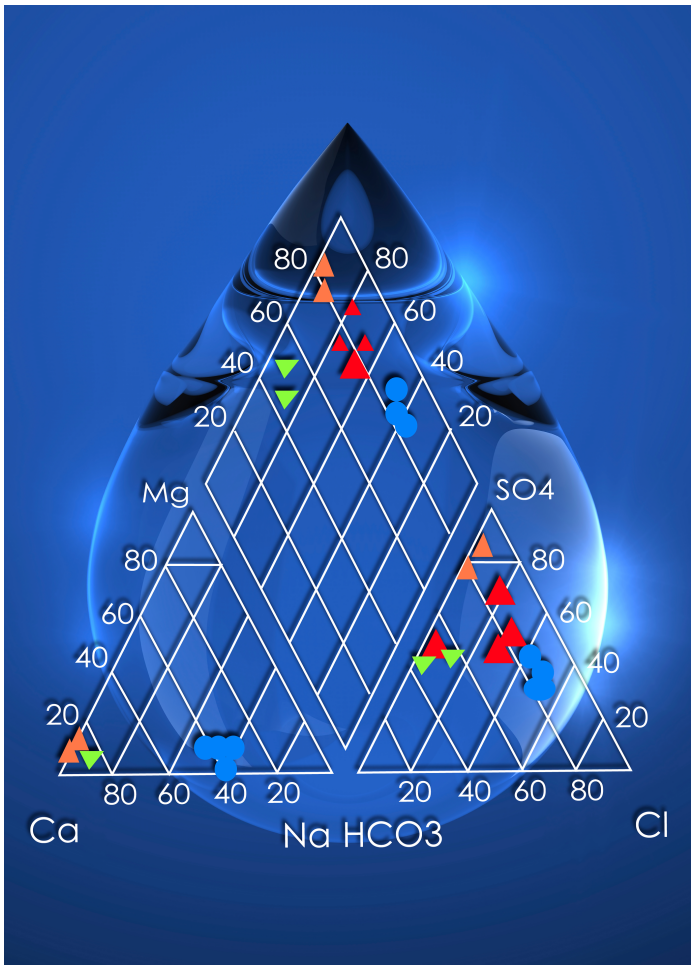
User's Manual



AquaChem 10.0

Water Quality Analysis Software

Waterloo HYDROGEOLOGIC

NOVA METRIX

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Specifications are current at the time of printing.
Errors and omissions excepted

Table of Contents

Chapter 1 Introduction to AquaChem

Welcome to the documentation site for AquaChem 10.0.

AquaChem 10.0 is the next generation version of the popular water quality software application by Waterloo Hydrogeologic. If you are looking for documentation on version AquaChem 2014, please click the link on the right below:

AquaChem 10.0 Documentation

AquaChem 2014.2 Documentation

AquaChem is a software package developed specifically for managing, analyzing, and plotting water quality data. It features a fully customizable database of physical and chemical parameters and provides a comprehensive selection of analysis tools, calculations, and plots for interpreting water quality data.

AquaChem provides a wide range of functionalities and calculations including unit conversions, charge balances, sample comparison, statistical summaries, and much more. AquaChem also contains a customizable database of water quality standards with support for multiple action levels for each parameter. Any samples exceeding the selected standard(s) 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:

- **Geochemical Plots:** Piper, Stiff, Durov, Schoeller, Wilcox, Giggenbach, Meteoric Water Line, Ludwig-Langelier, Ternary;
- **Statistical Plots:** Box and Whisker, Histogram, Probability, Quantile, Detection Summary
- **General Plots:** Scatter, Line, Pie, Stacked Bars, Radial, Time Series; and
- **Map Plots:** Uniform Symbols, Proportional Symbols, Pie Chart, Radial Chart, Stiff Diagram

Each of these plots facilitates interpretation of the many complex interactions between groundwater and aquifer materials and helps you identify important data trends and groupings.

AquaChem also contains a console for the R scripting language that puts the vast set of R libraries for statistical analysis, visualization, classification, clustering, modeling, and more at your fingertips. Save and load scripts within R to automate working with your data. Note that R and its libraries must be downloaded separately and is available through the Comprehensive R Archive Network (CRAN) which can be found on the main R website.

Once you start using AquaChem, you will see that it is truly one of the most powerful tools available for managing and interpreting any water quality data set.

1.1 Installing AquaChem

Hardware Requirements

To run the latest version of **AquaChem**, you will need the following minimum system configuration:

Operating System	Windows 10 Pro or Enterprise **NOTE:** Administrative rights may be required to install the software
Processor	32-bit or 64-bit (Pentium 4 or higher)
RAM	8GB or more recommended
Hard Disk	500 MB Free Space, plus extra space for your projects
Networking Hardware	Network Card (required for soft key licensing)

Software Requirements

To run the latest version of AquaChem, the following software pre-requisites are required:

Microsoft .NET Framework v.4.0 installed (provided with installation)
Microsoft Office OR Microsoft Access Runtime - *see the Installing Access Runtime Engine instructions*
R (optional) - *see the Installing R instructions*

If you have any problems with your particular system configuration, please contact your system administrator, or technical support: support@waterloohydrogeologic.com

Installation and Licensing

When you purchase AquaChem, you will receive download and installation instructions. Please consult these for the latest instructions.

Starting AquaChem

Once AquaChem has been installed on your computer, simply double-click on the AquaChem shortcut icon () located on your computer's desktop.

Alternatively, you can access the software via the start menu by clicking on Start/Programs/ ...

Please Note: If you are using dongle-based hardware licensing, please ensure that your dongle is connected to your computer AFTER you have installed the software, and that you have properly configured your installation.

1.1.1 Installing Access Runtime Engine

AquaChem 10.0 uses the Microsoft (MS) Access database file format to store the data associated with each project. In order for AquaChem to connect to and work with the data in your project, you will need a functioning Access database connection provider that matches the bit-level of AquaChem, which is a 32-bit application. The following configurations will provide the necessary Access database connections required by AquaChem:

- 32-bit (x86) version of MS Office 365 Access or MS Office 2019 Access
- 32-bit (x86) version of MS Access Runtime Engine 2007 or newer

Please Note: if you have a 64-bit version of Microsoft Office, you will need to install a 32-bit version of the MS-Access Runtime Engine that is *different* from the your Office version. For example, if you have Office 2019 x64 installed, you can install the 32-bit version of the Access Runtime Engine 2010, 2013, or 2016.

Download Links:

- Access Runtime 2010
- Access Runtime 2013
- Access Runtime 2016
- Access Runtime 365

1.1.2 Installing R

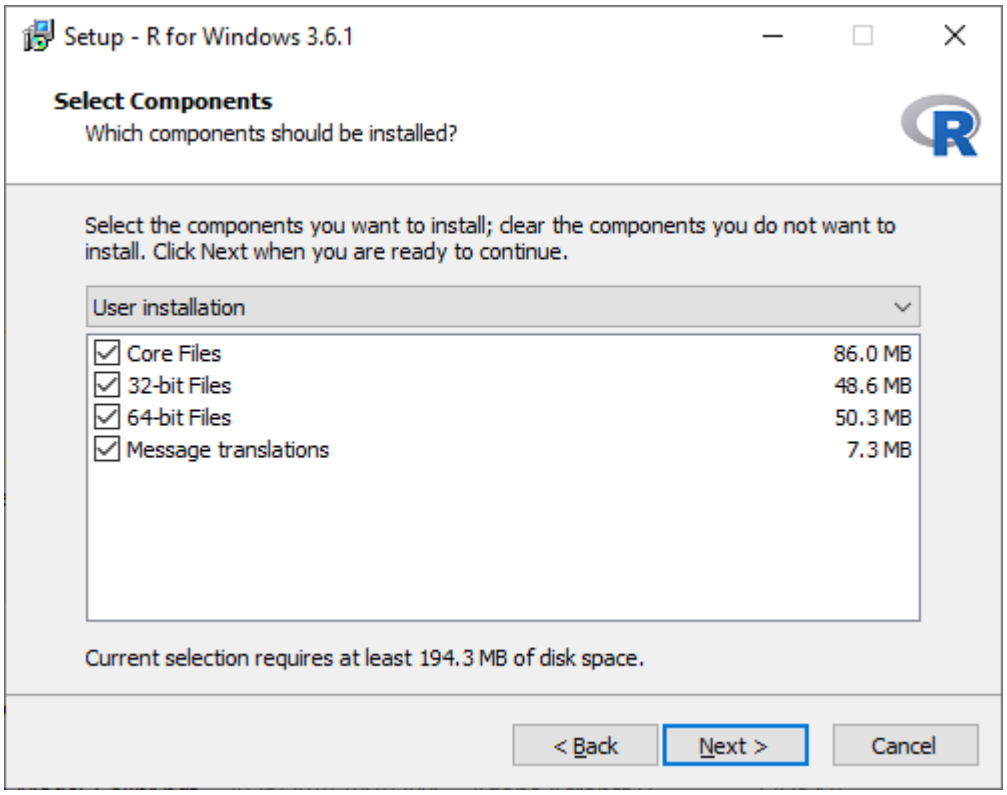
R is a freely available scripting language and environment for statistical computing developed by the R Foundation and an active user community which provides a vast variety of statistical and graphical procedures.

