Demonstration Guide

AquaChem

A Professional Application for Water Quality Data Analysis, Plotting, Reporting, and Modeling

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Introduction to AquaChem

AquaChem is a software package developed specifically for graphical and numerical analysis and modeling of water quality data. It features a fully customizable database of physical and chemical parameters and provides a comprehensive selection of analysis tools, calculations and graphs for interpreting water quality data.

AquaChem's data analysis capabilities cover a wide range of functionalities and calculations including unit conversions, charge balances, sample comparison and mixing, statistical summaries, trend analysis, and much more. AquaChem also has a customizable database of water quality standards with up to three different action levels for each parameter. Any samples exceeding the selected standard are automatically highlighted with the appropriate action level color for easily identifying and qualifying potential problems.

These powerful analytical capabilities are complemented by a comprehensive selection of commonly used plotting techniques to represent the chemical characteristics of water quality data. The plot types available in AquaChem include:

- Correlation plots: X-Y Scatter, Ludwig-Langelier, and Wilcox
- Summary plots: Box and Whisker, Frequency Histogram, Quantile, Detection summary
- Multiple parameter plots: Piper, Durov, Ternary, Schoeller
- Time-Series plots (multiple parameters, multiple stations)
- Geothermometer and Giggenbach plot
- Single sample plots: Radial, Stiff, and Pie
- Thematic Map plots: Bubble, Pie, Radial and Stiff plots at sample locations

Each of these plots provides a unique interpretation of the many complex interactions between the groundwater and aquifer materials, and identifies important data trends and groupings.

In addition, AquaChem features a built-in link 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. For more advanced simulations, you may link to the USGS programs

PHREEQC-I or PHREEQC for Windows, and use your AquaChem samples as input solutions for these modeling utilities.

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 any water quality data set.

1.1 Installing AquaChem

System Requirements
AquaChem requires the following minimum hardware configuration:

Supported Operating Systems:
- Windows 7 Professional, Enterprise or Ultimate
- Windows Vista Business, Ultimate or Enterprise
- Windows XP Pro (SP3)

Note: Home and Starter Versions are not supported.
Processor: Pentium 4, 32-bit or 64-bit
Hard Disk: 100MB
RAM: 2GB or more Recommended
Networking Hardware: Network Card (required for soft-key licensing)

The AquaChem installation package requires the following software configuration:
Microsoft .NET Framework 4.0 or higher
Microsoft Access or Access Run-time Engine

Installation
AquaChem is distributed on one CD-ROM. To install, please follow these directions:
Place the CD into your CD-ROM drive and the initial installation screen should load automatically. Once loaded, an installation interface with several different tabs will be presented.

Please take the time to explore the installation interface, as there is information concerning other Schlumberger Water Services products, our worldwide distributors, technical support, consulting, training, and how to contact us.

On the initial Installation tab, you may choose from the following two buttons: AquaChem Installation and AquaChem User's Manual
The User's Manual button will display a PDF document of the manual, which requires the Adobe Reader to view. If you do not have the Adobe Reader, a link has been created in the interface to download the appropriate software.
The Installation button will initiate the installation of AquaChem on your computer. AquaChem must be installed on your local hard disk in order to run. Follow the installation instructions, and read the on-screen directions carefully. You will be prompted to enter your name, company name and serial number. Please ensure that you enter your serial number exactly as is it appears on your CD case or invoice. Be sure to use capital letters and hyphens in the correct locations.

Once the installation is completed, you must re-boot your computer for the system changes to take effect. After the installation is complete and your system has re-booted, you should see the blue AquaChem icon on your Desktop screen labeled AquaChem 2014.1. To start working with AquaChem, double-click on this icon.

To install the software from the CD-ROM without the aid of the installation interface, you can:
Open Windows Explorer, and navigate to the CD-ROM drive
Open the Installation folder
Double-click the AquaChem_Setup.MSI to initiate the installation
Follow the on-screen installation instructions, which will lead you through the install and subsequently produce a desktop icon for you.

For more detailed instructions on installing and licensing AquaChem please download a copy of the AquaChem Installation and Licensing Guide:

http://trials.swstechnology.com/software/AquaChem/AquaChem Installation & Licensing Guide.pdf

PHREEQC-I Installation

The USGS's PHREEQC-Interactive program is a graphical interface for preparing and running complex geochemical modeling scenarios. AquaChem has a built-in link to the PHREEQC-Interactive program that is capable of launching this program with all selected samples already formatted as modelling input.

The PHREEQC-I must be installed separately; the installation file is available on your CD-ROM under the PHREEQC directory.

Once installed, the PHREEQCI executable must be registered in the Aquachem preferences. It can then be launched from AquaChem (Tools / Modeling / PHREEQC (Advanced) and the input file will automatically be initialized with the chemical composition of the samples that are highlighted in the AquaChem sample list.

PHREEQC for Windows Installation

AquaChem also supports a link to the PHREEQC for Windows program. This program is an alternative graphical interface that also allows for preparing and running advanced geochemical simulations.

If you wish to install and use the PHREEQC for Windows program, the installation is available in the PHREEQC folder on the installation CD-ROM.

These files are also available for download from the USGS - PHREEQC home page: http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

1.2 Uninstalling AquaChem

There may be instances where you will need to uninstall (remove) AquaChem from your system (i.e. if the software is to be transferred to another computer, or you need to reinstall on the current computer). To uninstall AquaChem:

- Locate the **Add/Remove Programs** option in your **Windows' Control Panel**.
- Select **AquaChem 2014.1** as the program to be removed
- Follow the on-screen instructions.
- Once you are finished, re-boot your system to ensure all system files are updated.

1.3 In-Program Help

To view the In-Program help, select Help / Contents. Some AquaChem windows and dialogs contain buttons, which load the appropriate help section for the current active component. The AquaChem Help window is divided into three main areas:

- A Navigation Frame on the left displays the Contents, Index, Search, and Favorites tabs.
- A Toolbar across the top displays a set of buttons to help navigate through the HGA Help system.
- A Topic Frame on the right displays the actual Help topics included in the On-Line Help.

The tabs in the Navigation Frame provide the core navigational features as described below.

Contents
The Contents tab displays the headings in the "Table of Contents" in the form of an expandable/collapsible tree. Closed book icons represent Table of Contents headings that have sub-headings.

Index
The Index tab displays the list of Help topics. You can scroll to find the index entry you want, or you can type in the first few letters of the keyword in the text box, and the index will scroll automatically as you type. Double-click an index entry to display the corresponding Help topic. Alternately, you may select an index entry and then click the Display button to open the Help topic.

Search
The Search tab is used to search the On-Line Help documents for a word or phrase of interest. Simply type the search word(s) or phrase(s), then press Enter or click the Display button.

Favorites
You can add frequently accessed Help topics to a personal list of favorites, which is displayed in the Favorites tab. Once you have added a topic to your list of favorites, you can access the topic by double-clicking it. Click Add to add the currently displayed topic to your favorites list. Select a favorite and then click Remove to delete a topic from your favorites list.

1.4 On-Line Help

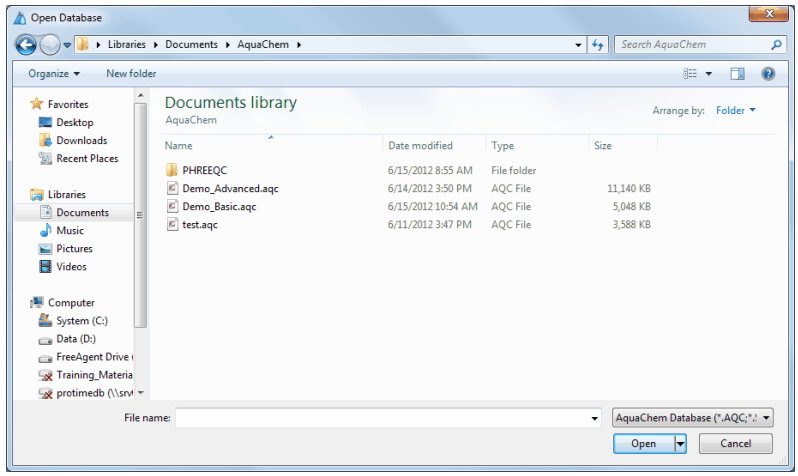
You can also find the AquaChem help on-line:
http://www.swstechnology.com/help/aquachem/2014/

This online version of the Help can be updated more regularly than the help within the program, so check it out for the latest updates to the documentation!

1.5 Starting AquaChem

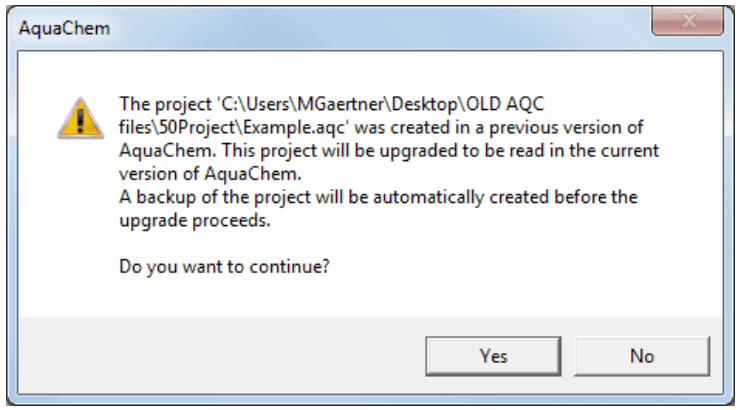
To start AquaChem, you must have the program installed on your hard disk. If you have not yet installed AquaChem, please refer to the section, Installing AquaChem, which is described above. Otherwise start AquaChem by double-clicking on the desktop icon (as shown on the left-hand side), or by accessing
SWS Software/Aquachem 2014.1 from your Start > Programs Windows menu.

Upon starting AquaChem, the following Open Database dialogue will be displayed prompting you to select a valid AquaChem database.



Select the Demo.aqc file to open the demonstration database; to open a different database, browse to the appropriate folder. Otherwise, to create a new database click [Cancel] in this dialogue and select File > New from the main menu.

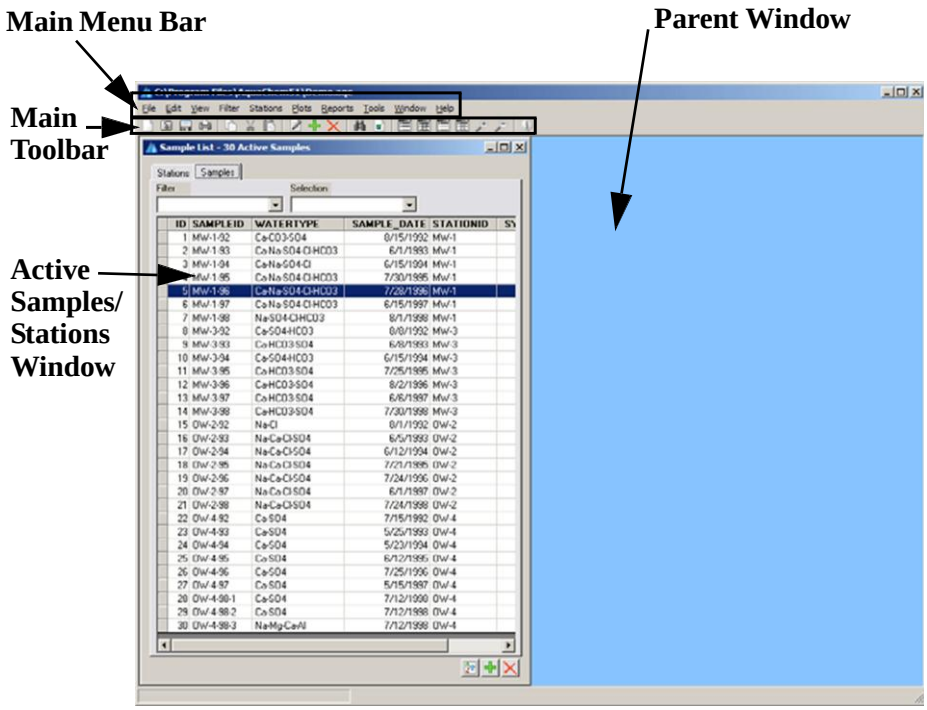
Opening Old Projects
You may open an .AQC file from previous versions of AquaChem.
To open a project from v.4.0 or higher, use the File > Open command. You will be prompted with an Open Database dialogue. Browse to the folder which contains your database and press [Open]. The following message will appear.



If you select [Yes], the AquaChem database will be opened with a screen layout as shown on the next page, or if you select [No] then the option of opening the old project sets will be canceled.

1.6 AquaChem Interface Layout

After opening an AquaChem database file, a screen layout similar to the following figure will appear.



Parent Window is the main AquaChem window which houses all other windows.

Main Menu Bar contains specific menus for graphs and dataset. Depending upon the currently selected window, each window has a distinct set of menu options. A detailed description of each main menu options associated with various windows is provided in Chapter 3: AquaChem Menu Commands of the User's Manual.

Main Toolbar contains specific tool buttons for different options. A detailed description of each main toolbar item is provided in section 1.6 of this chapter, AquaChem Toolbar.

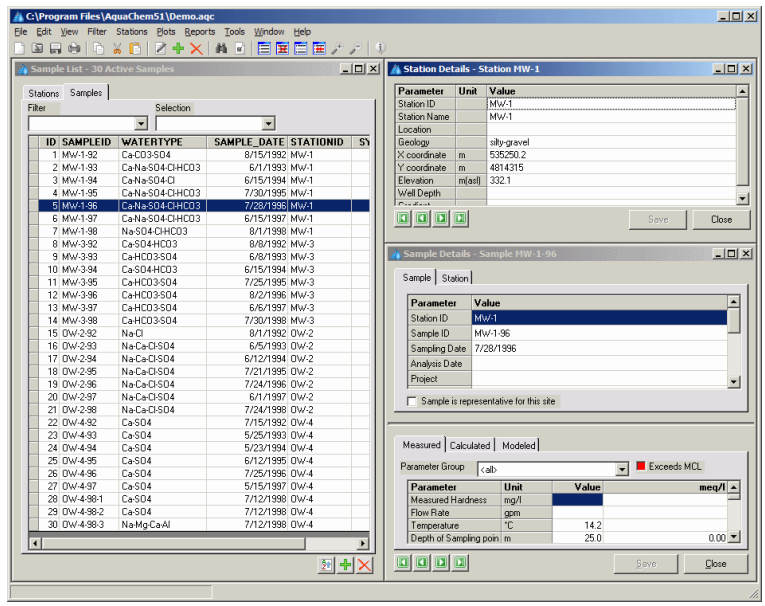
Active Samples/Stations Window will always appear when you open an AquaChem database and will remain on-screen as long as the project database is open (i.e. the Active Samples/Stations window cannot be closed unless the project database is closed). This window displays the list of samples and stations in the currently selected database. Two further windows can be accessed through the **Active Samples/Stations** tab to display and manipulate the dataset:

- **Sample Details Window** contains details for the selected sample.
- **Station Details Window** contains details for the selected station.

The following remaining ‘Child’ windows are used to display and manipulate the data which can be accessed through the main menu commands:

- **Table View** available under **View** menu allows you to view and edit the data in the database as a table.
- **Template Designer** available under the **File** menu contains options for designing print templates for plots and reports.
- **Reports** loads pre-defined data analysis reports, or user-designed reports. The **Report Designer** available under the **Reports** contains options for designing data reports.
- **Tools** loads several tools for data analysis and interpretation. **Modeling > PHREEQC** available under the **Tools** loads the interface for the PHREEQC modeling utility, and provides direct links to PHREEQC-I or PHREEQC for Windows. Now there is also an option to create an input file for PHT3D modeling software.

AquaChem follows most standard Windows interface conventions. Each window can be minimized to the bottom of the Parent window and re-opened as needed. Likewise, window sizes can be adjusted by dragging and releasing the corners of the window frame. Windows can be arranged (as shown below for example) on the Parent window using the **Windows > Tile Horizontal** or **Tile Vertical** command which are available from the main menu.

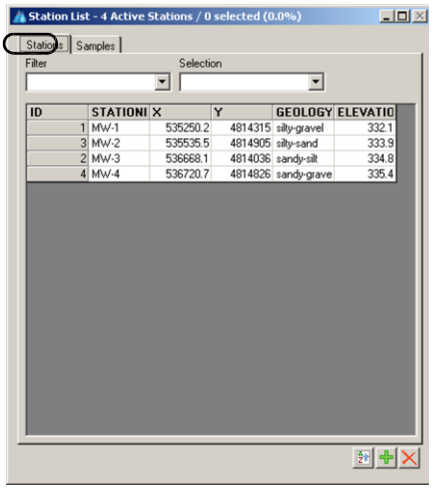


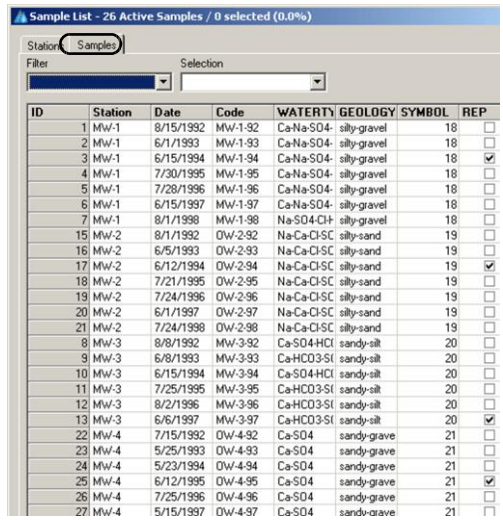
The following section summarizes the features of each of the main AquaChem windows.

1.6.1 Active Samples/Stations Window

AquaChem follows a database hierarchy of stations followed by samples. This means that each sample must have a corresponding station. When you create a new sample, a corresponding station must be assigned to it.

The **Active Sample/Stations** window contains summarized information about every active sample and station in the database; the fields in this window are read-only which means that fields in this window cannot be edited. This window contains two tabs: **Stations** and **Samples**. Clicking on these tabs displays the following windows.





The first column in these windows will always contain an ID value; each sample and station in your database will have a unique database ID value. This allows AquaChem to manage the data and perform internal calculations.

