samples and the Lithinee samples will now be plotted relative to the Total Dissolved Solids (TDS) value for each sample.

☞ **[Apply]** (to accept the new settings)

The scatter graph should clearly show that the samples from the Lithinee site have a higher level of TDS than the samples from the Arsene site.

Radial Plots

The first step is to select any two records from the **Record List** (preferably one from the Arsene site and one from the Lithinee site). To select two records you must click on one records and then press the **<Ctrl>** key while you select another record.

To create a radial plot,

☞ **Graphic/New/Radial**

☞ **[OK]** (to accept the default settings)

Two radial plot will appear for the two records that you selected. To edit the appearance of either of these radial plots simply right-click on them and a **Radial plot** graphic options dialogue box will appear.

At the top of the **Radial plot** graphics option dialogue box there is a combo box that provides a list of the samples that are displayed as radial plots. To view the graph settings for a particular sample you simply select that sample from the list and all of the graphic options will be displayed for that sample.

Now you should have four **Graphics** windows and the **Record List** window displayed on your screen. To arrange these windows,

☞ **Windows/Tile Vertical**

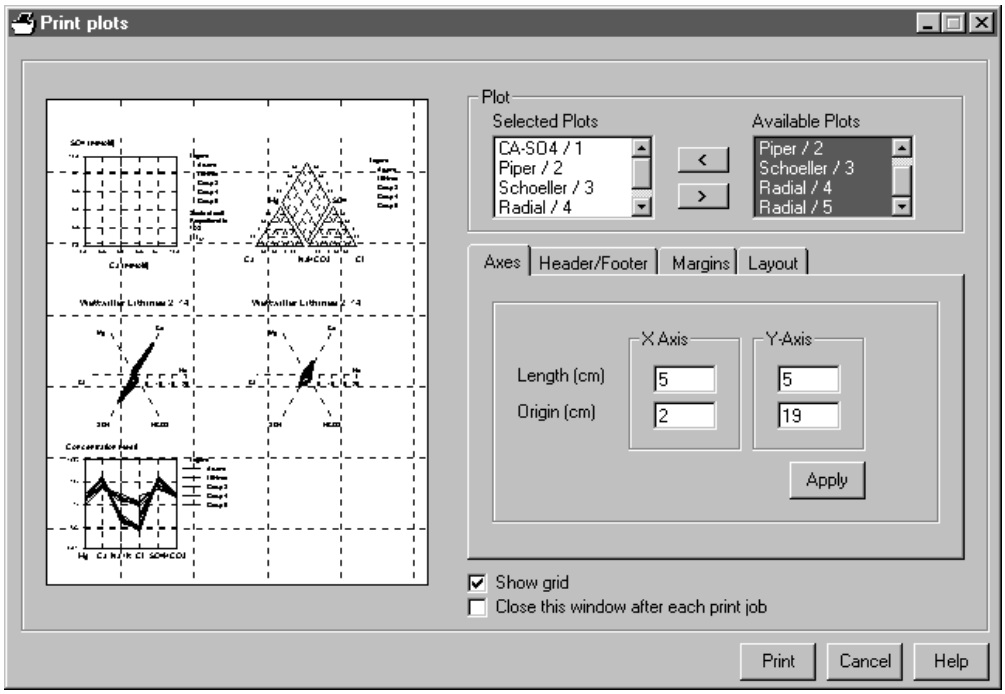
All of the open windows will be automatically arranged on the screen.

Next you will see how you can print these graphs.

Printing the Graphs

From the **Graphics Menu**, select **File\Print** (one of the graphs must be selected first).

You will see the following screen:



A list of **Available plots** will appear on the right-hand side of the **Print plots** dialogue box. Each of these plots will be highlighted indicating that they are selected. To print these plots you must move each of them plots into the **Selected Plots** list.

☞ 

All of the highlighted plots in the **Available Plots** list will be moved into the **Selected Plots** list and will be automatically sized and positioned to fit on the print page. If the default settings are not acceptable, you can easily change the layout settings by selecting the **Layout** tab, or manually change the individual size and position using the **Axes** tab.

Before printing the graphs, you can specify a title and a footer for the plots.

Select the **Header/Footer** tab.

type **Wattwiller Graphs** (in the text field below **Title 1**)

Select the arrow button under the **Header/Footer** tab, and

☞ **Footer** (from the pull down menu which appears)

type **AquaChem, WHI Software** (in the text field below)

Select the option to **Close this window after each print job.**

Once you have finished adding the titles and footer, and adjusting the size and position of the plots to your liking,

☞ **[Print]** (to print the graph)

This concludes the tutorial guide for AquaChem.

Although the purpose of this tutorial guide is to highlight some of the key features and analysis capabilities of AquaChem, it really only scratches the surface of the potential applications for this software package for managing, analyzing, interpreting and plotting aqueous geochemical data. Please continue to explore the program and discover for yourself how truly powerful it is.

If you have any specific questions regarding the features and analysis capabilities of AquaChem, please contact a Waterloo Hydrogeologic technical representative.

To purchase a fully functional version of AquaChem please contact:

Waterloo Hydrogeologic, Inc.
180 Columbia St. W. - Unit 1104
Waterloo, Ontario, Canada, N2L 3L3
Ph. (519) 746-1798
Fax (519) 885-5262
E-mail info@flowpath.com