Getting R

To get Started with R, please visit the R homepage: www.r-project.org. There you will be able to download a copy from one of the members of the Comprehensive R Archive Network (CRAN) and find many resources including the manual and answers to FAQs. AquaChem has been tested with the base version of R for Windows, which is available from many mirror websites, including: https://cloud.r-project.org/bin/windows/base/release.htm.

32-Bit vs. 64-Bit

Since AquaChem is currently only available as a 32-bit application, you will need to install the 32-bit version of R. Please note that you can install both the 64-bit and 32-bit versions of R (in fact this is currently the default installation setting):



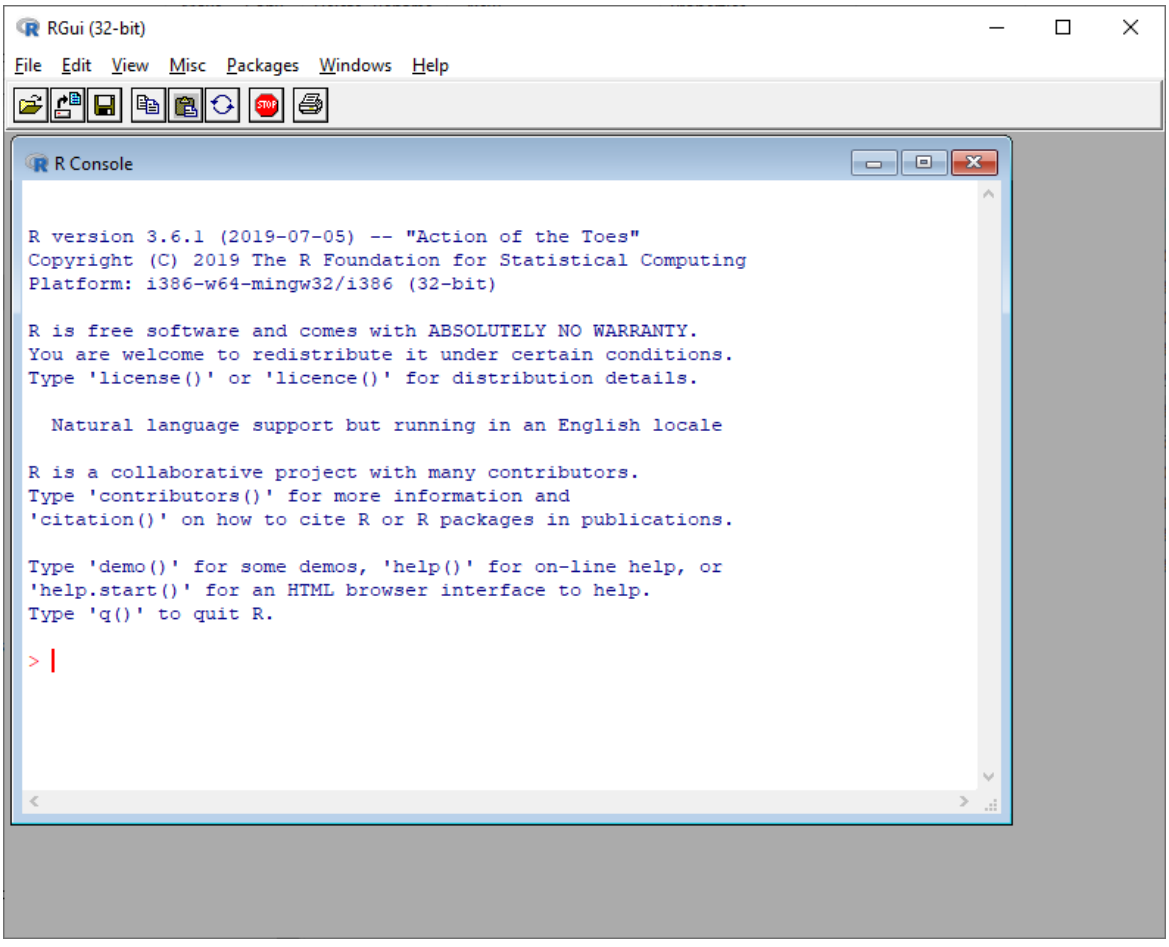
Package Libraries

The R scripting language is powerful in its own right; however, it is made significantly more useful by facilitating the use of thousands of external package libraries developed by the wider community; common examples include **ggplot2** (which facilitates plotting) and **leaflet** (which facilitates mapping).

In order to install package libraries from within AquaChem, you will need to call at least one library using a native R interface (e.g. RGui or RStudio). The following steps will guide you through the process of installing your first package which also installs the necessary files for installing more package libraries in AquaChem.

1. Go to the folder where you installed R, by default, this will typically be: *C:\Program Files\R\R-4.0.5\bin\i386*

2. Double-click the file called: RGui.exe. This will open the graphical user interface (GUI) which is distributed with R:



3. At the prompt, install one package (that you will likely use). For example, you can type:

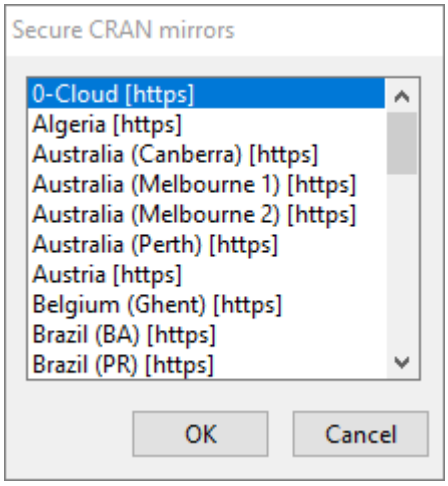
> *install.packages('ggplot2')*

Please Note: if the package fails to install; a likely cause is that R is attempting to install the library packages to a folder that requires administrative rights. If this is the case, you can do one of the following:

a. close RGui and reopen it by right-clicking and selecting the "Run as Admin..." option.
b. install R to a local folder that does not require administrative rights
c. set the libPaths option before installing packages in your script. For example if you want to install libraries into "c:\users\user_name\documents\R\libraries", at the beginning of each script you can add:

> *.libPaths(c("c:/users/user_name/documents/R/libraries" , .libPaths())*

4. Press <ENTER> to execute the command. You will be prompted to select which of the secure CRAN mirror sites from which you want to download the package:



Once you select a CRAN mirror site for the package, RGui will begin installing the package library along with the prerequisites to install other packages, including in the R-console module in AquaChem. Note that you will be similarly prompted each time you install a package using the *install.packages()* command in the R-console module within AquaChem.

5. Close RGui.

6. Open AquaChem and select Project > AquaChem Settings from the main menu

7. Select the R-Console tab and set the R location to where the 32-bit version of *R.dll* is installed on your machine. The default location is: *C:\Program Files\R\R-4.0.5\bin\i386\R.dll*; however, your installation location may be different.

8. Click Apply and OK

You should now be ready to start working with the R-Console in AquaChem.

1.1.3 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, you need to reinstall on the current computer, or update to a newer version).

Please Note: If you intend to uninstall AquaChem and reinstall it (whether on the same computer or a different one), please verify that you have a supported installation file that is covered under a maintenance agreement. This is particularly important if you need to transfer a standalone softkey license from one computer to another. If you are unsure of your eligibility to transfer or upgrade your software, please contact our licensing team: licensing@waterloohydrogeologic.com before uninstalling AquaChem.

To uninstall AquaChem:

- Locate the Add/Remove Programs option in your Windows' Control Panel.
- Select AquaChem as the program to be removed and follow the on-screen instructions.

1.2 Features

AquaChem is an environmental software package specifically designed for anyone working with water quality data, ideally suited for projects requiring management, analysis, and reporting. The analysis tools provided in AquaChem cover a wide range of functions and calculations used for analyzing, comparing, evaluating, and interpreting water quality data. These tools include simple unit transformations, charge balances, and statistics to more complex functions including those facilitated by the R-Console. These powerful analytical capabilities are complemented by an extensive selection of commonly used geochemical plots and graphs to represent the chemical characteristics of water quality data.