NOTE: The internal database ID value cannot be edited, nor can this column be removed from the active list. This ID is automatically created when you create a new sample or station.

In addition to the ID column, there will be columns containing sample or station description parameters. These columns can be modified and the sorting options can be modified as well. For more details on sorting the active list, please see the **View > Options - Active List** section in Chapter 3.

The bottom of the **Active Sample/Stations** window contains the following three buttons:

The **[Sort]** button will load the sort options for the active list. This will allow you to change which parameters appear in the active list and their order.

The **[New]** button will create a new sample or station, depending on which mode is active (i.e. which tab is selected).

The **[Delete]** button will delete the selected sample or station.

In order to edit the data for a specific sample or station, you need to open the **Sample Details** or **Station Details** window. These windows are explained in greater detail in the following sections.

1.6.2 Sample Details Window

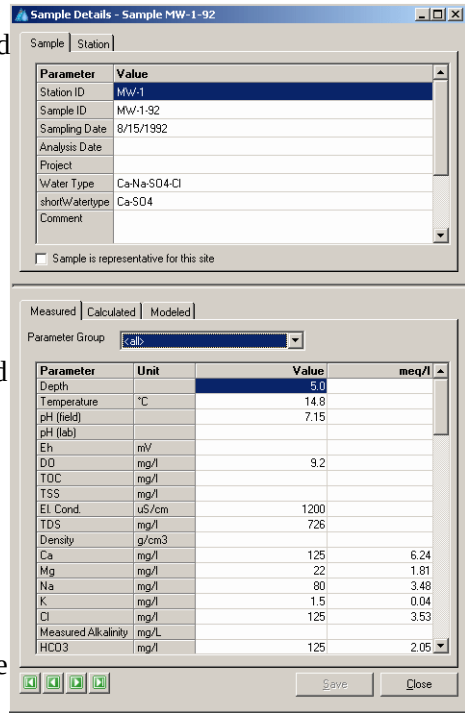
The **Sample Details** window is a read/write window, which means data can be entered, saved, and read from this window. Individual samples can be viewed and edited using this window.

To load this window for one of the samples in your active list, you can:

- select a sample from the active list and **double-click** the left mouse button on it; OR
- select a sample from the active list and press the **<Enter>** key on your keyboard; OR
- select a sample from the active list and click **Sample > Edit** from the main menu; OR
- right-click the sample from the active list and select

[Edit]. An example of the **Sample Details** window is shown

below:



To enter data in the **Sample Details** window, simply double-click in the desired field and type in the appropriate information. Alternatively, data can be imported into your database using the **Import** feature (see the **File > Import** section of the User's Manual for more details).

The **Sample Details** window is separated into two frames: the top frame includes general details on the sample (**Sample** and **Station** tabs), and the bottom frame contains the **Measured**, **Calculated,** **Modeled**, and **Description** tabs.

Data can be entered for the **Sample** tab at the top of this window, and in the **Measured** and **Description** tabs in the bottom half of this window. Under the **Measured** Parameters tab, you will see the label **Parameter Group** with a corresponding combo box. This allows you to select different groups of Measured Parameters, and focus on just desired groups (for example you may want to view just Anions or Cations). The **Show analyzed values only** group will hide all parameters for which there is no data recorded, and display only those samples which have measured values.

Parameter groups can be created and edited in the **File > Database** screen using the parameter group tab dialogue.

For Measured Parameters, you may also right-mouse click on a parameter in order to view the Parameter Details. The Parameter Details displays all the data available for the selected parameter including description, formula weight, and the CAS Registry number.

The **Calculated** tab contains function values based on measured data from the current sample. These entries cannot be edited (this data is read-only). However you may define which of the available functions should be displayed and what unit is to be displayed (e.g. for hardness) on this tab using the Sample Detail Options.

The data in the **Modeled** tab is obtained from PHREEQC simulations (as such, there will be no values for Modeled Parameters when you build a new database). There are three ways in which you can copy PHREEQC results into the **Modeled** tab:

[1] Click the PHREEQC button at the bottom of the window, and PHREEQC will calculate the Saturation Indices for the available Modeled Parameters in the database. This will be done only for the current sample;
[2] Select multiple samples in the Active Samples list, and use the menu option **Tools > Modeling > Calculate Sat. Indices and Activities**.
[3] Manually create a PHREEQC input file, using the **PHREEQC (Basic)** option under the **Tools > Modeling** menu. This option is recommended only for users that are familiar with the PHREEQC modeling program. The results from the simulation must be manually inserted into your AquaChem samples.

The scroll buttons at the bottom of the **Sample Details Window** can be used to scroll through the Sample Details for other samples:

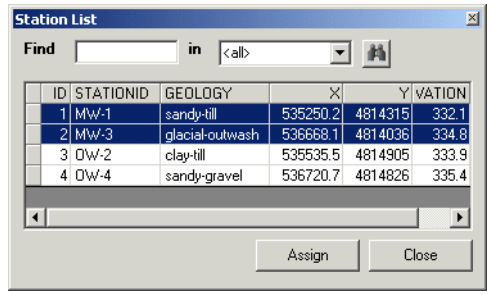
The order of these buttons (from left to right) is as follows:

First sample - loads the sample details for the first sample in your active list.

Previous sample - loads the sample details for the previous sample in your active list. **Next sample** - loads the sample details for the next sample in your active list.

Last sample - loads the sample details for the last sample in your active list.

The first field in the Sample Details window is the **Station ID**. As mentioned earlier, every sample must have a station assigned to it. To assign a station to a sample, click once in this field then click the ... button which will appear near the right side of this field. Alternatively, you may click **Samples > Assign Station** from the main menu. This will load a list of available stations, similar to the dialogue shown to the right side.



From this dialogue, you may select a station directly from the list; or if you have a

long list of stations, the **Find** feature at the top of this window can be helpful. Simply enter the Station ID or any other parameter from the station you are looking for into the **Find** field, and press the **Find** icon to run a search for this expression. If this expression
might be found in several fields of the station table then you might want to choose a category from the combo box beside this field in order to narrow down the fields which are searched by the query.

Once you have located the desired station for this sample, press the **[Assign]** button at the bottom of this dialogue and this will return you to the **Sample Details** window.

When you are finished in the **Sample Details** window, press the **[Save]** button at the bottom to save new data and/or changes to your database. Once you are finished, press **[Close]** to return to the Active List.

The data under the **Station** tab is read-only, and as such cannot be edited. The **Station** tab contains information on the station which corresponds to the current sample. To edit the station parameters, open the **Station Details Window** as described in the next section.

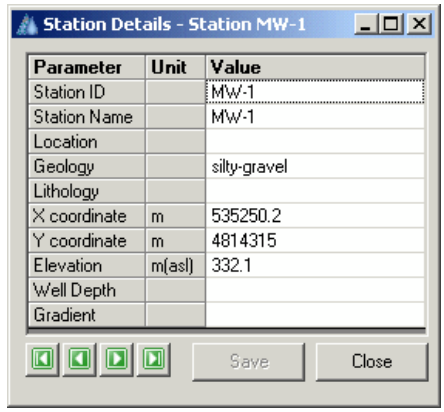
1.6.3 Station Details Window

The **Station Details** window is a read/write window, which means data can be entered, saved, and read from this window. Individual stations can be created, edited, or viewed using this window.

To load this window for one of the stations in your active list, you can:

- select the station from the active list, then **double-click** the left mouse button on it; OR
- select the station from the active list, then press the **<Enter>** key on your keyboard; OR
- select the station from the active list and click **Station > Edit** from the main menu; OR
- right-click on the station from the active list and select **[Edit]**.

An example of the **Station Details** window is shown below.



To enter data in the **Station Details** window, simply double-click in the desired field and type in the appropriate information. Alternatively, data can be imported into your database using the Import feature (see the **File > Import** section for more details). To

save new data and/or changes to the database for this station, press the **[Save]** button at the bottom of this window. Once you are finished, press **[Close]** to return to the active list.

The scroll buttons at the bottom of this window are similar to the Sample Details window; these buttons can be used to scroll through the details for other stations in your active list.

1.6.4 Plots Window

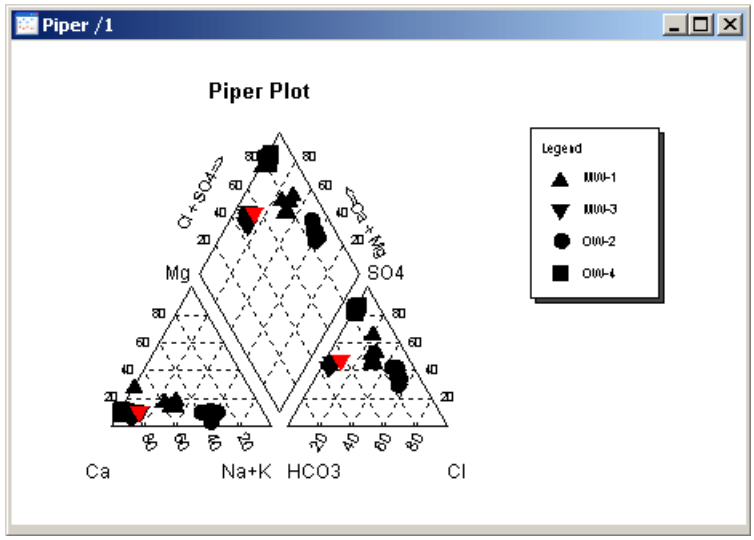
AquaChem provides a comprehensive selection of 27 different plotting techniques commonly used for aqueous geochemical data analysis and interpretation. Each of these plot types can be used to graphically represent information for all samples in the Active Samples List, or for selected samples only.

To create a new plot:

- Ensure the **Samples** tab is the current active window.
- Select **Plots > New** from the main menu.
- Choose the desired plot type from the list in this menu.
- Modify the plot options or click **[OK]** to accept the defaults.

This will create a Plot window displaying the selected plot for all or selected samples in the Active Samples List.

An example below shows a plot window containing a **Piper** plot:



Any samples selected in the **Active List** will be highlighted on the **Piper** plot. Shapes and sizes of the symbols can be modified and the plot options can be adjusted to show just the selected samples, or all the current active samples available in your database. In certain plots the data points may be labeled.

It is important to remember that the data plotted on all open plots are directly linked to the database samples. Any changes to the data are immediately reflected in each of the open graphs. Clicking a data point on the graph will highlight the corresponding sample in the Active samples list window (the corresponding data point in all other

open plot windows will also be highlighted). This can be effective for identifying outlier points on the plot. Similarly, selecting a sample in the active list will highlight the corresponding data point on all open graphs. Changing the number of samples in the active list automatically updates ALL open plots.

For more details on the various Plots and their respective options, please refer to
the User's Manual.

1.6.5 Table View

The **Table View** window is loaded when you select **View > Table View** from the main menu. You can then load any of the previously created table views, or use the **Create** option to design a new Table (spreadsheet) View.

For more details on the Table View options, please see the **View > Table View** section in Chapter 3 of the User's Manual.

1.6.6 Reports Window

A **Report** window provides reported and/or calculated information for a selected sample, group of samples, or all active samples in the database. The reports can be produced by selecting a sample from the active list and then selecting one of the report types from the **Reports Menu** option.

The text reports can be edited, printed, or saved to a .TXT, .CSV or .XLS file. AquaChem generates several types of reports. Using the **Report Designer**, you can create and customize your own reports, to display whatever data and/or calculations you desire.

For more details, please refer to Chapter 5 of the User's Manual.

1.6.7 Tools

AquaChem provides you with the following pre-defined data analysis tools:

- AquaChem Function
- Decay Calculator
- Find Missing Major Ion
- Formula Weight Calculator
- Volume Concentration Converter
- Special Conversions
- Species Converter
- Unit Conversions
- Calculate Facies
- Corrosion and Scaling
- Oxygen Solubility
- Aggregate Samples
- UTM Conversion

There are also **QA/QC** checks, **Look Up Tables**, and options for the linking to the PHREEQC interface available under the **Tools Menu**. As well, there is a feature that allows you to create an input file for PHT3D modeling engine using the data entered

in the database.

For more details, please refer to Chapter 6 of the User's Manual.

1.6.8 PHREEQC Interface

AquaChem includes a direct link to the USGS modeling program PHREEQC (version 2.11). You may also run the USGS graphical user interfaces (PHREEQC-I or PHREEQC for Windows), utilizing more advanced options which are not available through the AquaChem interface.

For more details on PHREEQC and modelling, please refer to Chapter 7 of the User's Manual.

1.7 AquaChem Toolbar

This section describes each of the items in the AquaChem toolbar. Most toolbar buttons are context sensitive and react according to the active AquaChem window or dialogue. If there are no options available for the selected window or dialogue, the toolbar icons may become grey and inactive. The AquaChem toolbar is shown below.

For a short description of each item in the toolbar, place your mouse pointer over an icon and a hint will pop-up. The function of each toolbar item is described below:

 **New** button creates a new database (only available if no other database is open)

 **Open** button opens a database (only available if no other database is open)

 **Save** button saves the current database file

 **Print** button prints a plot, table, or a report

 **Copy** button copies currently selected data, or copies a plot to the Windows Clipboard

 **Cut** button cuts currently selected data

 **Paste** button pastes currently copied (or cut) data

 **Edit** button edits selected sample/station

 **Create** button creates new sample/station

 **Delete** button deletes selected sample/station

 **Find** button finds samples/stations

 **Options** for sample/station list, Table View options, Report, or Plot window

 **Show all** button shows all samples/stations in the active list

 **Omit all** button hides all samples/stations in the active list

 **Show only selected** button hides all samples/stations in the list that have not been selected

 **Omit selected** button hides all selected samples/stations in the active list

 **Zoom out/Zoom in** used to change the zoom extent in the **Map** and other X,Y plots

 **Identify** button identifies sample data used on the selected plot(s)

2

Demonstration Exercise

This chapter contains a step-by-step review of some of AquaChem's key features and analysis capabilities. This exercise will give you some practical experience using AquaChem and familiarize you with the AquaChem demo database. In this exercise, the following items will be reviewed:

- Viewing the Demo Database
  - Customizing the Active Sample List
  - Editing Sample Data
  - Viewing Station Data
- Querying the Database
- Plotting the Data
  - Assigning Symbol Groups
  - Piper Diagram
  - Schoeller Graph
  - Scatter Plots
- Mapping the Data
  - Loading Basemaps
  - Export Map Symbols to ESRI Shapefile
- Printing the Plots
- Creating Data Reports
  - Sample Summary Report
  - Statistics Report
  - Trend Analysis
  - QA/QC Tools
- PHREEQC - Calculate Saturation Indices and Activities

Terms and Notation

The following terms and notations will be used in this exercise:

type:	Type in the given word or value
☞	Click the left mouse button where indicated
☞☞	Double-click the left mouse button where indicated

<Tab> Press the Tab key on your keyboard

<Enter> Press the Enter key on your keyboard

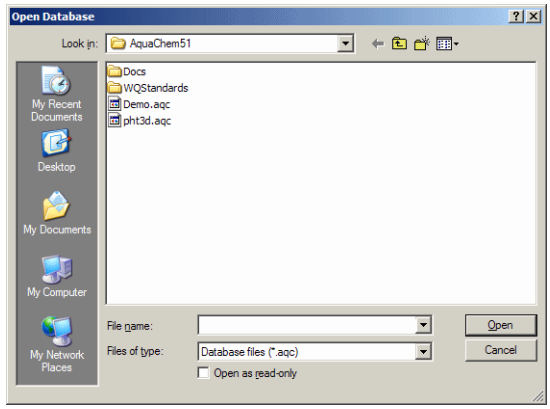
The **bold faced type** indicates menu or window items to click, or values to type.

The Main Menu items are the items available at the top of the AquaChem Parent window.

2.1 Viewing the Demo Database

To start AquaChem, click **Start** and choose **Programs/SWS Software/AquaChem 2014.1**, or double-click on the desktop  icon.

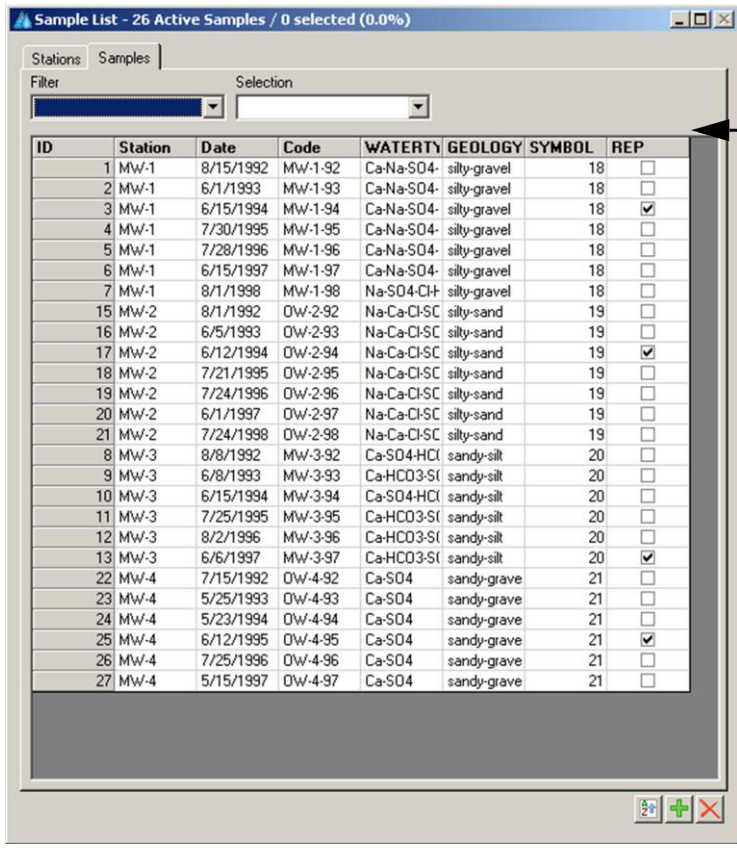
When AquaChem starts, it displays an **Open Database** dialogue (as shown below) prompting you to select an AquaChem database to open.



☞ **Demo_Basic.AQC** (located in C:\My Documents\AquaChem).

☞ **[Open]**

The Demo database file should then be loaded into AquaChem, and the following window should appear.



ID	Station	Date	Code	WATERTY	GEOLOGY	SYMBOL	REP
1	MW-1	8/15/1992	MW-1-92	Ca-Na-SO4-	silty-gravel	18	☐
2	MW-1	6/1/1993	MW-1-93	Ca-Na-SO4-	silty-gravel	18	☐
3	MW-1	6/15/1994	MW-1-94	Ca-Na-SO4-	silty-gravel	18	☑
4	MW-1	7/30/1995	MW-1-95	Ca-Na-SO4-	silty-gravel	18	☐
5	MW-1	7/28/1996	MW-1-96	Ca-Na-SO4-	silty-gravel	18	☐
6	MW-1	6/15/1997	MW-1-97	Ca-Na-SO4-	silty-gravel	18	☐
7	MW-1	8/1/1998	MW-1-98	Na-SO4-Cl-H	silty-gravel	18	☐
15	MW-2	8/1/1992	OW-2-92	Na-Ca-Cl-SC	silty-sand	19	☐
16	MW-2	6/5/1993	OW-2-93	Na-Ca-Cl-SC	silty-sand	19	☐
17	MW-2	6/12/1994	OW-2-94	Na-Ca-Cl-SC	silty-sand	19	☑
18	MW-2	7/21/1995	OW-2-95	Na-Ca-Cl-SC	silty-sand	19	☐
19	MW-2	7/24/1996	OW-2-96	Na-Ca-Cl-SC	silty-sand	19	☐
20	MW-2	6/1/1997	OW-2-97	Na-Ca-Cl-SC	silty-sand	19	☐
21	MW-2	7/24/1998	OW-2-98	Na-Ca-Cl-SC	silty-sand	19	☐
8	MW-3	8/8/1992	MW-3-92	Ca-SO4-HC(	sandy-silt	20	☐
9	MW-3	6/8/1993	MW-3-93	Ca-HCO3-S(	sandy-silt	20	☐
10	MW-3	6/15/1994	MW-3-94	Ca-SO4-HC(	sandy-silt	20	☐
11	MW-3	7/25/1995	MW-3-95	Ca-HCO3-S(	sandy-silt	20	☐
12	MW-3	8/2/1996	MW-3-96	Ca-HCO3-S(	sandy-silt	20	☐
13	MW-3	6/6/1997	MW-3-97	Ca-HCO3-S(	sandy-silt	20	☑
22	MW-4	7/15/1992	OW-4-92	Ca-SO4	sandy-grave	21	☐
23	MW-4	5/25/1993	OW-4-93	Ca-SO4	sandy-grave	21	☐
24	MW-4	5/23/1994	OW-4-94	Ca-SO4	sandy-grave	21	☐
25	MW-4	6/12/1995	OW-4-95	Ca-SO4	sandy-grave	21	☑
26	MW-4	7/25/1996	OW-4-96	Ca-SO4	sandy-grave	21	☐
27	MW-4	5/15/1997	OW-4-97	Ca-SO4	sandy-grave	21	☐

NOTE: You may need to adjust the size of this window in order to see all the rows and columns in the database table.

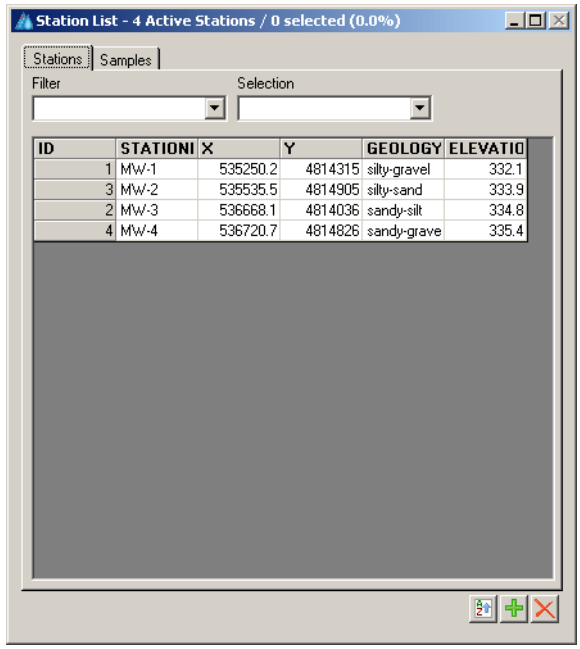
In the AquaChem database, the water chemistry data is stored as **Stations** and **Samples**. A **Station** is defined as a unique spatial location where a water **Sample** is collected. An example of a **Station** could be a monitoring well, a location where river effluent is collected, or a surface water location. The stations maintain a Parent-Child relationship with the samples, whereby each station is a Parent and each sample is a Child. While a station may 'own' many samples, each sample may only 'belong' to a single station.

The **Sample List** window is referred to as the **Active List** window and is the main AquaChem window. This window contains summary information for the samples provided in the Demo database. In the **Active List**, you can manage your working samples by selecting, showing, and hiding samples as necessary.

At the top of the **Active List** window, there are two separate tabs: one for **Samples** and a second for **Stations**. From here, you can switch between the list of samples and stations simply by choosing the proper tab. Take note of how the main menu items are refreshed based on the current mode:

- When the **Samples** tab is active, the main menu will show **File**, **Edit**, **View**, **Filter**, **Samples**, **Plots**, etc.
- When the **Stations** tab is active, the main menu will show **File**, **Edit**, **View**, **Filter**, **Stations**, **Plots**, etc.

☞ **Stations** tab (at the top of the Active List window). The Active list window will be refreshed, as shown below.



As you can see from the information displayed in the stations list, there are 4 stations in total (4 wells), each with a unique ID, name, and spatial location. For this database, 7 samples were collected from each station (well), to produce a total of 28 samples. A single sample was collected annually from each station from 1992 until 1998. The last sample (OW-4-98) was duplicated in the field (another sample taken at the same date, time, and place), so both samples were assigned the same Duplicate_ID to connect them to each other. The OW-4-98 sample was also cloned in the program to produce a blank sample, bringing the total number of samples to 30. It should be noted that this sample information has been fabricated for the purpose of this demonstration.

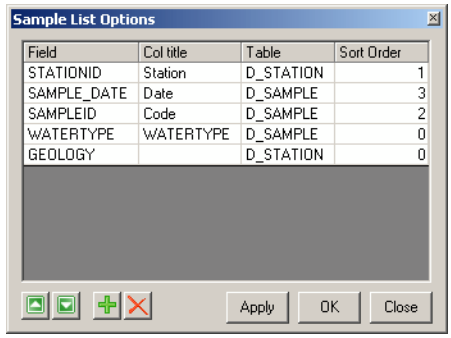
Customizing the Active Sample List

The information displayed in the active list window can be easily customized to your preferences. You may add/remove columns, and specify the sorting options.

To do so:

☞ **Samples** tab (at the top of the Active List window).

☞ **View** from the main menu and then select **Options**



In the **Samples List Options** dialogue that appears, you can modify the parameters that appear in the active list. Parameter Fields can be added or removed, and their order can be modified.

To add a parameter to the active list, simply press the button; then, place your mouse in the new blank line which appears at the bottom, and use the combo box to select a parameter from the list.

To remove a parameter from the active list, simply select the target parameter, then press the button.

To change an existing parameter, simply double click on the parameter name, and choose a new parameter from the combo box; then press **<Enter>** (on your keyboard).

To change the order of the parameters in the active list, select the target parameter and then use the or arrow buttons.

Feel free to experiment with active list options, by adding or changing fields in this dialogue.

Use the Sort Order column to change the sort options for the active list. For this exercise, you will leave the order as it is.

- ☞ **[Close]** to save the changes and return to the active list.

Editing Sample Data

The next step is to view and edit the sample data available in the database. To do so, you need to load the **Sample Details** window:

- ☞ **Samples** tab (at the top of the active list, to ensure it is the active tab)
- ☞ **MW-1-92** (SampleID), the first sample in active samples list
- ☞☞ This sample (or you can press the **<Enter>** key on your keyboard).

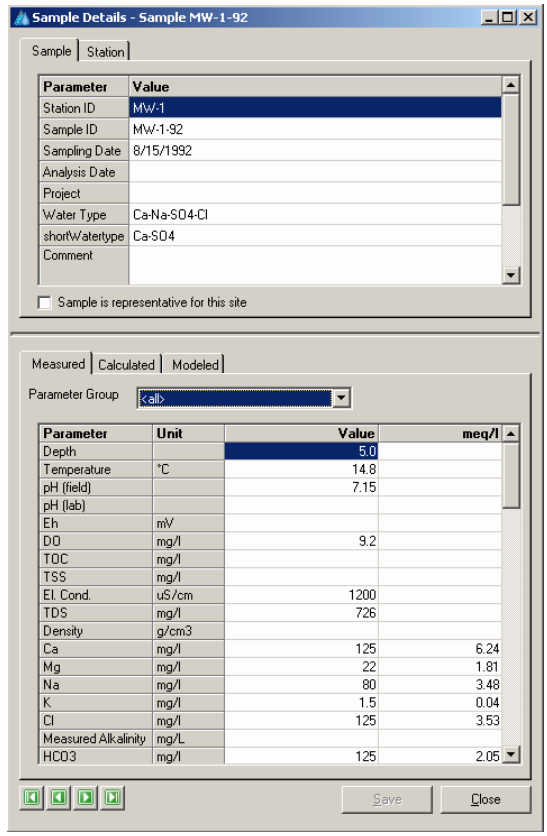
The **Sample Details** window (as shown below) displays all of the data for a single sample in the database:

The top of the **Sample Details** window includes:

- General sample information such as StationID, SampleID, Sampling Date, and Water type.
- A separate tab containing Station information (read-only)

The lower half of the **Sample Details** window includes the numerical data for the sample comprising:

- **Measured values** (analyzed chemicals, measured field data, etc.)
- **Calculated values** (basic geochemical calculations performed internally by AquaChem), and
- **Modeled values** (which may contain results from a PHREEQC simulation)



In the middle of the **Samples Details** window, you will see a label **Parameter Group**, with a corresponding selection box (with a default selection <all>). The **Parameter Group** allows you to quickly select a pre-defined group of parameters, so that you may focus on a specific set of measured values. AquaChem includes parameter groups for Anions, Cations, Gases, and others, or you can create and customize your own group.

The "Show analyzed values only" parameter group allows you to show only those parameters for which there are measured values.

☞ **Cations** from the list of available **Parameter Groups**.

You should now see only cations which are available in your database.

The **Sample Details** window will also indicate if any of your measured values exceed the selected Water Quality Standards specified in AquaChem; for instance the **Mn** value for this sample is shaded red. This indicates that the measured Mn value of 0.600 mg/L exceeds the guideline value of 0.400 mg/L (MCL, Level1). If you are viewing the Cations parameter group, Mn should be visible in this group.

The WHO (World Health Organization) Water Quality Standards are used for this demo

database; however, AquaChem also includes USEPA, CCME, and Health Canada Guidelines for you to gauge your data; you may also create and customize your own water quality standards.

After reviewing the sample data, it was determined that the Calcium value was incorrectly entered for this sample. You will now edit the data for the selected sample, and enter the correct value for Calcium.

To edit the value for Calcium:

- **Cations** from the list of available **Parameter Groups**
- Locate **Calcium** (Ca) in the list of **Parameters**
- Click once in the cell beside Ca, which has a current value of 125 mg/L

type: a new value of **120** mg/L,

- press **<Enter>** key on your keyboard

At this point you would save the record by clicking the **[Save]** button at the bottom of the Sample Details window.

Feel free to navigate through all of the samples in the Demo database using the  and  (previous and next) buttons in the lower left corner of this window.

Notice that when you open another **Sample Details** window, the window title is updated to show the Sample ID of the newly selected sample. As well, the sample will be highlighted in the Active List, allowing you to easily locate the sample and station information simultaneously. (You may need to adjust the size and position of the Sample Details window in order to see both windows on your display simultaneously).

Once you are finished reviewing the other samples,

- **[Close]** to close the **Sample Details** window.

Next, you will take a quick glance at the **Station Details**.

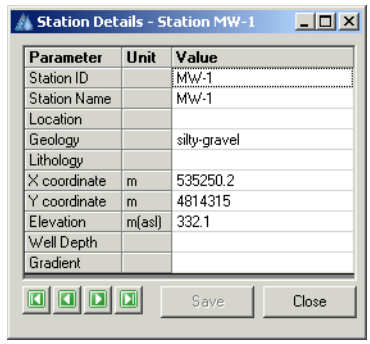
Viewing Station Data

To view the station characteristics for one of the wells in the Demo database, you must load the **Station Details** window.

To do so, first switch to stations mode:

- **Stations** tab (at the top of the active list window)
- **MW-1** (Station ID), the first station in active stations list
- **Stations > Edit** from the main menu (or you can press the **<Enter>** key on your keyboard).

You should then see a **Station Details** window, similar to the figure shown below:



The **Station Details** window displays all of the data for a single station in the database, and includes: Station ID, Location, Geology, and World Coordinates. The station X,Y coordinates are required if you want to plot samples on a site map, or to export sample attributes to ESRI Shape files. For the Demo database the station coordinates are saved in **NAD 1983 UTM Zone 17**.

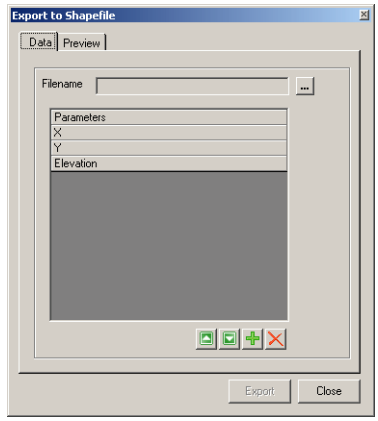
Simply enter or modify data in the appropriate fields, then **[Save]** and **[Close]** this window. For this exercise, there are no changes required for this station.

- ☞ **[Close]** at the bottom of the Station Details window.

Export Stations to ESRI .SHP File Format

In AquaChem, you can export station and any sample attributes to ESRI point scheme Shapefile format.

- ☞ **Samples** tab
- ☞ **File / Export / ESRI Shapefile** from the main menu. The following dialog will appear:



By default, X, Y coordinates and Elevation will be included as parameters.

- ☞  to add other parameters
- ☞ **Measured Values** from the combo box at the top of the dialogue
- ☞ Select Na, Ca, Mg, Cl, SO4, and HCO3 by holding down the **Ctrl** button

on your keyboard and clicking on each parameter

- **[Select]**
- **[Close]**
- ... button to specify the file name.

type: DemoStations

- **[Save]**
- **[Export]** at the bottom of the dialog to create the Shape file
- **[No]** in the warning message that appears

The Shape file can be loaded into a GIS Application, such as SWS's **Hydro GeoAnalyst**, where you can create thematic or contour map with the sample attribute data.

- **[Close]** to close the **Export** dialogue

The next section will demonstrate AquaChem's query features.

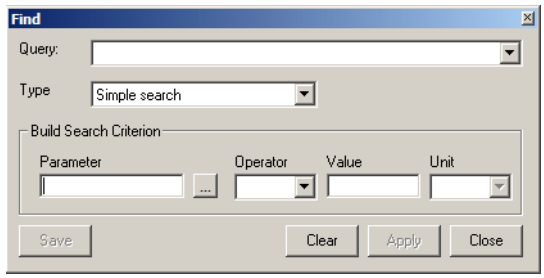
2.2 Querying the Database

The database querying function in AquaChem allows you to search and select a single sample or group of samples satisfying a specified search criteria. Once a query is executed, you can save the selection for easy recall in the future, and export the results to .TXT, .XLS, or ESRI Shapefile format.

To use the AquaChem database querying option, first ensure that the active list window is selected, and the **Samples** tab (at the top of the active list window) is the active tab.

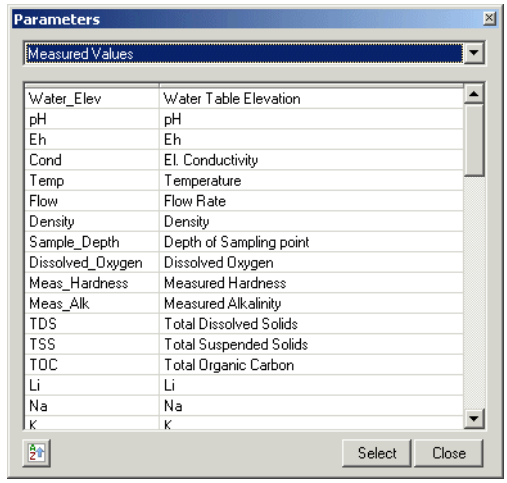
- **Edit > Find** from the main menu

The **Find** dialogue will appear as shown below.



In this example you will search the database for all samples which exceed a sodium **(Na)** concentration of 200 mg/L, and were sampled after 1996. You will execute the query, and display only those samples which meet this criteria.

- **Complex Search** from **Type** combo-box.
- ... button (beside the **Parameter** field). This will load **Parameters** dialogue with a list of available parameters.



From the combo box (at the top of the **Parameters** dialogue), you can select the desired parameter group (e.g. **Measured**, **Calculated**, **Thermometers** or **Modeled values**), and the desired parameter from the list below.