Data Management

AquaChem includes many data management features:

- Easily **import** data from various file types (.txt, .csv, .xls, .xlsx, .mdb, and .accdb) and formats (samples as rows, samples as columns, one analyzed value for each row).
- **Export** stations, analysis data and geochemical plots to various file formats including MS-Excel spreadsheets (.xlsx), text files (.txt, .asc), MS-Access databases (mdb, .accdb), and customizable print-ready Excel and PowerPoint templates (.xlsx, .pptx)
- Define sets of samples and sampling locations based on static lists (such as locations at a given site, watershed, or regulatory status) or dynamic criteria such as exceedances or sample collection time horizons so that you can easily and quickly generate periodic reports and drill down to the specific information that you need
- Data management workflows include **data quality** checks ensuring users have completed/included required information and that it meets specified conditions including lists of values or valid numeric ranges
- Import and manage Water Quality Standards in your project so that you can track project-specific regulatory requirements

Interactive Plots

AquaChem is capable of generating a wide variety of plots to help you better understand your data:

- **Geochemical plots**: Piper, Stiff, Durov, Schoeller, Wilcox, Giggenbach, Meteoric Water Line, Ludwig-Langelier, Ternary;
- **Statistical Plots**: Box and Whisker, Histogram, Probability, Quantile, Detection Summary;
- **General Plots**: Scatter, Line, Pie, Stacked Bars, Radial, Time Series; and
- **Map Plots:** Uniform Symbols, Proportional Symbols, Pie Chart, Radial Chart, Stiff Diagram

AquaChem allows you to create multiple plots for the same datasets and view these plots simultaneously side-by-side. The plots can be made interactive which means when you chose to base your data on dynamic sources, you can click on data points in the plot and the corresponding samples are highlighted in the sample list. Similarly, you can select samples from the Sample List and they will be highlighted on any plots in which they appear. This is useful for exploring and analyzing the data, and for identifying outliers or otherwise interesting data.

Water Quality Analysis

AquaChem comes with a comprehensive set of calculators and converters that allow you to perform quick, on-the-fly analyses of your water quality data. AquaChem is capable of the following calculations and conversions:

- **Unit Conversion**: AquaChem manages measurement and concentration units for you – switch between mass-, molar-, and equivalent-based concentrations on the fly
- **Ionic Functions**: Water Type, Electroneutrality/Ion Balance, Sum of Anions, Sum of Cations, TDS, Hardness, Alkalinity
- **General**: Date functions, Exceedance counts, Total Organic Carbon, Total Organic Halogens
- **Corrosion and Scaling Indices**: Langelier Saturation, Ryznar Stability, Puckorius Scaling, and Larson-Skold
- **Agricultural/Irrigation Metrics**: Sodium Absorption Ratio, Magnesium Hazard, Residual Sodium Carbonate
- **Enthalpy**: Enthalpy of water (liquid or vapor) based on temperature or dissolved silica
- **Isotopes**: Estimates of infiltration elevation and temperature based on Oxygen-18 and Deuterium isotopic fractionation

Automatic Reports

In just a few clicks, AquaChem delivers ready-made reports that contain key information about your water quality data. The following automatic reports are supported:

- **Sample Report**: A standardized sample report that tabulates sample results; optionally compares results to active Water Quality Standards and calculates summary statistics, including min/max, specified quantiles, and the mean
- **Data Reports**: Export data tables to print-ready MS-Excel templates that you can customize

Scripting with R-Console

AquaChem includes a console that allows you to run scripts in the R scripting language and leverage the thousands of available libraries that facilitate data analyses, visualization, and categorization and much more.

1.3 What's New

Version 10.0 - Jun 2020

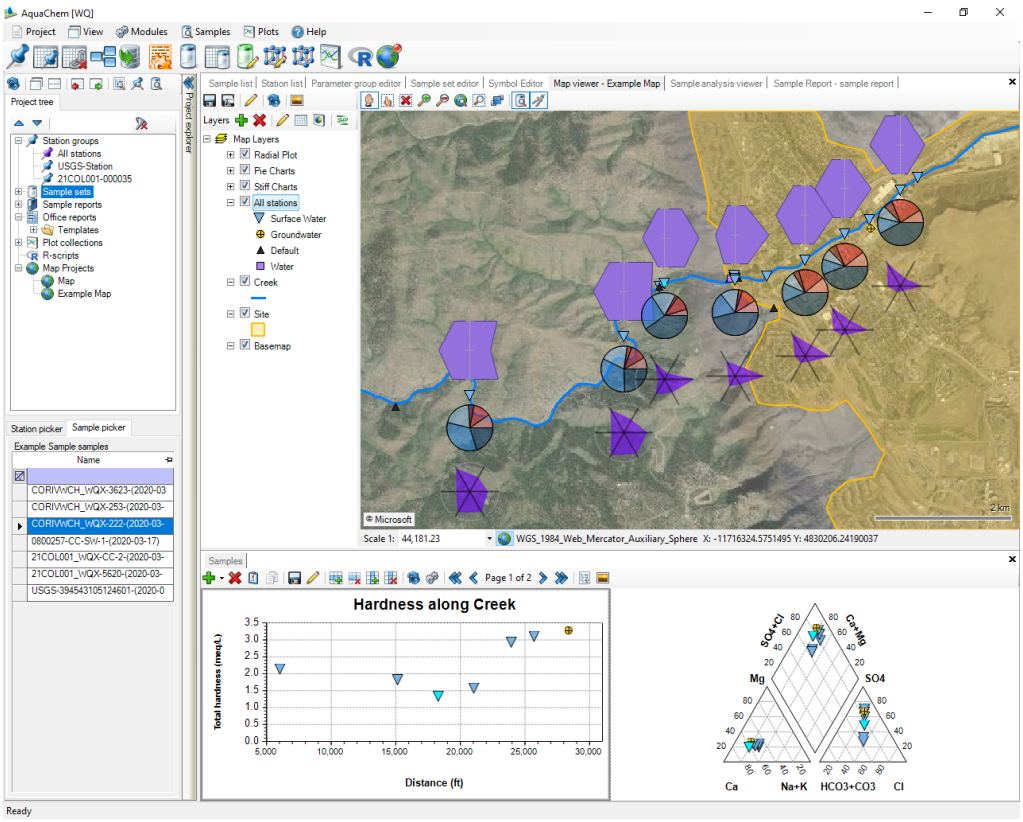
Map Viewer Module

- Create simple maps with station and sample symbols based on project data
  - Map Samples from station groups or sample sets as:
    - Symbols from the sample editor,

- Proportional symbols,
- Categorized symbols,
- Pie charts,
- Stiff diagrams, or
- Radial plots

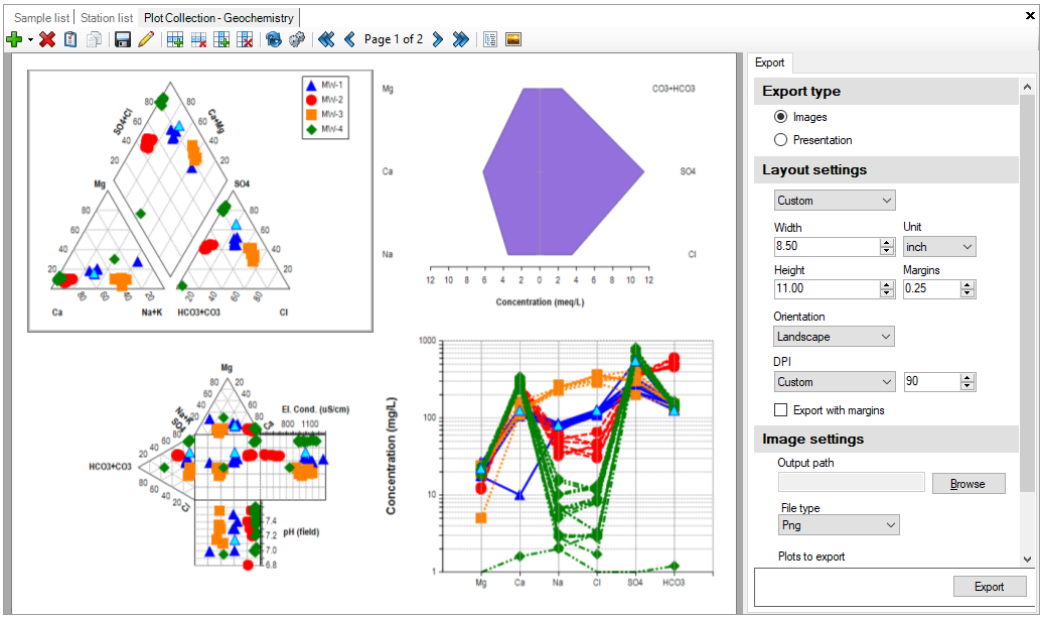
o Add shapefiles and georeferenced images to the map