- **Measured Values** (from the combo box at the top of the dialogue).
- **Na**. You may need to scroll through the list of parameters in order to locate this parameter). You can use the button at the bottom of this dialogue to sort the parameter list alphabetically, allowing you to quickly locate the desired parameter. Once the parameter is selected it will become highlighted in blue to indicate that it has been selected.
- **[Select]**. The parameter **Na** should now appear in the **Parameter** field.
- The button and choose the "**>**" symbol from the combo box beside **Operator**.

type: **200** in the **Value** field

- **[Add to Criteria]** button

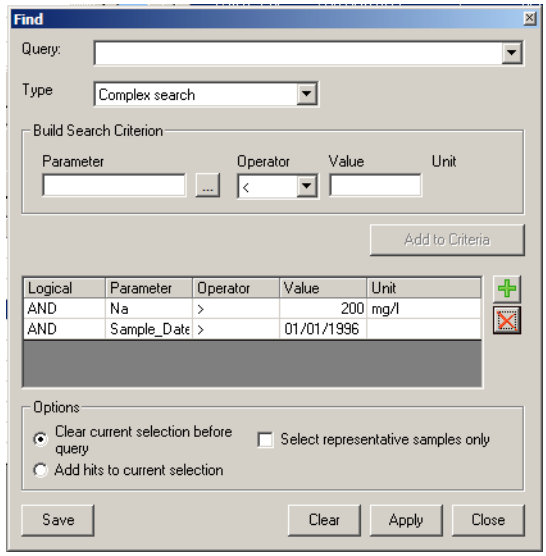
Next, add the sample date parameter:

- ... button (beside the **Parameter** field). This will load **Parameters** dialogue with a list of available parameters.
- **Sample Description** (from the combo box at the top of the dialogue).
- **Sample_Date**
- **[Select]** and the parameter should now appear in the **Parameter** field.
- The button and choose the "**>**" symbol from the combo box beside **Operator**.

type: **01/01/1996** in the **Value** field

- **[Add to Criteria]** button

Once you are finished, the **Find** dialogue should appear similar to the one shown below:



- **[Apply]**, and
- **[Save]** to save the query

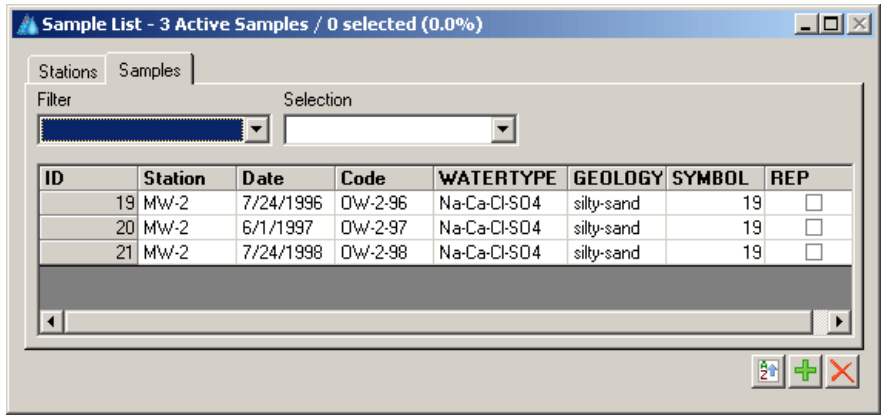
type: **Na Exceedences after 1996**

- **[OK]**
- **[Close]** to close the **Find** dialogue

Upon returning to the active samples list, you should see that there are 3 samples highlighted; these samples satisfy the query criteria. To omit the records that do not satisfy this criteria,

- **Filter / Show Only Selected** or click Ctrl-N on your keyboard

There should be 3 Active Samples shown, all corresponding to the **OW-2** Station (as shown below)



ID	Station	Date	Code	WATERTYPE	GEOLOGY	SYMBOL	REP
19	MW-2	7/24/1996	OW-2-96	Na-Ca-Cl-SO4	silty-sand	19	
20	MW-2	6/1/1997	OW-2-97	Na-Ca-Cl-SO4	silty-sand	19	
21	MW-2	7/24/1998	OW-2-98	Na-Ca-Cl-SO4	silty-sand	19	

Any calculations, reports, and plots will now only consider this subset of the data.

In the **Filter** combo box (at the top left corner of the dialogue shown above) the newly created query can be retrieved in the future.

The results of this query can now be exported to .XLS, .TXT, or .SHP file format, using the **File / Export** menu option.

In order to proceed to the next section of this exercise, you need to restore all the samples to the active list:

- ☞ **Show All** from the **Filter** combo box
- ☞ **Demo Tutorial Stations** from the **Filter** combo box

In the next section of this exercise, you will learn about the plotting options available in AquaChem, how to assign symbols to samples, and produce analysis graphs and plots.

2.3 Plotting the Data

AquaChem allows you to create more than 27 different types of graphs commonly used for aqueous geochemical data analysis and interpretation. The following sections of this demonstration exercise will describe how you can easily create, customize, and display multiple graph types.

Assigning Symbol Groups

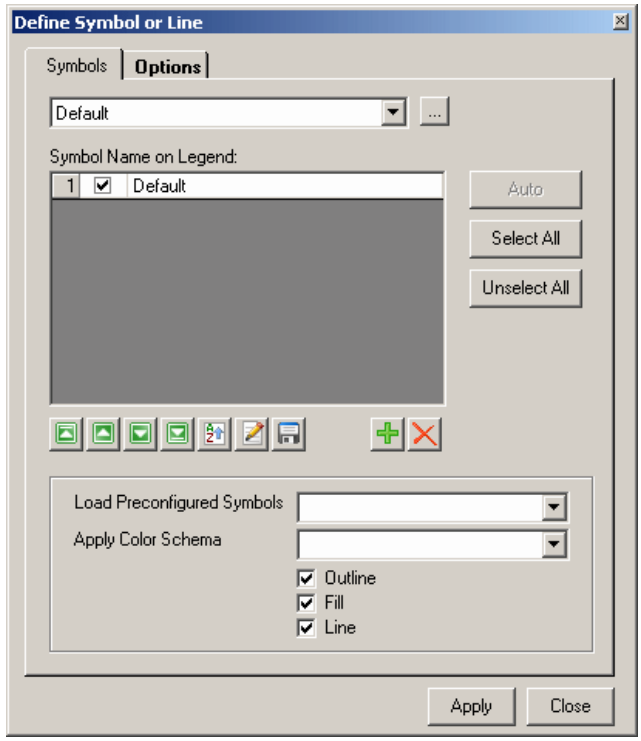
In order to easily identify the data points from each sample location, you must first assign a specific symbol to each group of samples. Each symbol is associated with a specific number, shape, and color for easily identifying the associated samples in the Active Sample list and on a graph.

By default, a new database will include three symbol groups: a **Default** symbol group with just one symbol assigned to each sample, a **Station** symbol group, with a unique symbol for each unique station in the database, and a **Geology** symbol group with a unique symbol assigned to each geology type; the station and geology symbols are automatically assigned to the appropriate corresponding samples.

For this demonstration, the symbols have been created for you. You will view them and modify them as you see fit.

To do so:

- ☞ **Plots** from the main menu and then select **Define Symbol or Line**.

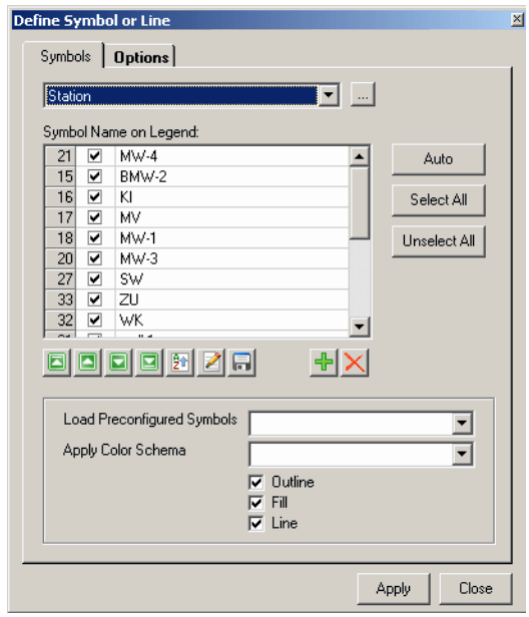


In this dialogue, you can create new symbols which will be added to the **Default** symbol group; you can create a new symbol group, and automatically generate symbols for the available samples; or select another symbol group and modify symbols in it. For this exercise, you will use the latter option.

To select a new symbol group:

- ☞ Select **Station** from the combo box under **Symbol Group** (at the top of this dialogue).

You should now see a bunch of symbols listed in the **Define Symbol or Line** dialogue. These symbols are named after each station in the demo project.



At this time, the symbol shape, color, and size may be customized. Simply select a symbol from the list, and then select the **Edit** button.

Note: This tutorial only uses four of these stations, namely: MW-1, MW-2, MW-3, MW-4. Feel free to edit any of these four symbols. All other symbols can be ignored.

The **Stations Symbols** dialog will appear on your screen, allowing you to change the properties of the symbol. Once you have made the desired changes, click the **Close** button.

The check box beside each symbol is used to indicate which symbols are active; only active symbols are plotted on the graphs. The names of the symbols will be displayed in the legend of each plot. These names can be easily changed by clicking on the symbol name and entering a new name in the **Symbol Name on Legend** field.

Once you are satisfied with the symbol settings

- ☞ **[Close]** to return to the active list.

In the active list window, under the **Symbol** column you can now see the symbol number which corresponds to each sample.

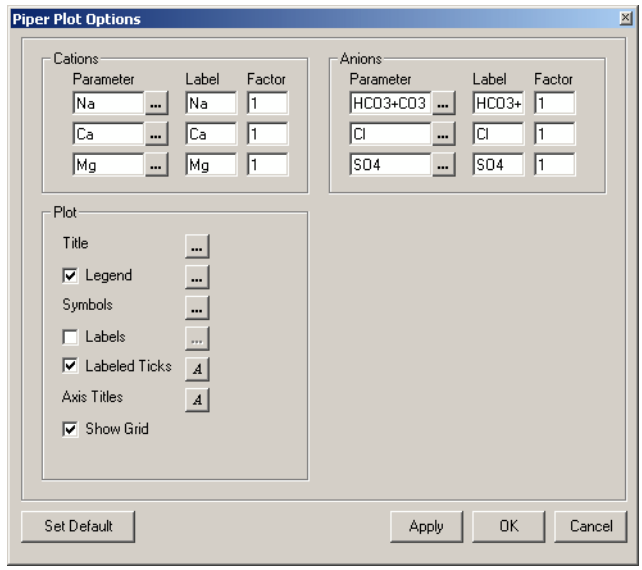
The following section will demonstrate how to plot the sample data with these new symbols.

Piper Diagram

Piper diagrams provide an overview of the chemical composition of multiple samples. You may find it useful to start your analysis with a Piper diagram. In this section, you will create a Piper diagram for all samples in the Demo database:

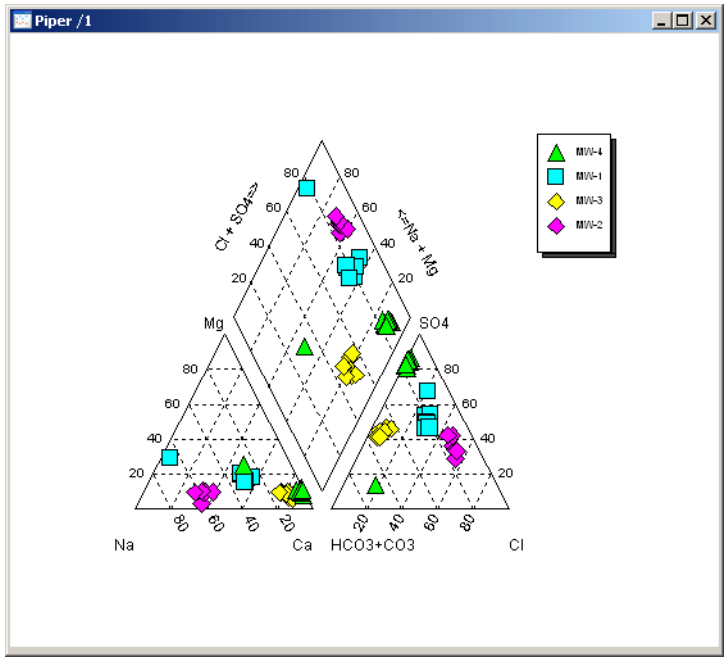
- ☞ **Plots / New / Piper**

The **Piper Plot Options** dialogue will appear with default settings for which parameters will be plotted. These parameters can be modified at any time, but for now you will accept the default plot settings.



☞ **[OK]** (to create the plot with the default settings).

A **Piper** plot window will appear as shown in the figure below:



You may need to enlarge the graphics window to see the full view of the plot. To do this, click once on one of the plot window corners, and drag this corner outwards.

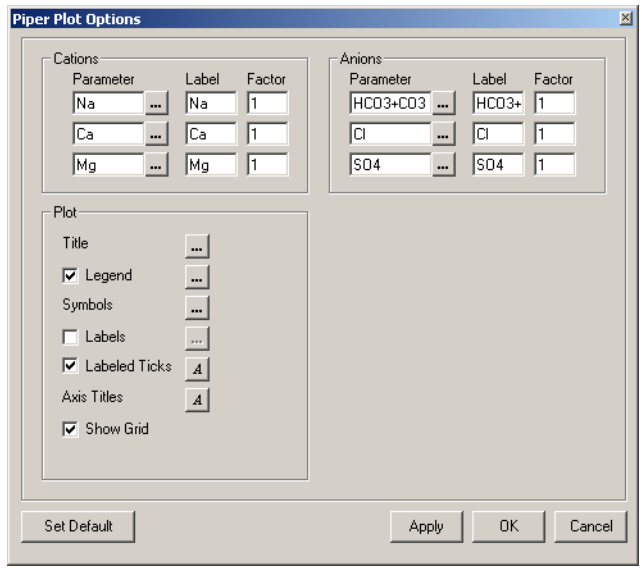
This plot clearly indicates that there are four distinct groups of samples, each with distinctly different water chemistry.

Notice that if you click on a sample point in the graph, the corresponding sample will be selected in the Active sample list. In addition, if you click on a sample in the active list, the symbol will be highlighted (in red by default) on the Piper diagram (you may need to rearrange the position of the windows in order to see this feature).

In the **Piper** plot, you can modify the appearance of the graph by adding a title, changing the fonts, adding labels, adding a legend, or removing the grid lines.

To do so,

- ☞ Right-click on the center of the **Piper** plot (or select **View > Options** from the main menu). A **Piper Plot Options** dialogue will load as shown below.



This dialogue allows you to select which parameters are used for the plot, grid, intervals, axis titles, and display formats.

- ☞ **...** beside **Title** to see the plot title options. The **Title** options include title, position and the font size.
- ☞ **[Cancel]** to return to the main options dialog
- ☞ **[OK]** to apply these changes to the open plot.

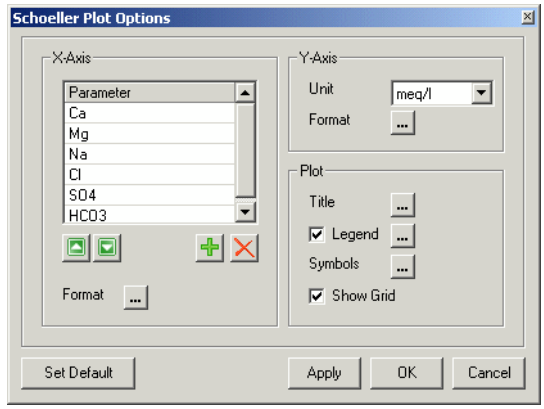
Schoeller Graph

The **Piper** plot provided a good overview of the data; next you will create a **Schoeller** graph to get more details on the concentrations of the major ions for each sample in the Demo database.

To do so,

- ☞ **Plots** from the main menu, then select **New** and then **Schoeller**.

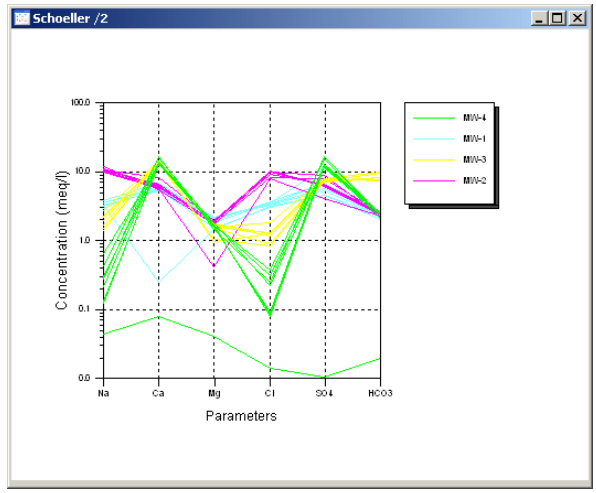
A **Schoeller Plot Options** dialogue will appear with default plot settings.



These settings can be modified at any time, but for now, you will accept the default parameter settings.

- **[OK]** (to accept the default plot settings).

A **Schoeller** graph will appear as shown in the figure below:



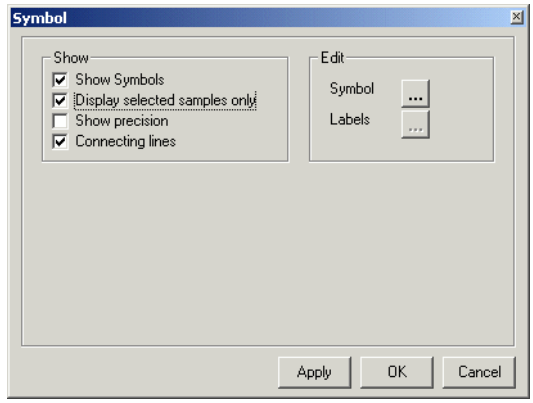
This graph provides a comparison of the log of the concentrations of the major ions for each sample in the database. The highlighted line on the graph corresponds to the selected sample in the active sample list window.

To display the symbols for each sample, you need to modify the plot options.

To do so,

- **View** from the main menu then **Options**, or right-mouse click on the centre of the **Schoeller** plot.
- ... beside **Symbols** to see the symbol options.

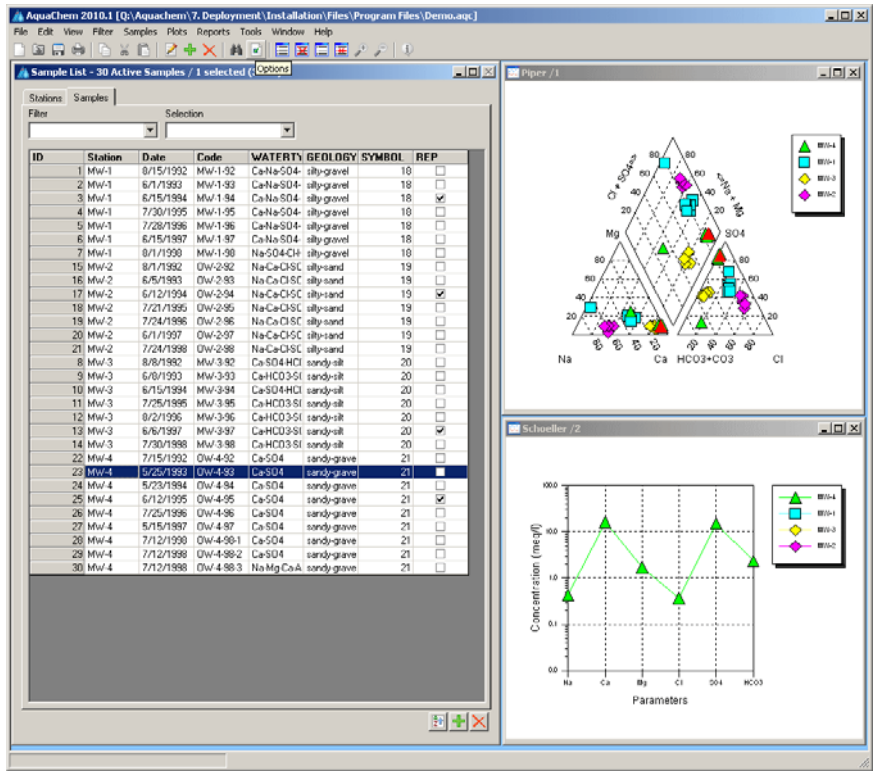
Under the **Symbol** options, you want to show symbols on the plot and enable the option to show selected samples only.



- ☞ Place a check mark in the box beside **Show Symbols**
- ☞ Place a check mark in the box beside **Display Selected Samples only**
- ☞ **[OK]** to apply the changes and close the **Symbol** dialogue
- ☞ **[OK]** to close the Schoeller plot options dialogue

You should now see only one line on the plot. This line corresponds to the selected sample in the active sample list. This occurs as a result of using the **Display Selected Samples only** option.

You should now have both a **Piper** plot and a **Schoeller** graph displayed on your screen. You may need to modify the sizes and positions of each plot window in order to see each one fully. After rearranging the plot windows, your display should be similar to the one below:

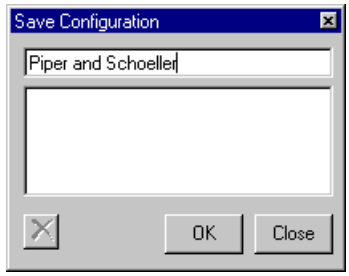


Notice that if you select a new sample in the Active Samples List, this sample is highlighted on both the **Piper** plot and the **Schoeller** graph. In addition, any changes that are made to the sample data will be immediately reflected on both of these plots.

You will now save this plot configuration so that these plots can be quickly recalled later.

To do so,

- ☞ **Piper** plot window (to make this the active window).
- ☞ **Plots** from the main menu, and then **Save Configuration**



type: ***Piper and Schoeller*** (a name for the Plot Configuration).

- ☞ **[OK]**

This plot configuration can now be recalled in the future, by using the **Open Configuration** option from the **Plots** menu. For now, you will close these plots to allow for more work space in the windows environment.

- ☞ **Plots > Close All Plots** from the main menu.

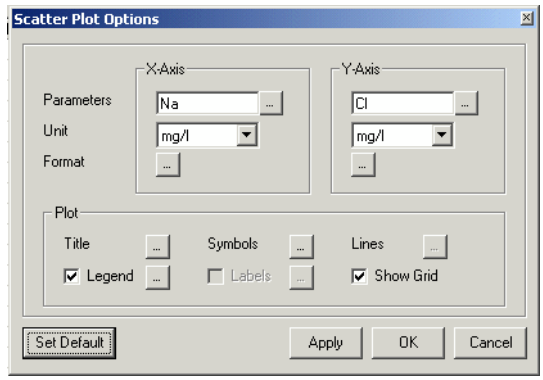
Scatter Plots

The **Scatter** plot allows you to visualize the degree of correlation between two parameters. Such correlation can also be visualized with a **Correlation Matrix** report. In this section, a scatter plot for Ca and SO4 concentrations is presented.

To create a **Scatter** plot,

- ☞ **Plots** from the main menu, then **New** and then **Scatter**

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

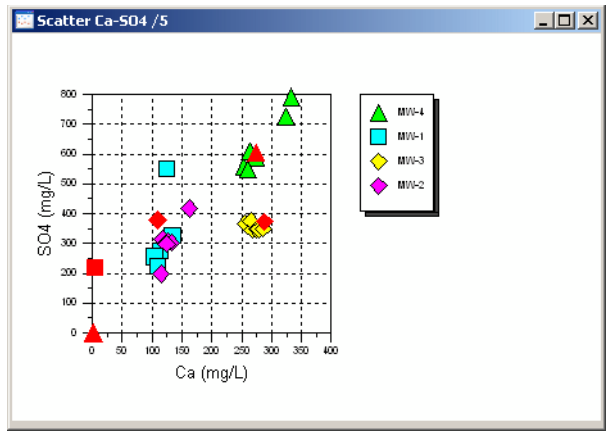


- **Parameters** field, under **X-Axis**
- The ... button to load the list of available parameters.
- **Measured Values** (from the combo box at the top of the dialogue
- **Ca**
- **[Select]**

Repeat the same steps to change the parameter for the **Y-Axis**:

- **Parameters** field, under **Y-Axis**
- ... to load the list of available parameters.
- **Measured Values** (from the combo box at the top of the dialogue
- **SO4**
- **[Select]**
- **[OK]** to accept the new plot settings and produce the plot

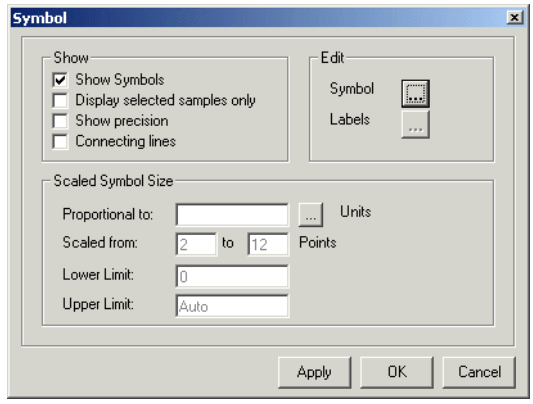
A **Scatter Ca-SO4** graph will appear similar to the one shown below.



This graph clearly indicates a much higher ratio of Ca to SO4 for those samples taken from the MW-3 site (in the middle of the plot). 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

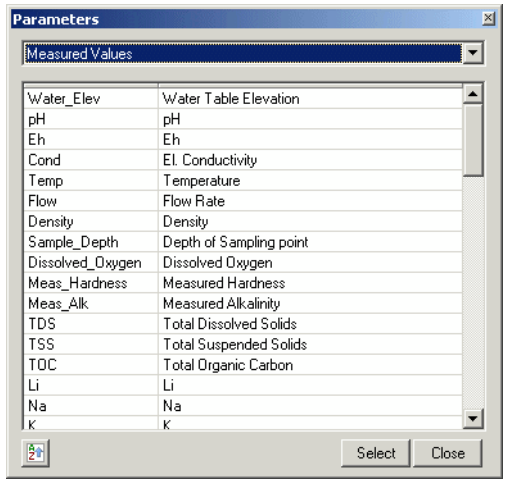
parameter in the database. To do so,

- ☞ Right-click on the graph to produce the **Scatter Plot Options** dialogue
- ☞ ... beside **Symbols** to see the symbol options. You may need to adjust the position of your plots windows, so that you can see the **Scatter** plot window and the options dialogue at the same time.



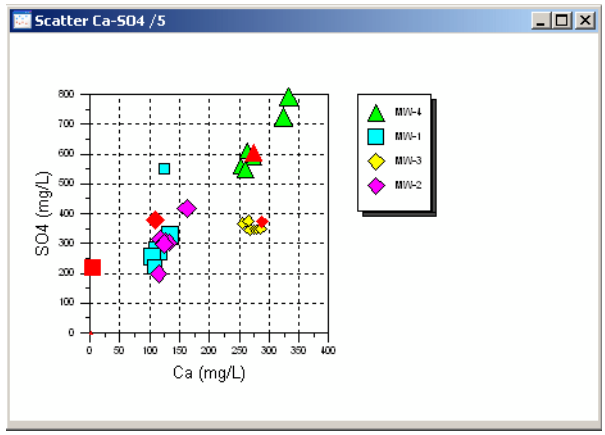
Locate the **Scaled Symbol Size** options at the lower half of the options dialogue.

- ☞ ... button beside the **Proportional to:** field. This will load a parameter list.

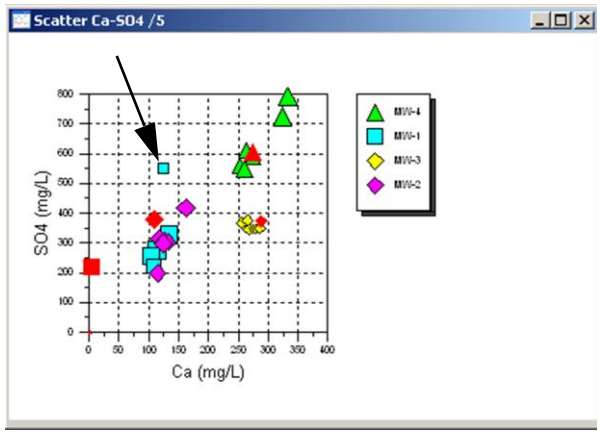


- ☞ **Measured Values** from the combo box
- ☞ **TDS** (Total Dissolved Solids)
- ☞ **[Select]**
- ☞ **[OK]** to accept the new plot settings.
- ☞ **[OK]** to close the **Scatter Plot Options** dialogue.

The symbol sizes for all samples will now be plotted relative to the Total Dissolved Solids (TDS) value for each sample. Your plot should be similar to the figure shown below.

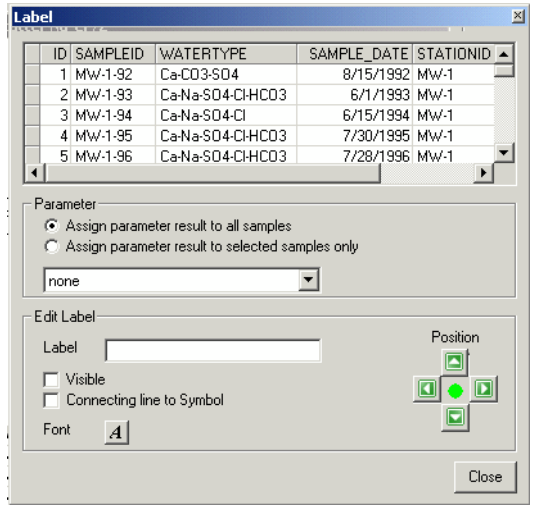


The **Scatter** graph should clearly show that the samples from station MW-3 have a lower level of TDS than the remaining samples, indicated by the slightly smaller symbol size for samples at this station.



After analyzing the plot, you can see that a sample from MW-1 may be an outlier. You will now label this sample accordingly.

- ☞ Click on the data point on the graph to select it
- ☞ Right-click on the plot to load the **Scatter Plot Options** dialogue
- ☞ **Labels** (place a check mark in the box)
- ☞ ... beside **Labels** to see the symbol label options, where you can customize the appearance of the symbol labels.



- ☞ **Assign parameter result to selected samples only** radio button.
- ☞ **SAMPLEID** (from the combo box below).

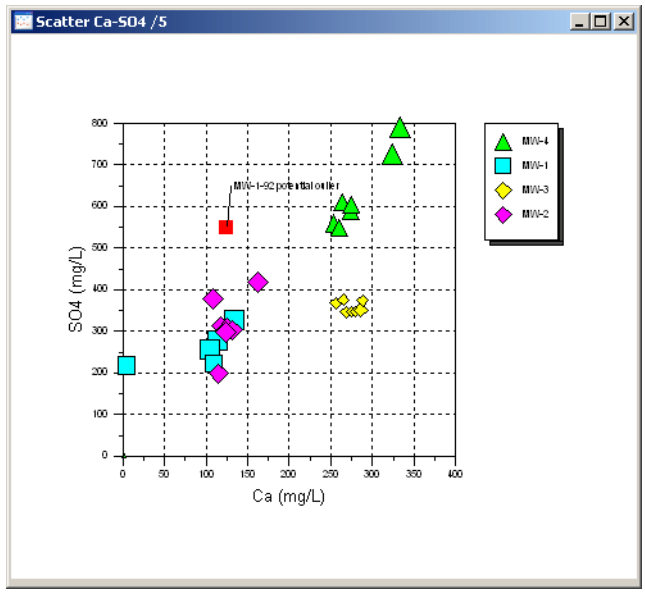
This will assign the Sample ID label to that symbol on the plot. It will also fill in the **Label** field in the **Edit Label** frame and put a check mark beside **Visible**.

- ☞ In the Label field beside "MW-1-92".

Type: "potential outlier", after the Sample ID

- ☞ Check the box beside **Connecting line to Symbol**
- ☞ Use the **Position** arrows to move the label so it is above the data point and is not blocking any other data points
- ☞ **[Close]**
- ☞ **[OK]** to close the **Scatter Plot Options** dialogue

Your **Scatter** plot should look similar to the following:



Before proceeding, close the **Scatter** plot.

☞ **[X]** in the upper-right corner of the **Scatter** plot window.

In the next section, some of the mapping features will be reviewed.

2.4 Mapping the Data

AquaChem has introduced GIS support into the map plot. You may import ESRI Shapefiles for site maps, or georeferenced raster images (air photos, topographic maps). In addition, you may also export map symbols (Radial, Stiff) to shape file format, for analysis and interpretation in GIS software packages, including Schlumberger Water Services' **Hydro GeoAnalyst**. Some of the map features are demonstrated below.

Loading Basemaps

To create a new site map,

☞ **Plots** / **New** / **Map**

The first step is to add the air photo as a background basemap.

☞  button under the **Base Map** frame.

Change the **Files of Type** to "Common Graphic Files", browse to the folder \Documents\AquaChem, and locate the Airport_color.bmp file.

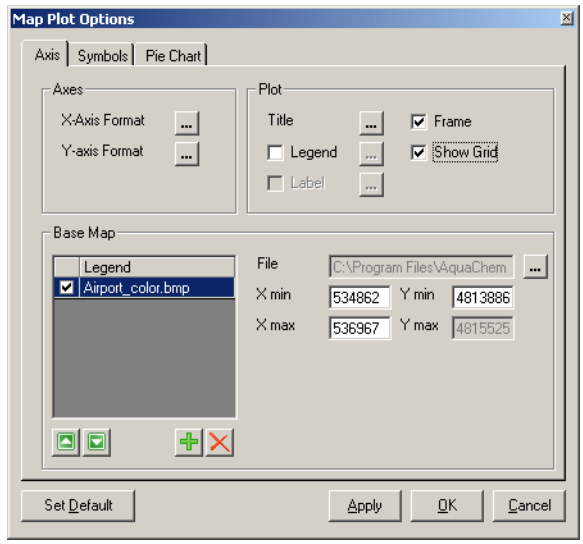
- **[Open]**

In order to map the pixels of the image to a coordinate system, the image must have two georeference points with known coordinates. AquaChem uses the coordinates of the lower left corner of the image (X min, Y min), and the upper right corner (X max, Y max). These georeference points can be defined using the procedure described below.

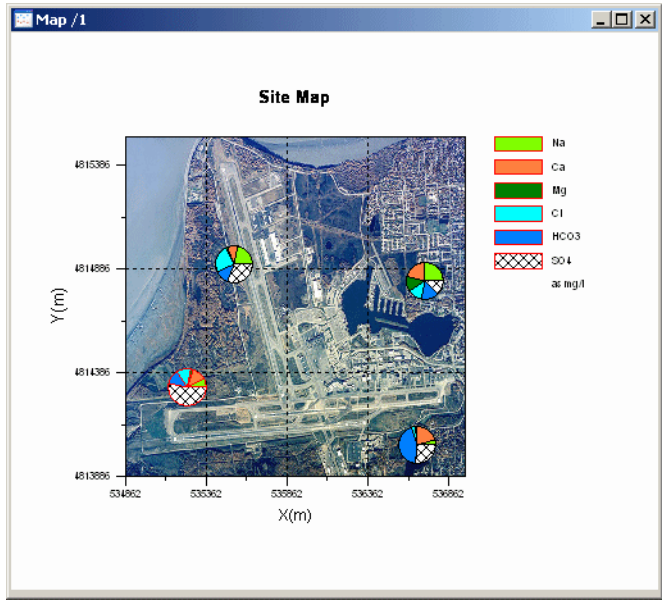
Enter the following values in the X and Y fields:

- **X min: 534862**
- **Y min: 4813886**
- **X max: 536967**

The last coordinate is calculated automatically and should be close to **4815525.**



- Put a check mark beside **Legend**
- **[Apply].** The airphoto should be loaded in the map window. An example is shown below.



The default symbol to represent the samples is a **Pie** plot and the default aggregation option is **None**.

Data aggregation tools have also been introduced to AquaChem. When there are multiple samples collected at the same sampling location (station), it is difficult to distinguish these samples on a map, since they are "stacked" on top of each other. With the data aggregation features, you can specify which samples should be plotted on the map, by selecting from one of the following "aggregation options":

- Selected Sample
- Representative
- Most Recent
- Oldest
- Smallest
- Highest
- Closest to Average

For this exercise you will create a **Stiff** plot and export it to ESRI Shapefile. To create a **Stiff** plot with customized aggregation options, return to the **Map Plot Options** dialogue.