o Map includes standard navigation tools

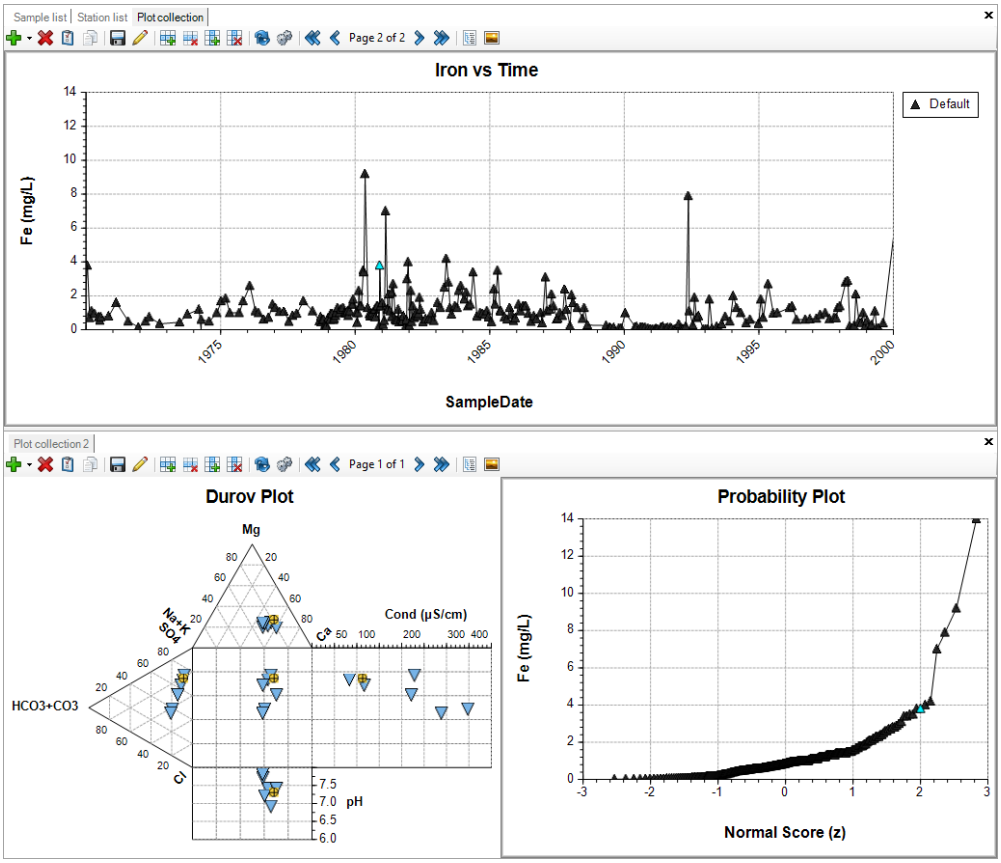


Plot Collections

- Plot collections include a What-You-See-Is-What-You'll-Get layout view for exports so that you can easily configure your plots for export to images or report templates. Choose from standard page sizes or set your own custom size



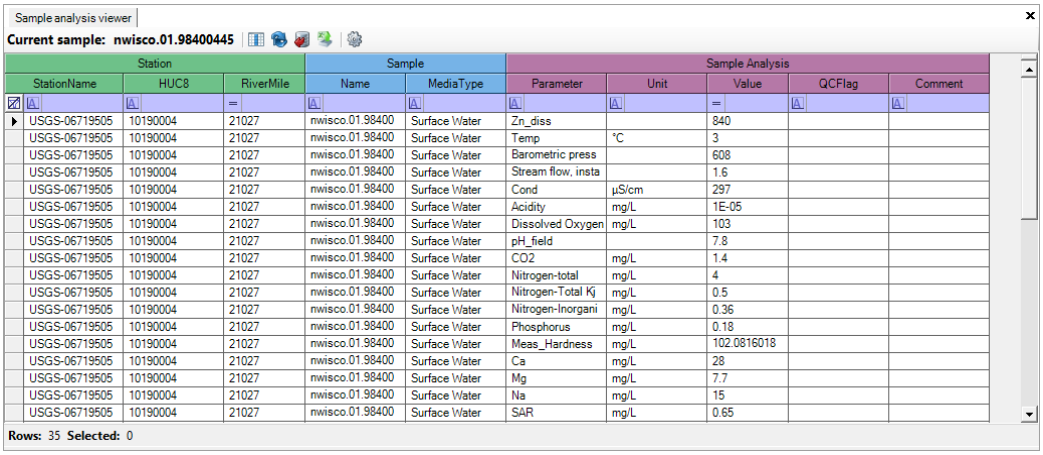
- Plots can use the currently selected sample(s) as a data source to make plot collections even more interactive
- Rectangular plots (e.g. Box and Whisker, Detection Summary, Histogram, Probability Plot, Time series, etc.) can be optionally stretched to fill their cell in the plot collection layout. Similarly, the right and bottom plot panels in a Durov Plot can be scaled relative to the central plot



- Axis labels on rectangular plots can be rotated
- Custom plot lines can be dynamically linked to a water quality standard and you can set x cutoff values
- Improved performance for Plots built using calculated parameters

Other Enhancements

- The new Sample Analysis Viewer allows you to quickly view a list of results and related metadata data for specified stations or samples with all the standard data handling tools available in AquaChem



Sample analysis viewer

Current sample: nwisco.01.98400445

Station			Sample		Sample Analysis				
StationName	HUC8	RiverMile	Name	MediaType	Parameter	Unit	Value	QCFlag	Comment
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Zn_diss		840		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Temp	°C	3		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Barometric press		608		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Stream flow, insta		1.6		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Cond	µS/cm	297		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Acidity	mg/L	1E-05		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Dissolved Oxygen	mg/L	103		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	pH_field		7.8		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	CO2	mg/L	1.4		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Nitrogen-total	mg/L	4		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Nitrogen-Total Kj	mg/L	0.5		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Nitrogen-Inorgani	mg/L	0.36		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Phosphorus	mg/L	0.18		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Meas_Hardness	mg/L	102.0816018		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Ca	mg/L	28		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Mg	mg/L	7.7		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	Na	mg/L	15		
USGS-06719505	10190004	21027	nwisco.01.98400	Surface Water	SAR	mg/L	0.65		

Rows: 35 **Selected:** 0

- Print-to-Office Templates support macro-enabled documents (.xlsm, .pptm) so you can automate building more powerful and advanced reports
- You can create a parameter group based on a field in the sample results table (for example Sample Method).
- Allow specification of a custom date field when importing data

Defects Addressed

- Labels are used instead of parameter names in plots
- Month-based ticks were not shown correctly in time series plots
- In some cases, custom lines were not shown correctly in Box and Whisker plots

For full version history, see the AquaChem readme file at:
https://www.waterloohydrogeologic.com/aquachem-readme/

Chapter 2 Quick Start Tutorials

The following tutorials provide a brief introduction on how to use AquaChem. The objective is not to teach you every detail, but to familiarize you with basic principles and the way the program works. The steps are intentionally kept brief so that you can actually start using the program as quickly as possible. You are encouraged to explore the more detailed sections of the Help documentation to further familiarize yourself.

- **AquaChem 10 Demo Project**: The first tutorial provides a guided tour through the 'AQC 10 Demo' project. The Demo Project contains a modest selection of data and represents an AquaChem project which has already benefited from considerable work. This Demo Project contains a number of pre-built sample groups, sample reports, water quality standards, plot collections, and R-scripts. If you're looking for a simple introduction to the features and capabilities offered in AquaChem 10.0, please review this tutorial.