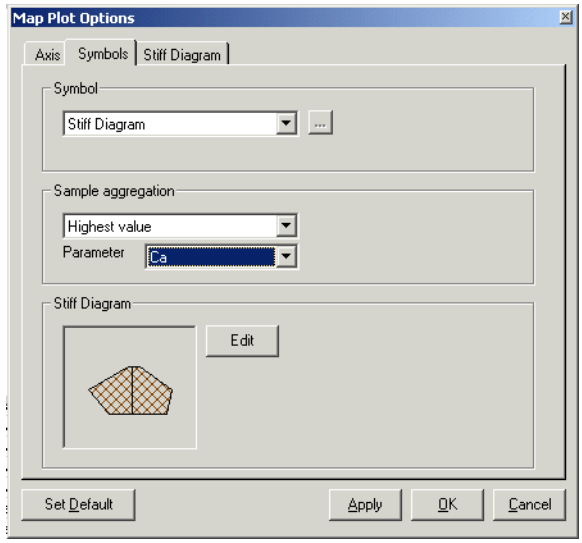
☞ **Symbols** tab

☞ **Stiff diagram** from the combo box in the **Symbol** frame

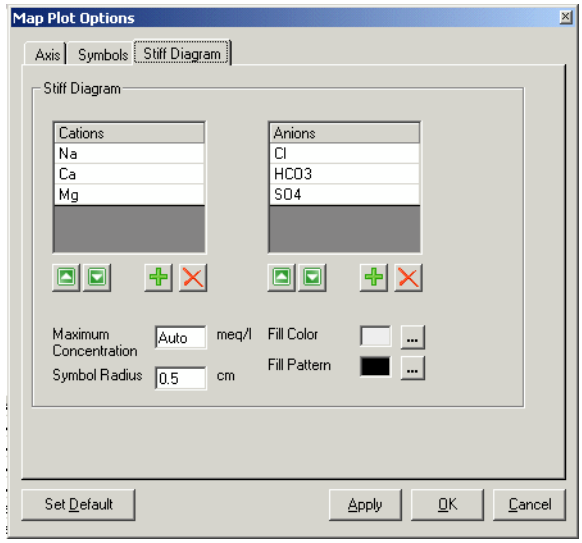
For this exercise, specify the following aggregation:

☞ **[Highest Value]** from the list

☞ **Ca** from the parameter list

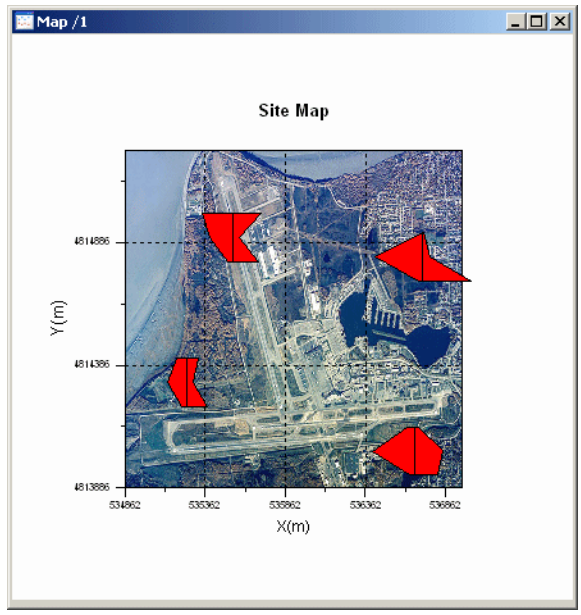


☞ **Stiff diagram** tab to customize the settings



This tab may be used to modify the parameters displayed on the **Stiff** diagram, it's color, size, and pattern. For this exercise, leave the parameters as they are, but change the **Symbol Radius** to 1 cm.

☞ **[OK]** to apply the changes and close the dialogue

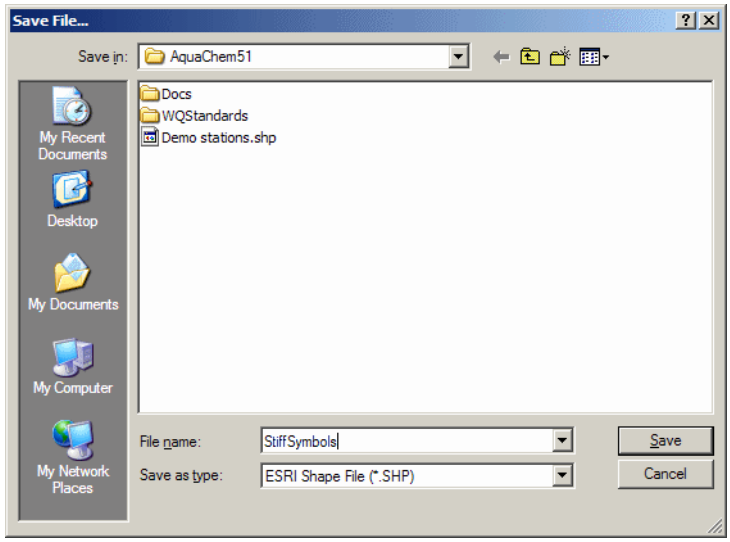


Export Map Symbols to ESRI Shapefile

Most GIS applications are limited to bar and pie thematic maps for data representation, which may not truly represent your water quality data; AquaChem allows you to export Stiff and Radial symbols (and their attribute data) to Polygon Shape file format, so that they may be imported for further analysis in a GIS package. Follow the directions below.

With the map plot window visible, and selected,

- ☞ **File / Export / ESRI Shapefile** from the main menu. The following dialog will appear:



- ☞ Specify the name for the Shape file (Stiff Symbols)
- ☞ **[Save]**

A confirmation dialog will appear.

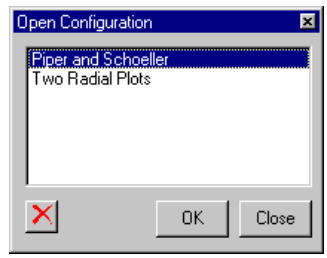
- ☞ **[OK]** to continue.
- ☞ **[X]** at the top of the **Map** plot to close it

You will now proceed to print one of the plots that was created earlier in this section.

2.5 Printing the Plots

In order to print the AquaChem plots, you will first load the plot configuration file which was saved earlier. Before proceeding, please ensure you have all other AquaChem windows and dialogues closed and only the Active Samples list window is visible and active.

- ☞ **Plots** from the main menu and then select **Open Configuration**



- ☞ ***Piper and Schoeller*** (from the list of Configurations)
- ☞ **[OK]**

You should then see one **Piper** diagram and one **Schoeller** plot, which was created earlier.

To print these plots,

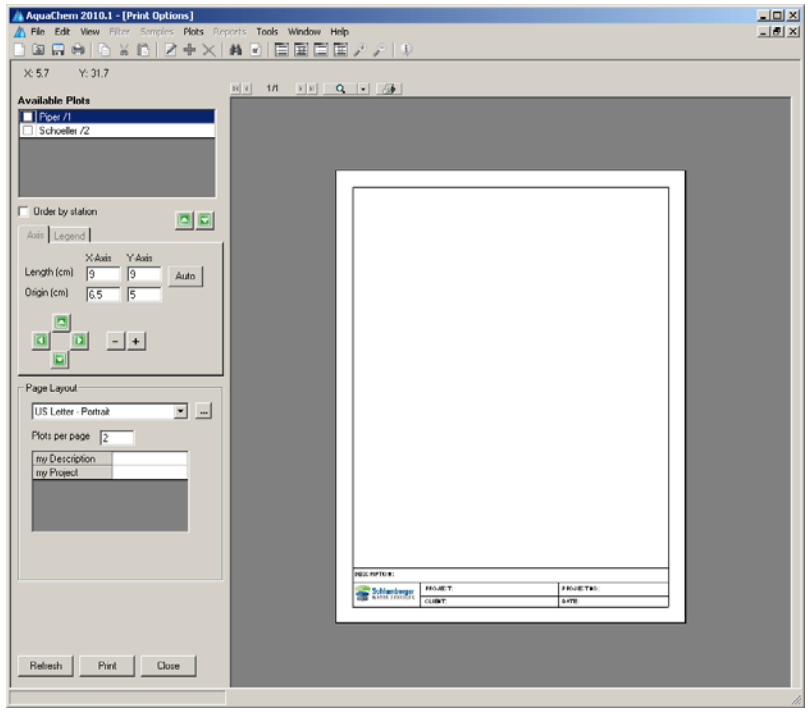
- ☞ **File** from the main menu and then select **Print**, or press  button in the toolbar.

You should then see the **Print Options**

window. Under Available Plots,

- ☞ **Piper /1** to uncheck this plot
- ☞ **Schoeller /2** to uncheck this plot

Your report should now appear blank, as shown below.



The **Print Options** allow you to choose which plots will be printed, their position, size, which plot template will be used, in addition to other Windows page layout and printer setup options.

In the **Available Plots** field (the upper-left corner of the **Print Options** window), a list of available plots will appear. This list includes the plots which are currently open in AquaChem and are available to be printed. In this example, you have a **Piper** Diagram and a **Schoeller** Plot available. However for this exercise you will print only the Piper diagram.

The first step, before you select which plot to print, is to select the page layout or to choose a print template. This will ensure that the plot is properly fit to the desired page dimensions.

Under the **Page Layout** options (on the left side of the window), ensure that the template setting is **US Letter - Portrait**.

As soon as the template is loaded, a list of plot descriptors will appear in the **Page Layout** dialogue, and the print preview window will be automatically updated to reflect the selected template settings.

Next, you will fill in the project specific plot description fields under the **Page Layout** options. Press the **<Enter>** key after each entry:

my Description:
type: Piper plot of samples collected from 1992 to 1998

my Project:
type: Demo Project

my Project #:
type: 2005-1

my Client:

type: Your name or a client's name.

my Date:

type: Current date

NOTE: The SWS logo shown in the bottom of the page can be easily replaced with your own company logo. This can be done using the **Template Designer** option. This option is not explored in this exercise.

Now, you are ready to load the **Piper** diagram onto this print template. To select the **Piper** diagram for printing,

- ☞ Click once in the first box beside **Piper /1** (under **Available Plots**, in the upper left corner), and a check mark will be added to the box. The presence of a check mark beside the plot name indicates that this plot will be loaded into the print preview. If the plot does not load automatically, click **[Refresh]** button at the bottom left corner of the screen.

If the default page settings are not acceptable, you can manually change the individual size and position of each plot using the options provided in the **Axis** tab. Alternatively, you can easily change the page layout by pressing the **[Printer Setup]** button.

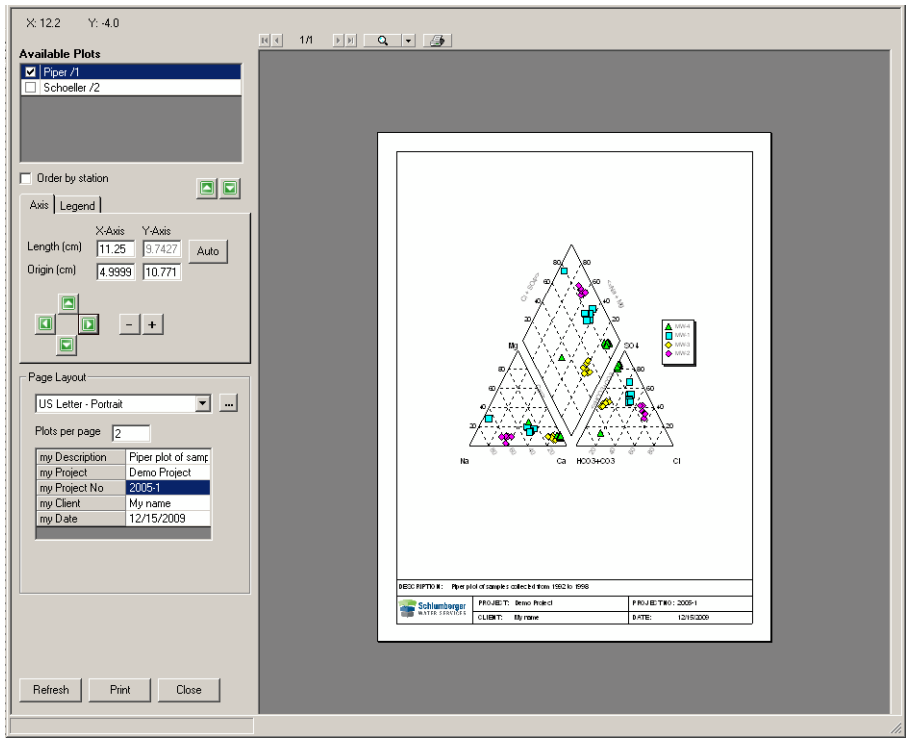
Next you must select the legend for the **Piper** plot, and position it on the page.

- ☞ **Legend** tab (below the list of **Available Plots**, and beside the **Axis** tab).
- ☞ **Visible** (click once in this box) to activate the legend for the **Piper**

plot. The **Piper** plot legend will appear in the upper-left corner of the page. To move the legend,

- ☞ **X-Axis** field and enter a value of 15.
- ☞ **Y-Axis** field and enter a value of 20.
- ☞ **[Refresh]** button (in the lower left corner) to refresh the Print

Preview. If you have loaded the plot successfully, your display should be similar to the one shown below:



- ☞ **[Print]** button (in the lower left corner) to print the plot to a printer.
- ☞ **[Close]** to return you to the main AquaChem window.

- ☞ **Plots > Close all Plots,** from the main menu.

In the next section of this exercise, you will explore the Report options available in AquaChem.

2.6 Creating Data Reports

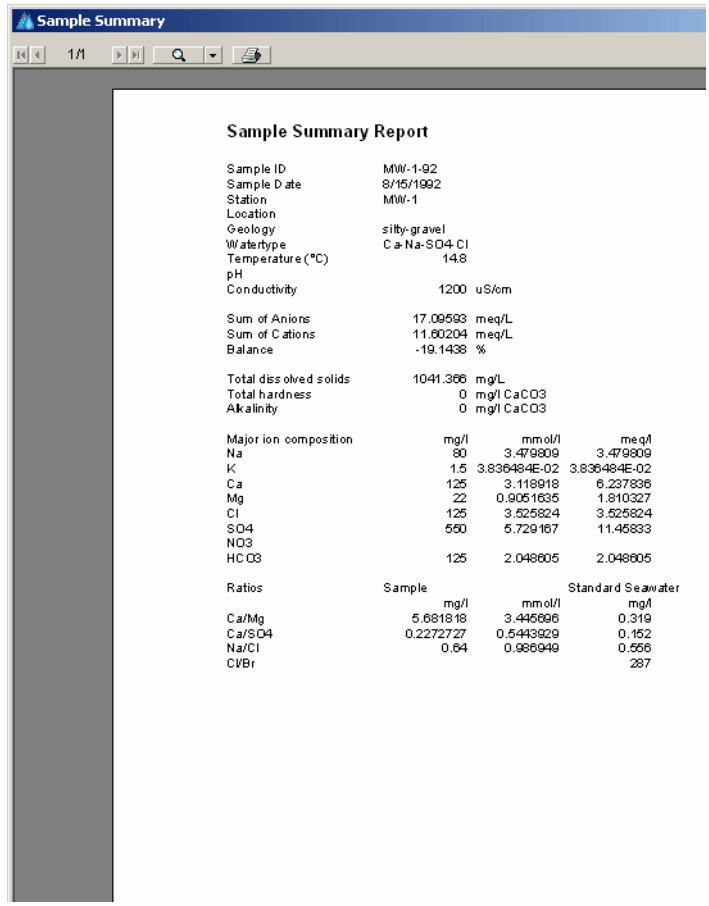
AquaChem allows you to visualize the data and present up to seven different types of reports, and also allows you to create your own report templates. The following section will briefly demonstrate two of these reports: Sample Summary and Statistics.

Sample Summary Report

The **Sample Summary** report provides a summary of the most common measured and calculated parameters for the selected sample. To visualize a **Sample Summary** Report:

- ☞ **MW-1-92** (SampleID) the first sample in the Active Samples list
- ☞ **Reports** from the main menu and then select **Sample Summary**

The **Sample Summary** window will be displayed as shown below:



This report provides general sample information, measured values for major ions, and calculated values (Sum Anions, Sum Cations, Hardness, etc.).

To view the **Sample Summary** report for other samples, use the

 scrolling buttons in the lower right corner of the report window. These will allow you to show a report for the first, previous, next, or last sample in the sample list.

The **Sample Summary** report can be printed or saved to a file. You may save the report content as .RTF (Rich Text format) or .HTM (web-ready format). To do so, select **File>Save** and specify the file location and name in the dialogue that loads.

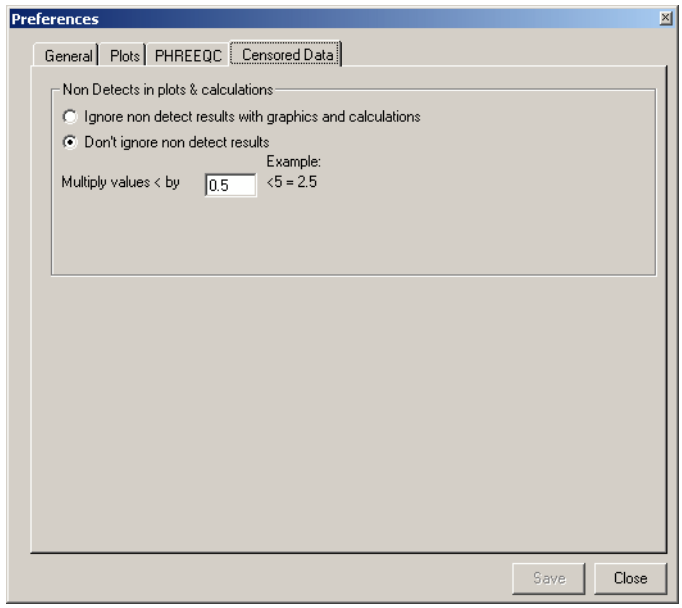
☞ **[Close]** to close the **Sample Summary** window.

NOTE: The **Sample Summary** report was created using the **Report Designer**. This report is included with any new database.

Statistics Report

Statistical calculations are an essential component of water quality data analysis. AquaChem now offers more advanced features for handling censored data sets (non-detect values). To see these options, view the user preferences.

- ☞ **File / Preferences** from the main menu.
- ☞ **Censored Data** tab, and the following dialog will appear.



In this dialog, there are several user-defined settings for handling data that is below the MDL for statistical calculations and in plots (settings are based on the USEPA Guidance for Data Quality Assessment document).

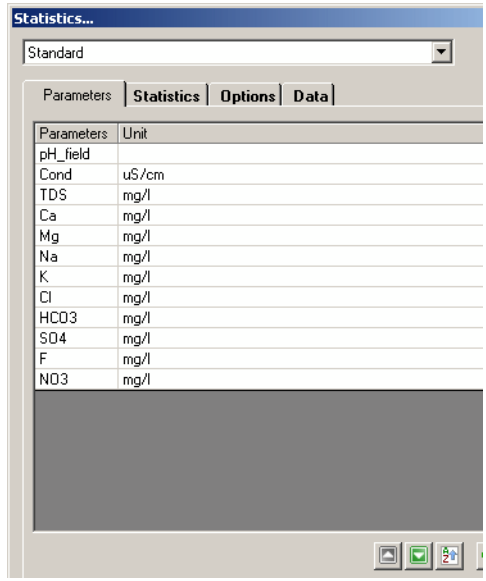
- ☞ **[Close]** to return to the main window.

The **Statistics Report** provides a statistical summary of selected parameters for all active samples.

To view a **Statistics Report** for all samples in the active list:

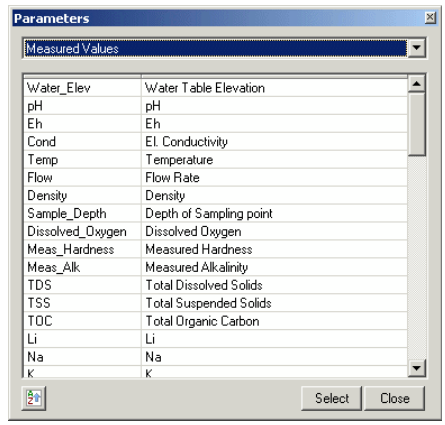
- ☞ **Reports / Statistics / Summary Statistics**

The following options dialog will appear:



There is an option to add / remove parameters, and also change the units for the selected parameters.

- ☞  button to add new parameters. The parameters dialog will appear:



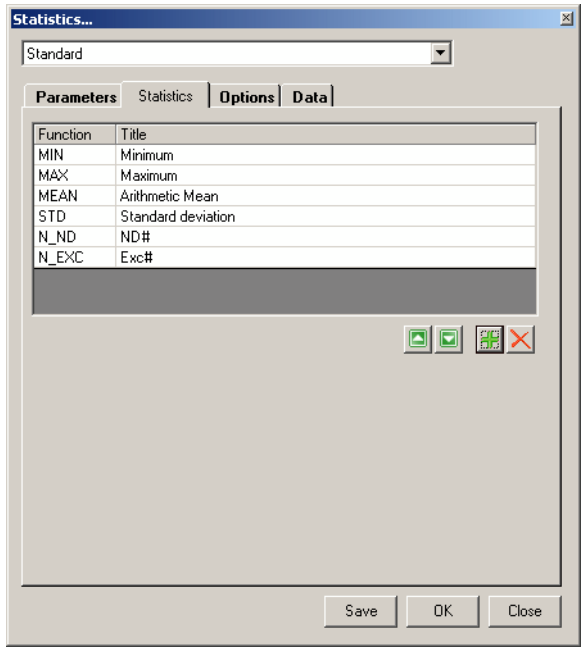
- ☞ **Calculated Values** from the picklist at the top of the window.
- ☞ **Sum of Anions** from the list.
- ☞ **[Select]**
- ☞ **Sum of Cations** from the list.
- ☞ **[Select]**
- ☞ **[Close]**

Select the desired units for these new parameters.

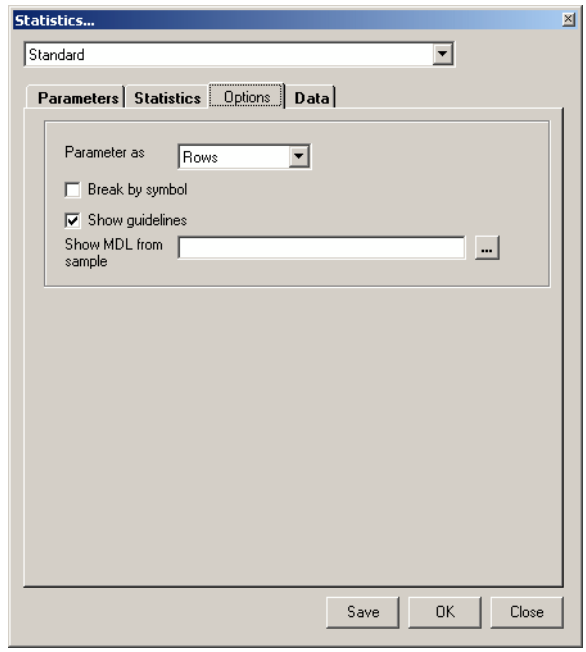
- ☞ Select **meq/l** for both new parameters by clicking in the corresponding cell of the **Unit** column and selecting the appropriate unit from the combo box.

Now you will add additional statistical calculations to the report.

- **Statistics** tab



-  button to add new statistical calculations.
- **Number of Non-Detects** and **Number of Exceedences** from the list.
- **[Select]** button
- **[Close]** button
- **Options** tab



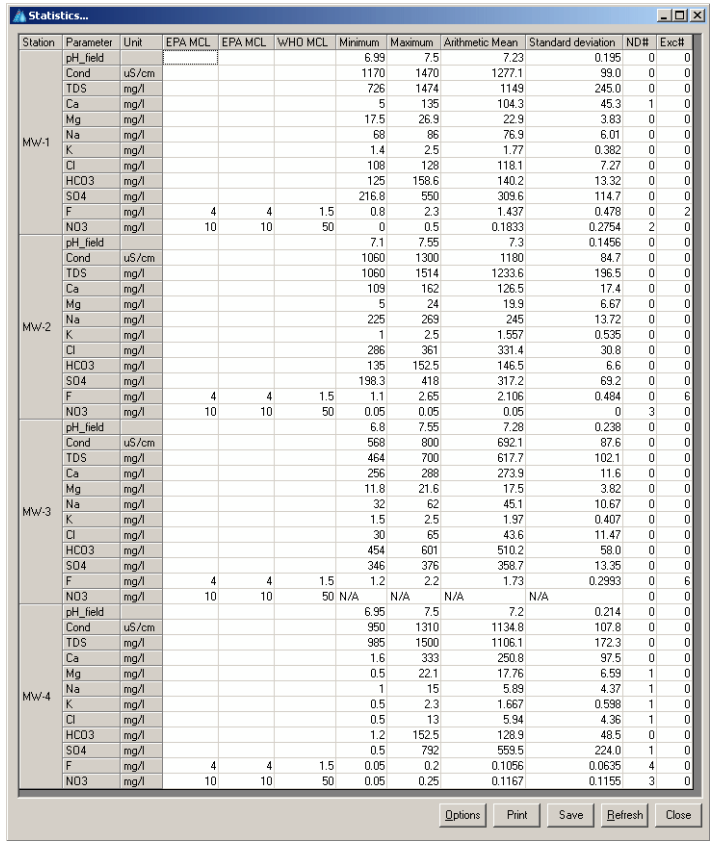
- ☞ Check the box beside **Break by symbol**.
- ☞ **Data** tab to see a preview of the data set.

You can save the statistics report configuration for easy recall in the future. To do so:

- ☞ **[Save]** button to save the statistics report as a

  template. type: MyExample for the name
- ☞ **[OK]**
- ☞ **[OK]** a second time, in the **Options** dialog, to generate the report.

The **Statistics Report** window should be shown on your display, similar to the one below.



Station	Parameter	Unit	EPA MCL	EPA MCL	WHO MCL	Minimum	Maximum	Arithmetic Mean	Standard deviation	ND#	Exc#
MW-1	pH_field					6.99	7.5	7.23	0.195	0	0
	Cond	uS/cm				1170	1470	1277.1	99.0	0	0
	TDS	mg/l				726	1474	1149	245.0	0	0
	Ca	mg/l				5	135	104.3	45.3	1	0
	Mg	mg/l				17.5	26.9	22.9	3.83	0	0
	Na	mg/l				68	86	76.9	6.01	0	0
	K	mg/l				1.4	2.5	1.77	0.382	0	0
	Cl	mg/l				108	128	118.1	7.27	0	0
	HCO3	mg/l				125	158.6	140.2	13.32	0	0
	SO4	mg/l				216.8	550	309.6	114.7	0	0
	F	mg/l	4	4	1.5	0.8	2.3	1.437	0.478	0	2
	NO3	mg/l	10	10	50	0	0.5	0.1833	0.2754	2	0
MW-2	pH_field					7.1	7.55	7.3	0.1456	0	0
	Cond	uS/cm				1060	1300	1180	84.7	0	0
	TDS	mg/l				1060	1514	1233.6	196.5	0	0
	Ca	mg/l				109	162	126.5	17.4	0	0
	Mg	mg/l				5	24	19.9	6.67	0	0
	Na	mg/l				225	269	245	13.72	0	0
	K	mg/l				1	2.5	1.557	0.535	0	0
	Cl	mg/l				286	361	331.4	30.8	0	0
	HCO3	mg/l				135	152.5	146.5	6.6	0	0
	SO4	mg/l				198.3	418	317.2	69.2	0	0
	F	mg/l	4	4	1.5	1.1	2.65	2.106	0.484	0	6
	NO3	mg/l	10	10	50	0.05	0.05	0.05	0	3	0
MW-3	pH_field					6.8	7.55	7.28	0.238	0	0
	Cond	uS/cm				568	800	692.1	87.6	0	0
	TDS	mg/l				464	700	617.7	102.1	0	0
	Ca	mg/l				256	288	273.9	11.6	0	0
	Mg	mg/l				11.8	21.6	17.5	3.82	0	0
	Na	mg/l				32	62	45.1	10.67	0	0
	K	mg/l				1.5	2.5	1.97	0.407	0	0
	Cl	mg/l				30	65	43.6	11.47	0	0
	HCO3	mg/l				454	601	510.2	58.0	0	0
	SO4	mg/l				346	376	358.7	13.35	0	0
	F	mg/l	4	4	1.5	1.2	2.2	1.73	0.2993	0	6
	NO3	mg/l	10	10	50	N/A	N/A	N/A	N/A	0	0
MW-4	pH_field					6.95	7.5	7.2	0.214	0	0
	Cond	uS/cm				950	1310	1134.8	107.8	0	0
	TDS	mg/l				985	1500	1106.1	172.3	0	0
	Ca	mg/l				1.6	333	250.8	97.5	0	0
	Mg	mg/l				0.5	22.1	17.76	6.59	1	0
	Na	mg/l				1	15	5.89	4.37	1	0
	K	mg/l				0.5	2.3	1.667	0.598	1	0
	Cl	mg/l				0.5	13	5.94	4.36	1	0
	HCO3	mg/l				1.2	152.5	128.9	48.5	0	0
	SO4	mg/l				0.5	792	559.5	224.0	1	0
	F	mg/l	4	4	1.5	0.05	0.2	0.1056	0.0635	4	0
	NO3	mg/l	10	10	50	0.05	0.25	0.1167	0.1155	3	0

The minimum, maximum, arithmetic mean, standard deviation, as well as other statistical values of interest will be calculated for the selected database parameters. Using the **Break by symbol** option the samples are separated into their appropriate stations.

NOTE: You may need to adjust the column widths in order to see the full column headings and the entire contents of the report.

With these new statistics features you can quickly and easily sort your data and determine the number of exceedences, number of samples below the method detection limit, minimum value, maximum value, and much more.

Export Report

This report can be printed or saved to a file. You may save the report content as .XLS, .TXT or .CSV.

- ☞ **File / Save** from the main menu, click on the  button in the toolbar, or click the **[Save]** button at the bottom of the window.
- ☞ **Excel (.XLS)** from the list of file types

For the filename,

type: StatsReport

- ☞ **[Save]**
- ☞ **[Close]** located at the bottom of the **Statistics Report** window. This will close this report window and return you to the main AquaChem

window.

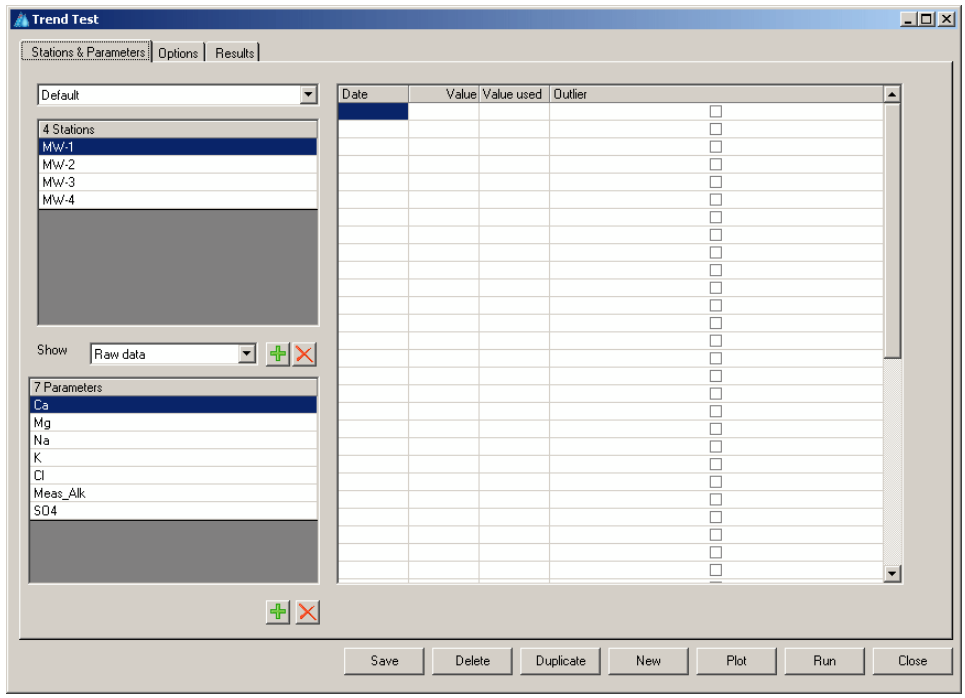
Trend Analysis

AquaChem allows you to quickly perform trend analysis on many stations and parameters simultaneously. In this example, you will perform a trend analysis on the samples collected from two stations in the database (MW-1, MW-2), to determine if benzene and PCE concentrations demonstrated a decreasing trend over time.

From the main menu,

☞ **Reports / Statistics / Trend Analysis**

The following options dialog will appear:



☞ **New** button located at the bottom of the dialog.

Adding Stations

To add stations to the trend analysis,

☞  button located beside the Show combo box

The Stations dialog will appear on your screen.

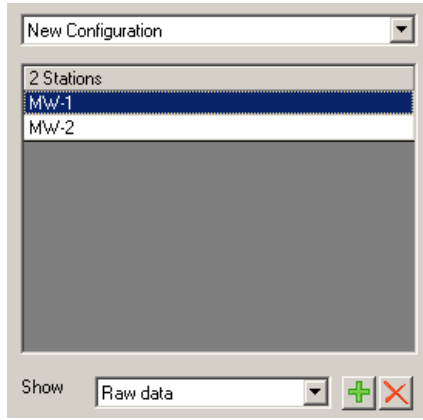
☞ **MW-1**

. ☞ **[Select]** button

☞ **MW-2**

- **[Select]** button
- **[Close]** button

The MW-1 and MW-2 stations should now appear in the station list.



Adding Parameters

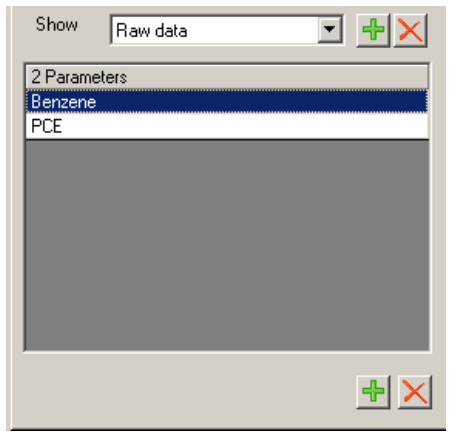
To add parameters to the trend analysis,

-  button located below the Parameters box

The Parameters dialog will appear on your screen.

- **Benzene**
- **[Select]** button
- **PCE (Tetrachloroethylene)**
- **[Select]** button
- **[Close]** button

The parameters Benzene and PCE parameters should now appear in the Parameters list.



The next step is to specify the input and output options for the trend analysis.

Trend Analysis Options

To set the trend analysis input and output parameters,

☞ **Options** tab

The input options will appear on the left side, and the output options will appear on the right side. First we will specify the input parameters for the trend analysis calculations.

In the **Title** field,

type: Trend Analysis Example

In the **Description** field,

type: Analysis of benzene and PCE trends for MW-1 and MW-2

In the **Start Date**

field, type:

1/1/1992

In the **End Date**

field, type:

1/1/1999

In the **Max %ND**

field, type: 80

In the **Historic ND, ignore >**

field, type: 5

In the **Min Years** field,

type: 4

In the **Confidence (%)** field,

type: 95

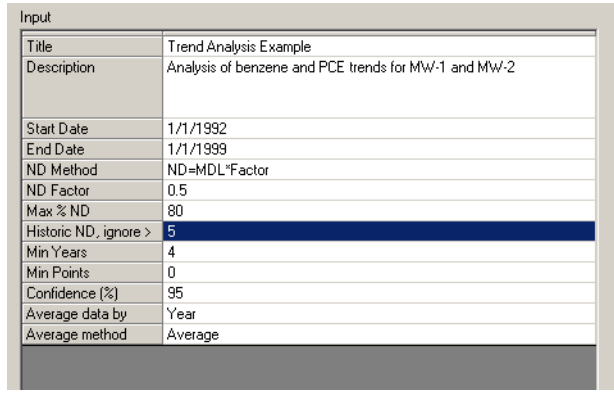
From the **Average data** by field:

☞ **Year**

From the **Average method** field:

☞ **Mean**

The input options grid should appear similar to the one shown below.



The next step is to specify the desired output options. The output options allow you to specify which tests to run and how the trend analysis results are displayed. For this example, the default options will used. As such, the Mann Kendall test, Sen's test, and Linear regression will be calculated and displayed in the results.

Running the Trend Test

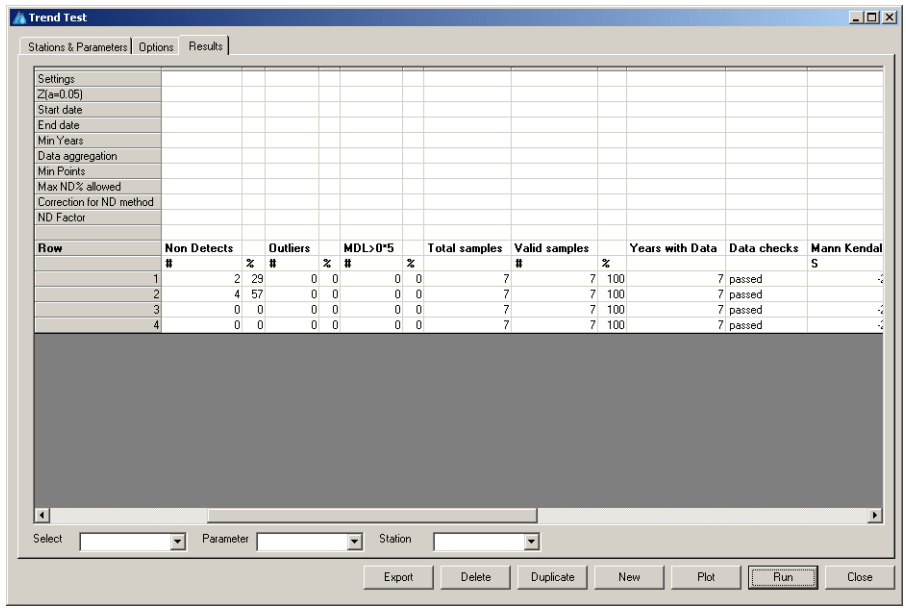
Now that the stations and parameters have been defined, and the options have been configured, you can run the trend test analysis.

To run the trend test analysis,

☞ **[Run]** button located along the bottom of the dialog.

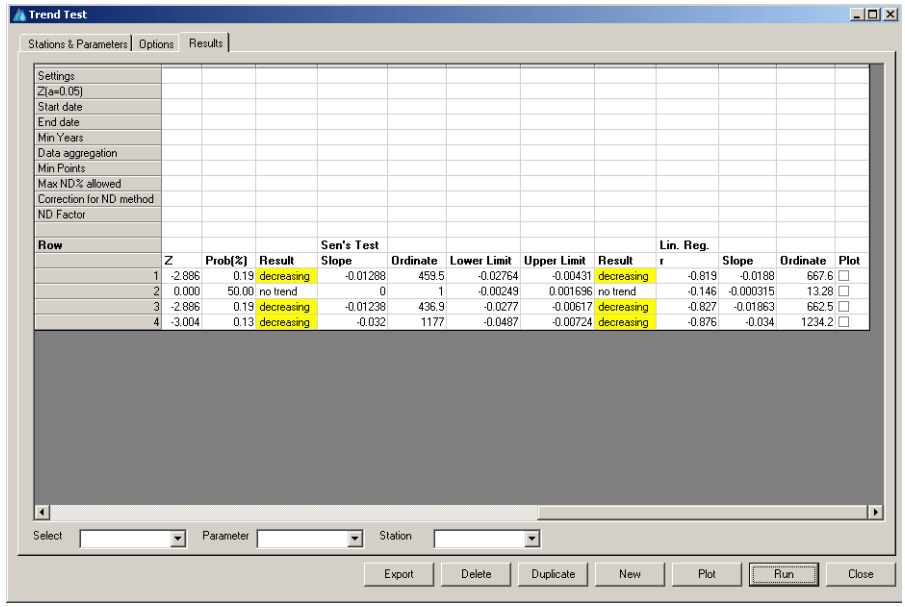
Depending on how many stations and parameters have been selected, this process may take a moment before the results are displayed. Because this example only uses two stations and two samples, the results should be returned immediately.

The results will be displayed under the **Result** tab in a spreadsheet view.



The first 10 rows in the spreadsheet provide an overview of the input parameters specified in the Options tab. The remaining rows display the trend test results for each station and parameter combination.

Move the horizontal scroll bar to the right, to view the results of the Mann Kendall test and Sen's Test. You will see that both tests indicate benzene to be decreasing overtime for both MW-1 and MW-2. However, for PCE the trend analysis shows a decreasing trend for MW-2, but no trend for MW-1.



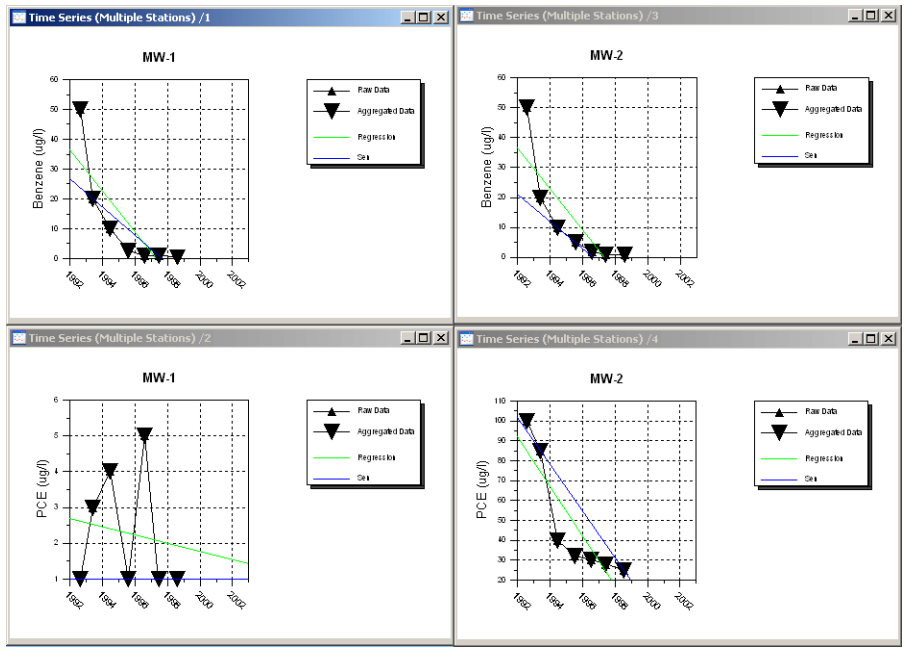
You can visualize the trend analysis for each station and parameter combination by plotting the results on time series plots.

The view the trend analysis on a time series plot,

Scroll across the spreadsheet table so that the last column in the table is shown. Under the Plot column,

- ☞ ☑ for each row under the Plot column
- ☞ **[Plot]** button, located along the bottom of the dialog.

Four time series plots will appear on your screen showing the raw data, aggregated data, regression line and Sen's line.



To close the trend analysis plots,

☞ **Plots > Close All Plots** from the main menu

QA/QC Tools

The **QA/QC** checks included with the new version of AquaChem allow you quickly and easily identify and compare duplicate samples, non-detects, outliers, etc. These validation tools are a critical component of data analysis and interpretation.

Compare Duplicates

To compare duplicate samples, you must first locate them. You can also do this with the **QA/QC** tools.

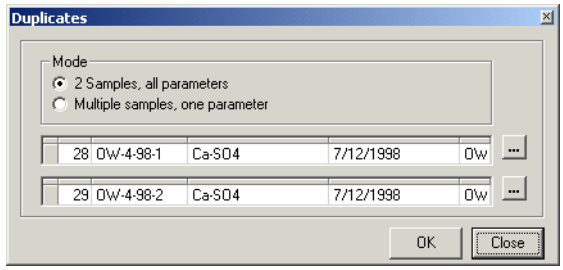
To view the **QA/QC** tools,

☞ **Tools >QA/QC** from the main menu and select **Highlight Duplicates**

AquaChem will search your database for all samples that have “Duplicate_ID” codes, which are assigned in the sample description parameter category and highlight them. There are two such samples in this database (which will be selected at the bottom of the samples list).

☞ **Tools >QA/QC** from the main menu and select **Compare Duplicates**

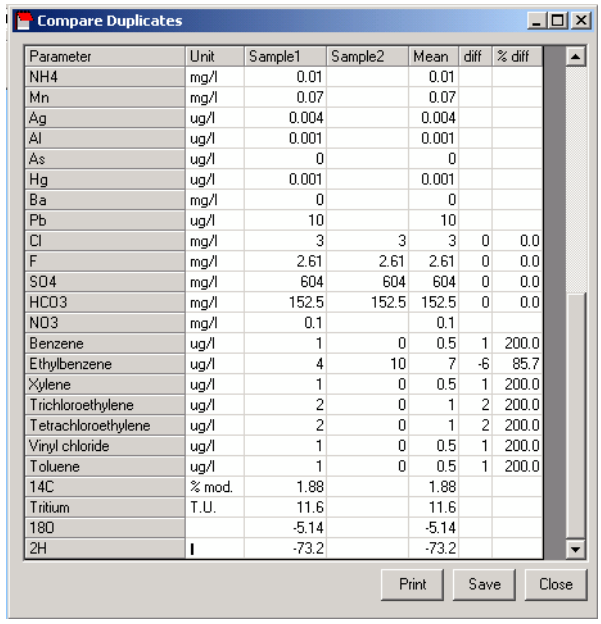
The Compare Duplicates dialogue will appear similar to the one below.



The two selected samples are entered automatically into the fields.

- ☞ **[OK]** to generate the report.

The report window will be displayed similar to the one shown below:



Parameter	Unit	Sample1	Sample2	Mean	diff	% diff
NH4	mg/l	0.01		0.01		
Mn	mg/l	0.07		0.07		
Ag	ug/l	0.004		0.004		
Al	ug/l	0.001		0.001		
As	ug/l	0		0		
Hg	ug/l	0.001		0.001		
Ba	mg/l	0		0		
Pb	ug/l	10		10		
Cl	mg/l	3	3	3	0	0.0
F	mg/l	2.61	2.61	2.61	0	0.0
SO4	mg/l	604	604	604	0	0.0
HCO3	mg/l	152.5	152.5	152.5	0	0.0
NO3	mg/l	0.1		0.1		
Benzene	ug/l	1	0	0.5	1	200.0
Ethylbenzene	ug/l	4	10	7	-6	85.7
Xylene	ug/l	1	0	0.5	1	200.0
Trichloroethylene	ug/l	2	0	1	2	200.0
Tetrachloroethylene	ug/l	2	0	1	2	200.0
Vinyl chloride	ug/l	1	0	0.5	1	200.0
Toluene	ug/l	1	0	0.5	1	200.0
14C	% mod.	1.88		1.88		
Tritium	T.U.	11.6		11.6		
18O		-5.14		-5.14		
2H		-73.2		-73.2		

With this report you can quickly compare the samples and determine potential sources of error during lab analysis, sample collection, or handling procedures.

- ☞ **[Close]** located at the bottom of the window to close the report
- ☞ **[Close]** to close the **Compare Duplicates** dialogue

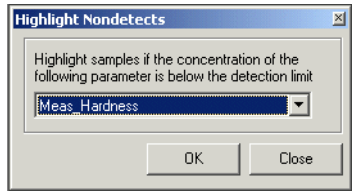
Highlight Non-Detects

Data generated from chemical analysis may fall below the method detection limit (MDL) of the analytical procedure. These measurement data are generally described as not detected, or nondetects, (rather than as zero or not present) and the appropriate limit of detection is usually reported. In cases where measurement data are described as not detected, the concentration of the chemical is unknown although it lies somewhere between zero and the detection limit. Data that includes both detected and non-detected results are called censored data in the statistical literature. (Office of Environmental Information, U.S. Environmental Protection Agency, 2000)

In AquaChem, you can highlight samples that have non-detect values for a specific parameter. You define a parameter, and AquaChem searches the database for all values for this parameter, and highlights any values which contain the "<" symbol (for example, <0.1)

- ☞ **Tools > QA/QC** from the main menu and select **Highlight Non-Detects**

The following dialog will appear, where you can select the parameter of interest.



- ☞ **Ag** from the list.
- ☞ **[OK]**
- ☞ **[Close]**

In the demo database, there are numerous samples for Ag that are below the MDL. Feel free to review one of the selected samples now.

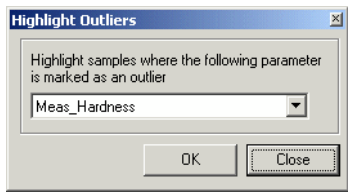
Highlight Outliers

Outliers are measurements that are extremely large or small relative to the rest of the data and, therefore, can cause misrepresentation of the population from which they were collected. Outliers may result from transcription errors, data-coding errors, or measurement system problems such as instrument breakdown. However, outliers may also represent true extreme values of a distribution (for instance, hot spots) and indicate more variability in the population than was expected. Not removing true outliers and removing false outliers both lead to a distortion of estimates of population parameters. (Office of Environmental Information, U.S. Environmental Protection Agency, 2000)

In AquaChem, you can highlight samples that have the outlier check enabled, to quickly identify potential errors in sampling or analysis.

- ☞ **Tools > QA/QC** from the main menu and select **Highlight Outliers**

The following dialog will appear, where you can select the parameter of interest.



- ☞ **Pb** from the list.
- ☞ **[OK]**

☞ **[Close]**

You should see two samples highlighted in the list. To view only these samples,

☞ **Filter > Show Only Selected**

To see the data for these samples, select one and

☞ **Sample > Edit.** The Sample details window will appear

Scroll down the list of values to see the value of Pb. You will see the value is 15 ug/l (or 10 ug/l), which is much different from the rest of the data set. You should now review the sample collection and analysis procedures to determine the potential source of error.

To restore all samples,

☞ **Filter > Show All**

In the last section of this Demo exercise, you will use PHREEQC to calculate saturation index values for a sample in the Demo database.

2.7 PHREEQC - Calculate Saturation Indices and Activities

PHREEQC is a geochemical modeling program designed by the USGS. The program can be used for speciation, batch-reaction, one-dimensional transport, inverse geochemical calculations, and much more. AquaChem includes several options for running PHREEQC with your water quality data. In this section, you will calculate saturation indices and activities for a sample in your database, with just a few clicks of your mouse.

The Saturation Index (**SI**) of a selected mineral phase is the degree of saturation. The SI can be a means of evaluating water quality data to determine if certain minerals have a tendency to dissolve or precipitate out of solution, in order to reach equilibrium. The SI is calculated as follows:

$$SI = \log(IAP/K_T)$$

where,

IAP = the ion activity product for the given material and
K_T = the reaction constant at the given temperature

If SI > 0, then the solution is super-saturated with respect to the mineral phase, and precipitation will be likely;

If SI < 0, then the solution is below saturation of the specified mineral phase, and dissolution will be expected;

If SI = 0, then the solution is in equilibrium with the specified mineral phase.

When you select an AquaChem sample from your database, an input file will

be
automatically created using the measured parameter values (ex.Ca, Fl, SO4, etc.). PHREEQC will calculate saturation indices and activities for all modeled parameters which are defined in the current database structure, provided that an appropriate measured value has been entered. The results of the simulation will be automatically written back to the database for the selected sample, provided that the fields exist in the database.

An example of how to Calculate Saturation Indices and Activities using PHREEQC is provided below:

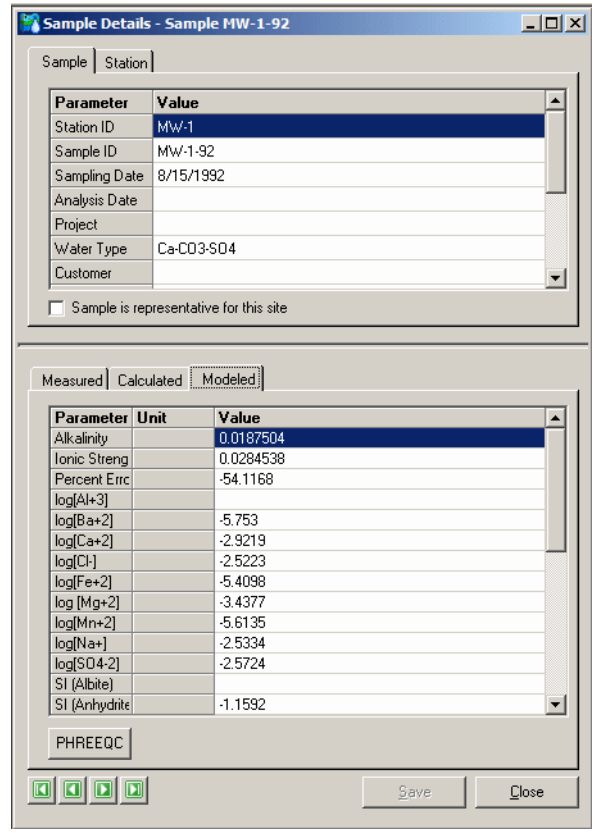
- **Samples** tab (at the top of the active list window).
- **MW-1-92**, the first sample in active stations list.
- **Tools > Modeling > Calculate Sat. Indices and Activities** from the main menu.

PHREEQC will then run in a DOS window (in the background) and calculate the appropriate SIs and activities. The modeled results will be saved automatically back to your database.

To view the PHREEQC results, you must load the **Modeled Parameters** tab in the Sample Details window for this sample:

- **Samples > Edit** from the main menu
- **Modeled** tab

In this window, you will see the modeled values for the available parameters. An example is shown in the figure below:



PHREEQC has calculated the appropriate SI and activity values for the defined modeled parameters. You may now do further processing and analysis with these parameter values, such as plotting, reporting, and querying.

This concludes the demonstration exercise for AquaChem 2014.1.