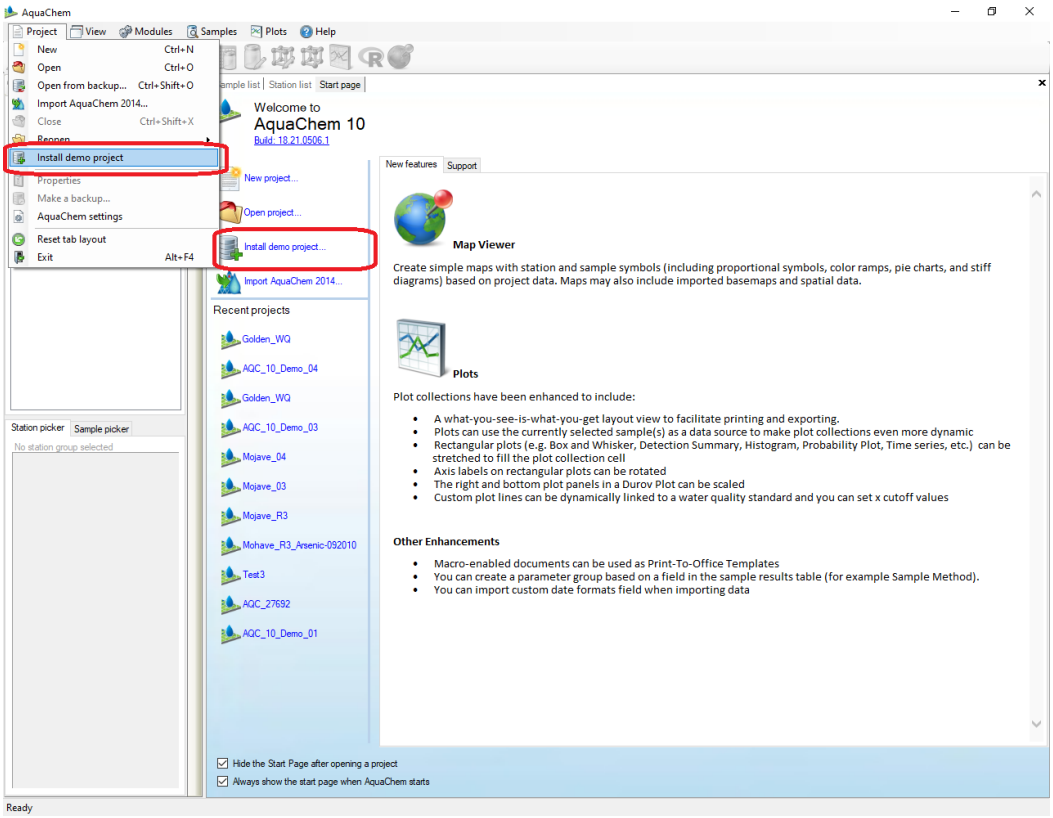
- **Creating a Project and Importing Data**: The second tutorial introduces you to the process of creating a new project in AquaChem 10.0, customizing the database structure using the template manager module, and importing a small dataset to the 'Station', 'Sample', and 'Sample Analysis' tables.

- **Importing Projects from AquaChem 2014**: Finally, the third tutorial provides a simple guide for importing existing AquaChem 2014 projects. This tutorial also offers a brief review of the database structures supporting both the original version of AquaChem 2014 as well as the corresponding structure of the AquaChem 10.0.

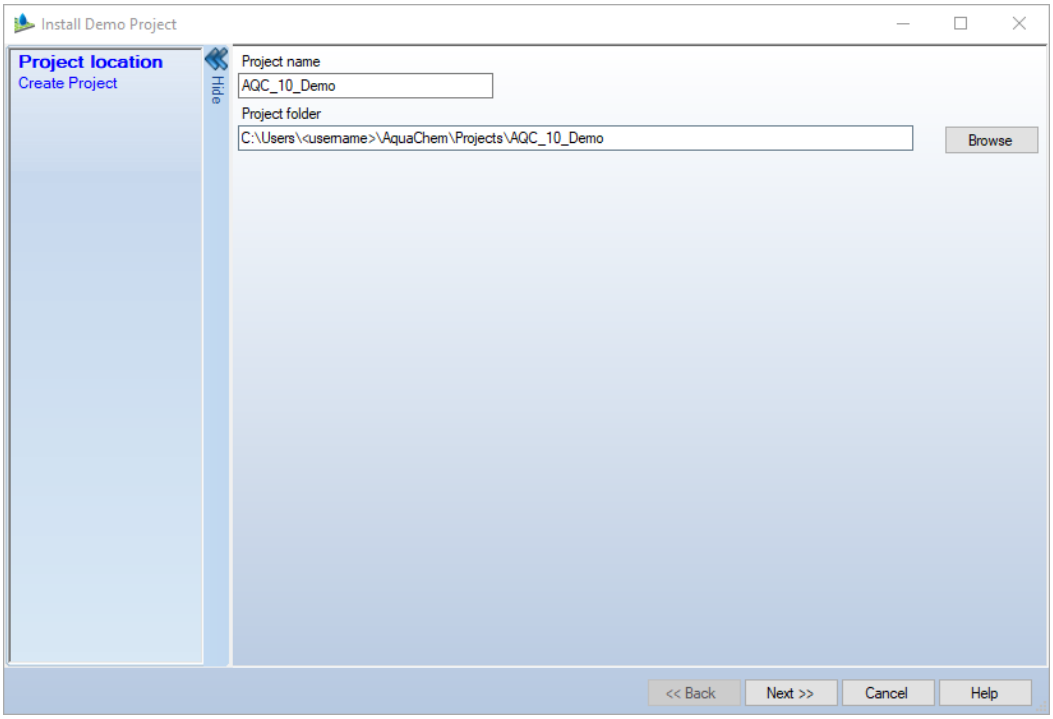
2.1 AquaChem Demo Project

The AquaChem demo project is a project with a relatively simple data set that comes with several pre-defined Station Groups, Sample Sets, Sample Reports, Plot Collections and R-Scripts.

To explore the AquaChem demo project, first launch AquaChem 10.0 and access the Start Page. On the Start Page you should see a button to '**Install demo project...**'. Alternatively, you can click '**Project > Install demo project**' from the main menu, as shown below:



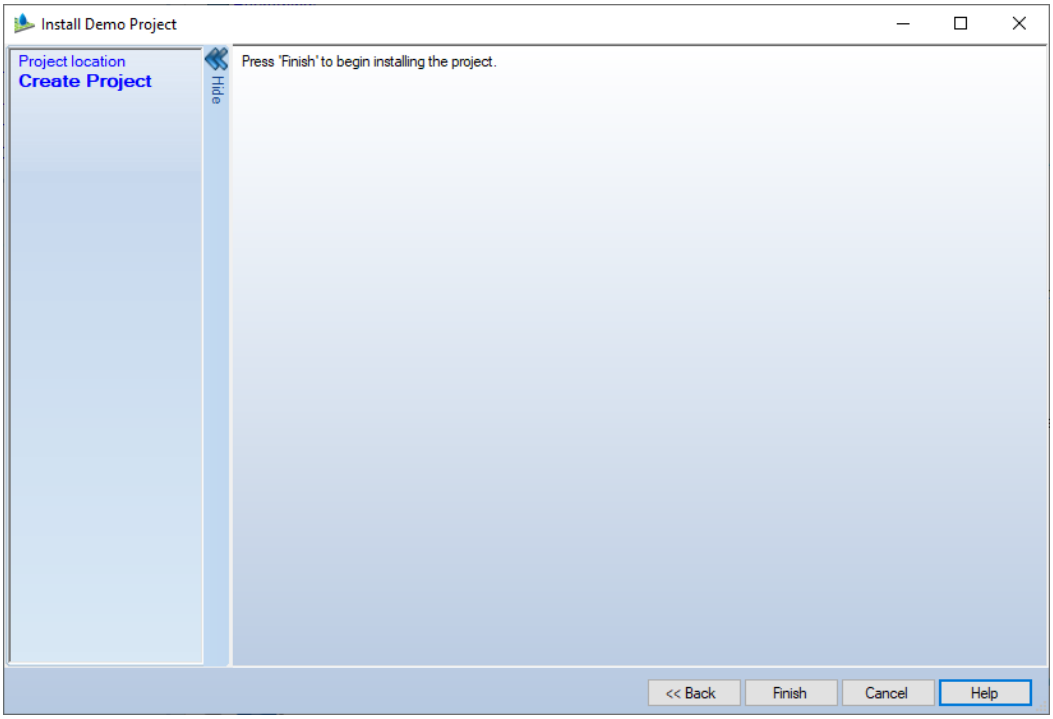
Clicking either of these buttons will open the '**Install Demo Project**' window, as shown below:



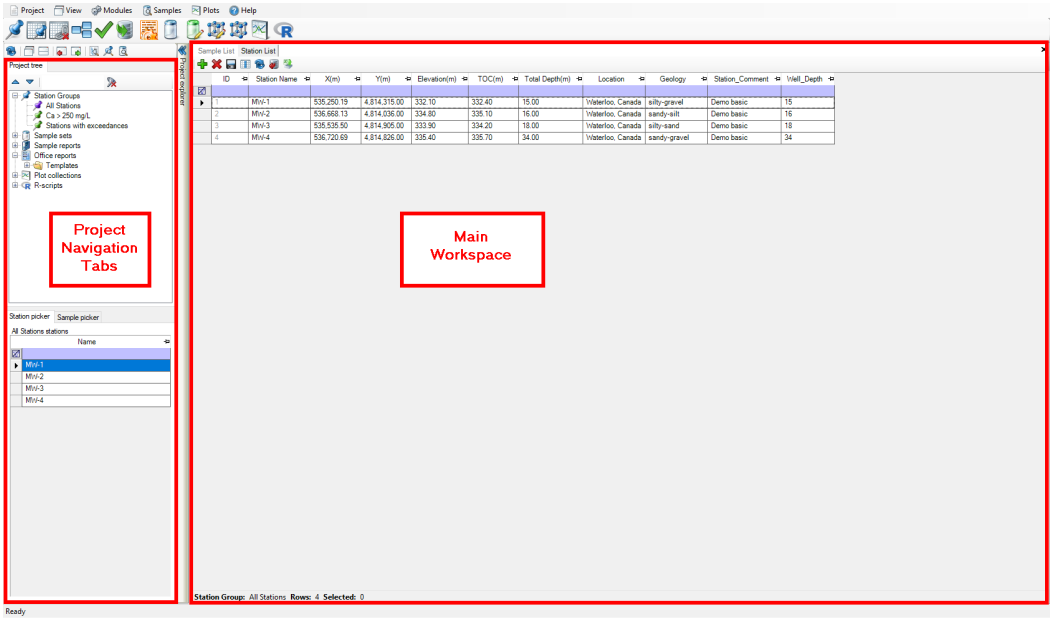
By default the demo project will be called '**AQC_10_Demo**' and will be saved to the default projects folder. This is typically:

'*C:\Users\<username>\Documents\AquaChem\Projects*'

where *<username>* is either your user account name or the Public user account, depending on how you installed AquaChem. You can can also specify a user-defined name by typing in the '**Project name**' field, and select a different project folder by clicking the '**Browse**' button. If you are happy with these defaults click the Next >> button to proceed to the next step:



Now simply click the Finish button to install the demo project. After a few moments, the project will be installed and the demo project will be opened, displaying the 'Station List' tab:



Now that the Demo Project is installed, you can begin to familiarize yourself with AquaChem 10.0. This introductory tutorial is split into several major sections. The Demo Project is already set-up and ready for you to review these particular sections. It is recommended that you carefully review each section of this tutorial in the order listed below, but if you're interested in one particular feature/function you may skip ahead.

The tutorial includes the following sections:

- **Review the Interface:** this section provides a brief walk-through of the main data tables/tabs (e.g. Station/Sample Lists, Sample Results, etc.) and a short introduction to the modules available in AquaChem 10.0.

- **Managing Data:** this section shows you how to manually enter data and how to create station groups, sample sets and parameter groups.

- **Creating Sample Reports:** this section shows you how to access and use the Sample Reports module. Existing sample reports will be reviewed, and a new sample report will be created.

- **Creating Plot Collections:** this section shows you how to access and use the Plot Collections module. Existing plot collections will be reviewed, and a new plot collection will be created.

- **Basic Scripting with the R-Console:** this section will introduce you to the R-scripting language and the R-console module within AquaChem. Three basic scripts which are pre-loaded in the Demo Project will be reviewed and executed.

Please note: several important concepts are not covered in this particular tutorial, but they are reviewed in subsequent tutorials:

- If you need to review how to create a new project, configure the database using the template manager, and import data using the Import Data System please review the **'Creating a New Project and Importing Data'** tutorial.
- If you need to review how to import a project from AquaChem v2014 please review the **'Importing Projects from AquaChem 2014'** tutorial.

2.1.1 Review the Interface

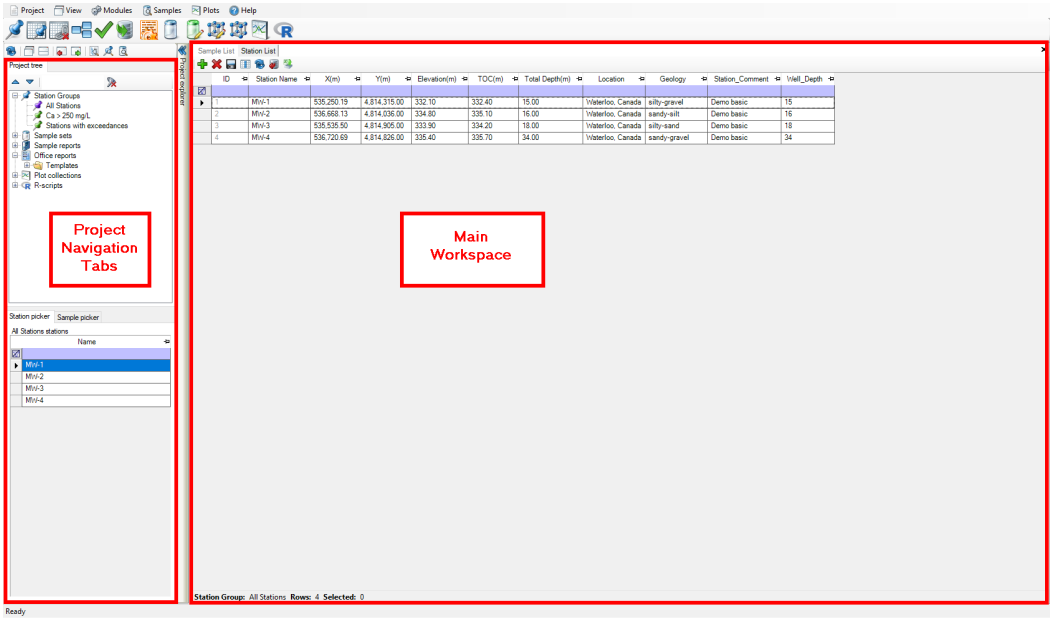
Before jumping into the contents of the demo project, spend a few moments familiarizing yourself with the general layout of the AquaChem interface. The following components of the interface are reviewed in this section:

- Project Tree
- Station/Sample Picker
- Sample/Station List tabs
- Sample Results/Details tab
- Review main modules (Plot Collections, Sample Report, R-Console)
- Review supporting modules (Template Manager, Data Import System, List Editor, Parameter Editor, Parameter Group Editor, Station/Non-Station Data Tables)

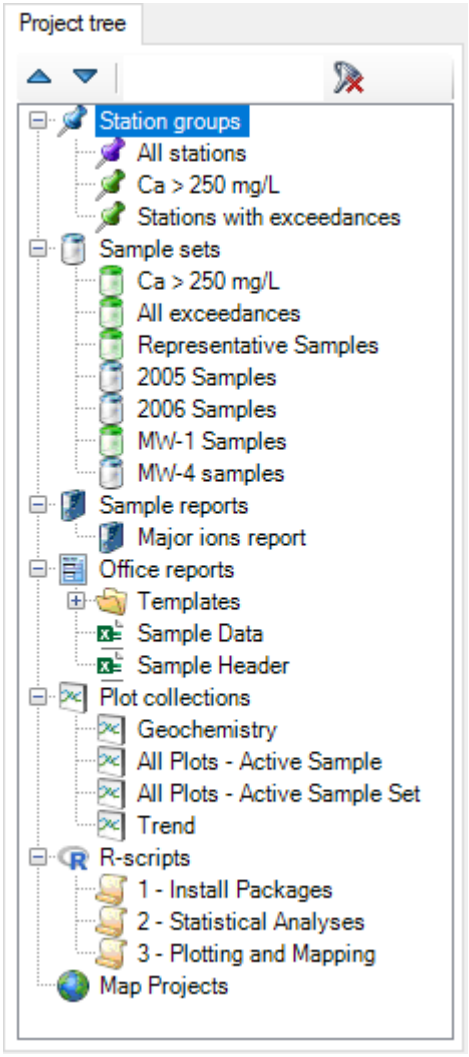
General Layout - Project Tree, Station/Sample Picker, Station/Sample Lists and Sample Results

When first opening AquaChem, the default window displays will appear. There are two tab groups:

- On the left is a tab group with the Project tree, Station picker, and Sample picker (i.e. project navigation tabs)
- On the right is a tab group with the Sample List, and Station List (i.e. the main workspace)

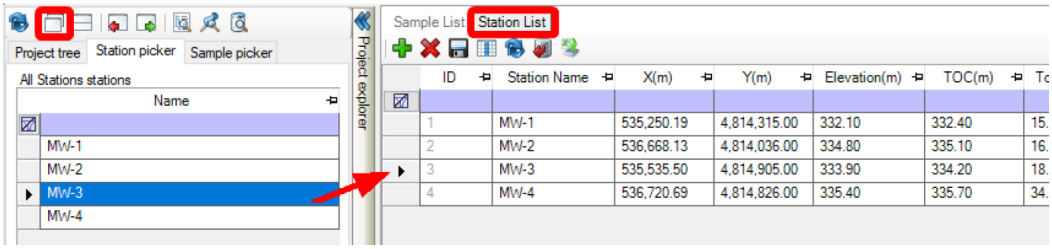


The project navigation tabs on the left side of the AquaChem interface can be used to access/activate a variety of project-specific items like Station Groups, Sample Sets, Sample Report, Plot Collections, and R-scripts. If you expand the contents of the **'Project Tree',** you should see the following:



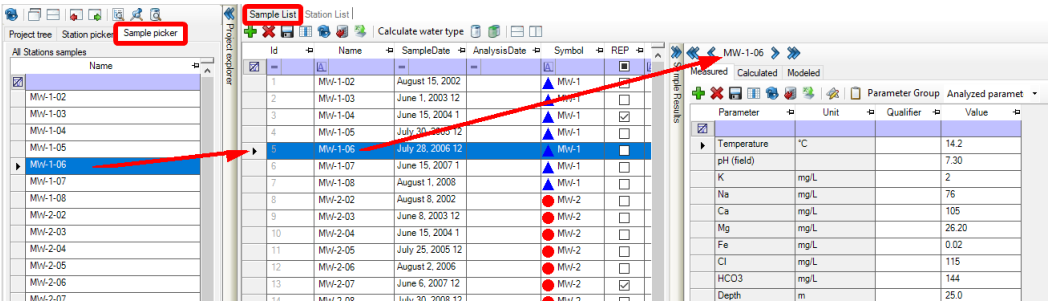
Using the **Project Tree** is the easiest way to navigate within your project and access previously saved work. From here you can open any existing plot collections, R-scripts, or sample reports or activate particular station groups or sample sets, simply by double-clicking any of the objects in the Project Tree. For now, let's set these options aside and review the other major components of the AquaChem interface.

Below the Project Tree, you will find the **'Station Picker'** and **'Sample Picker'**. These 'picker' menus display the currently active station groups and sample sets, and allow you to easily select from the available records. For example, if you click station 'MW-3' in the Station Picker the related record within the Station List (main workspace) will automatically be selected:



Please Note: in the image above, the Project Tree, Station Picker, and Sample Picker have all been combined into the same frame using the highlighted toolbar button ('**Combine tabs**'). These toolbar buttons can be used to combine or separate the tabs, dock them to the left or right of the AquaChem interface, or hide/show individual project navigation tabs.

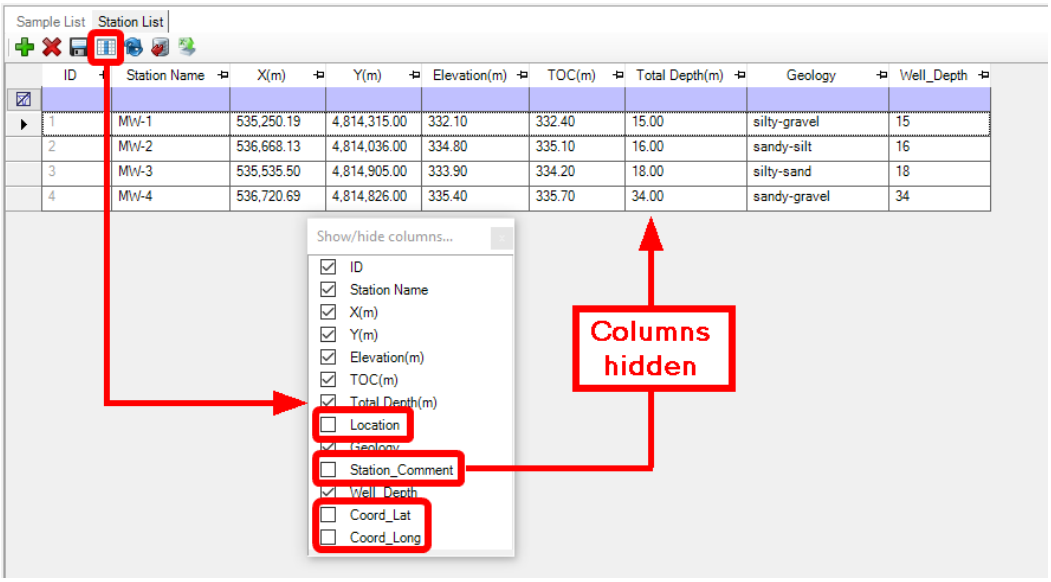
Similar to the function of the Station Picker, the Sample Picker navigation tab allows you to easily select from available samples within the currently active sample group. As an example activate both the **Sample picker** and the **Sample List**, and select one of the available samples from the Sample Picker. The associated record will automatically be highlighted within the Sample List, and the associated water quality measurement data will be displayed in the Sample Results pane to the right:



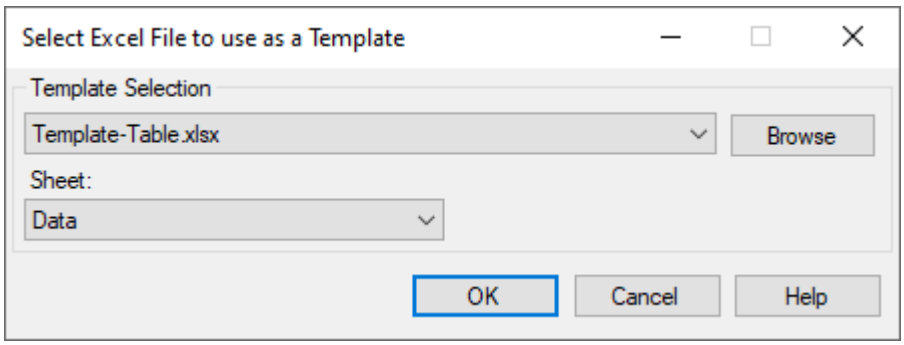
It should be clear at this point that the Station List and Sample List tabs display records from the Station Data table and the Sample Data tables respectively, while the Sample Results tab displays data from the Analysis Results table (see the Data Structure section of the manual for further info about the database relationships).

Each of these tables includes a number of common toolbar buttons which allow you to add/delete records [/], save changes [], export data [/] or refresh the data []. There are also some less obvious buttons included in these toolbars. For example, a button is available in the Station and Sample lists which allows you to 'Show/Hide Columns' from the tables [].

Open the Station List and click the '**Show/Hide Columns**' button [] to open the 'Show/hide columns...' window, as shown below. Feel free to make some customizations and hide unneccessary columns. For example, you might hide the 'Location', 'Station_Comment', 'Coord_Lat' and 'Coord_Long' columns, since they do not offer much helpful information in the context of the Demo Project:

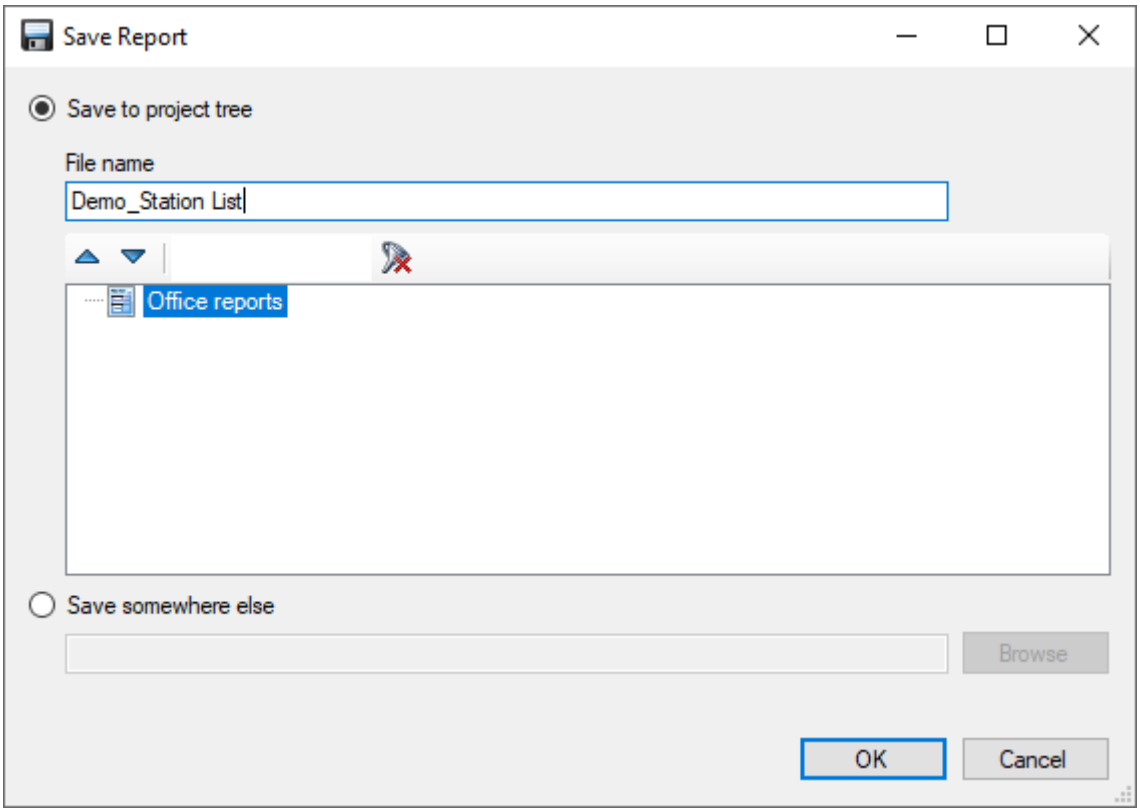


You can also test out exporting this data table to a print-ready MS Excel template by clicking the '**Print to Excel**' button [ ]. Clicking this button will open the '**Select Excel File to use as a Template**' window, as shown below:



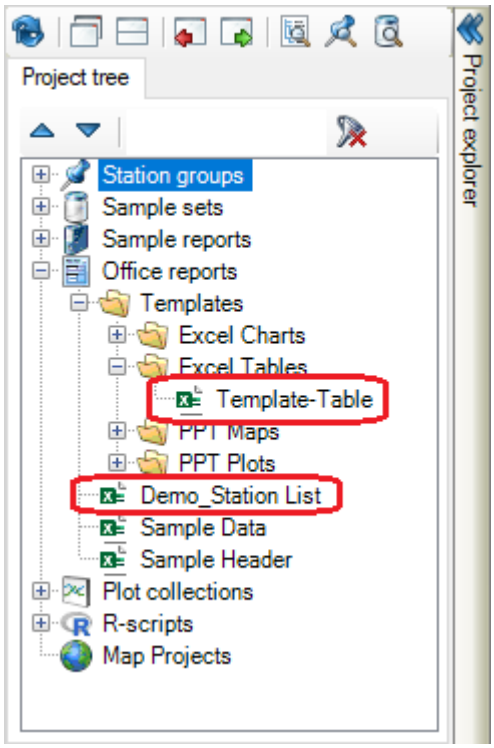
In your own projects, you will want to create and customize a number of your own print ready templates; but for this demonstration, simply proceed with the default template selection ('Template-Table.xlsx') and click 'OK'. A 'Print progress' window will appear as shown below, and when you click 'Close' a new window will appear which allows you specify where the resulting data file will be saved. You can save exported data files to the project tree, or you can export them to a folder of your choosing by selecting the 'Save somewhere else' option and clicking the Browse... button to select the location.

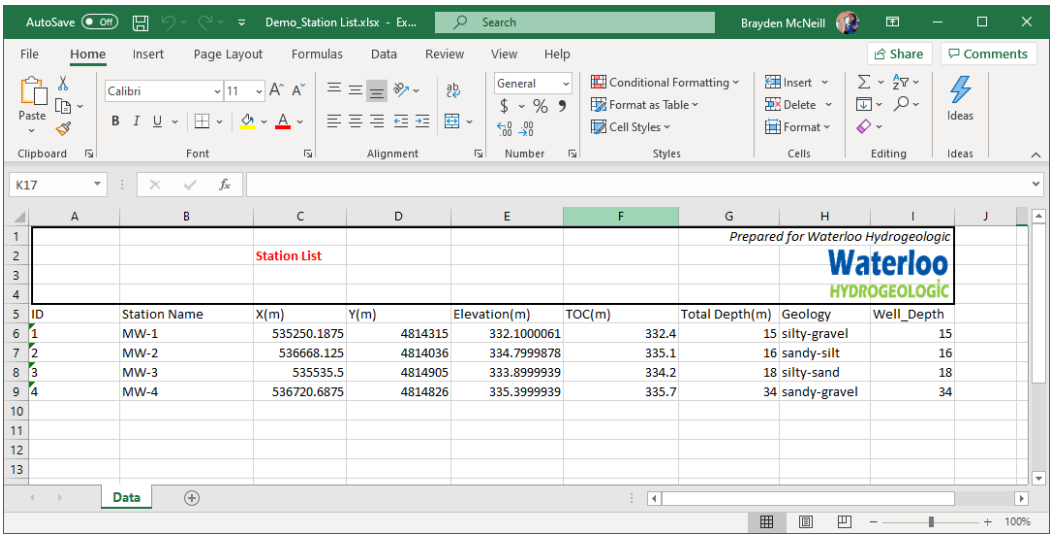
For now, save the exported data table to the project tree using the file name 'Demo_Station List', as shown below:



Please Note: it is assumed that MS-Office, including Excel, is installed on your machine. Without MS-Office installed you may experience an error.

When you click OK, the resulting MS-Exel file will be saved to the Project Tree under the '**Office Reports**' node and MS Excel will open and display the resulting data table.

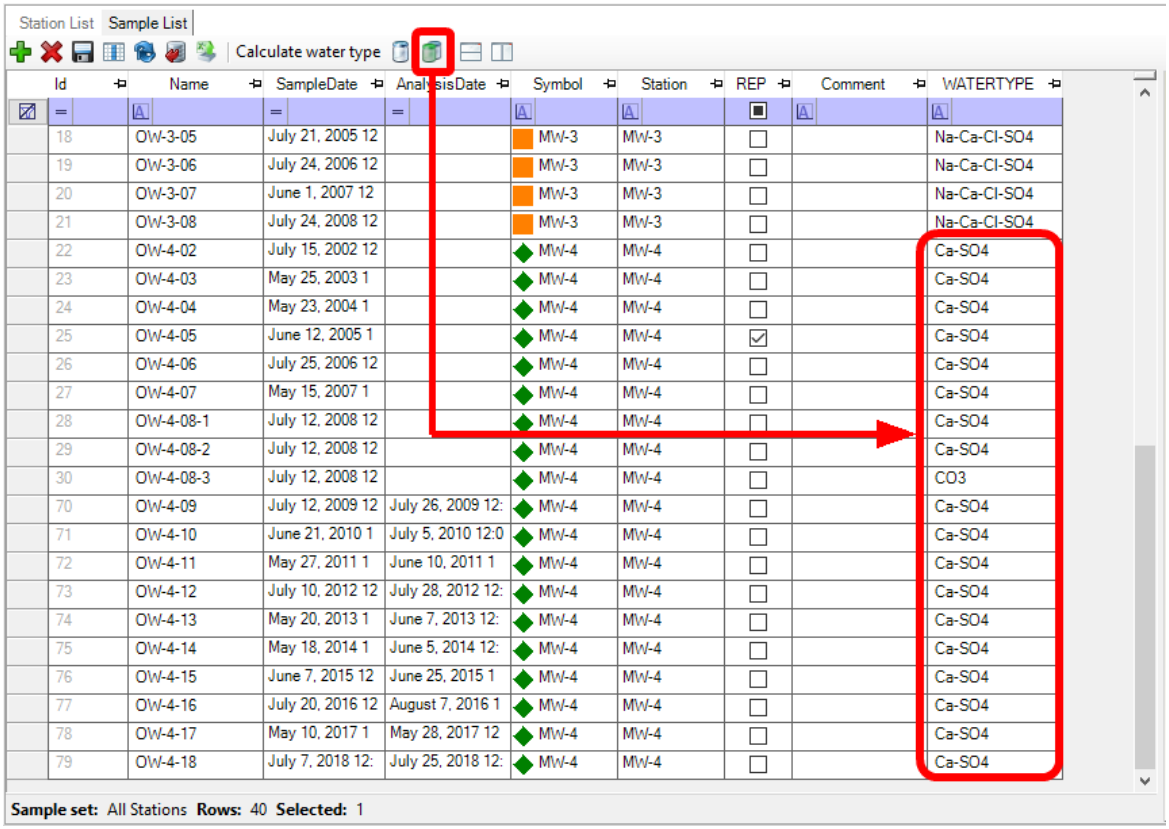




ID	Station Name	X(m)	Y(m)	Elevation(m)	TOC(m)	Total Depth(m)	Geology	Well_Depth
1	MW-1	535250.1875	4814315	332.1000061	332.4	15	silty-gravel	15
2	MW-2	536668.125	4814036	334.7999878	335.1	16	sandy-silt	16
3	MW-3	535535.5	4814905	333.8999939	334.2	18	silty-sand	18
4	MW-4	536720.6875	4814826	335.3999939	335.7	34	sandy-gravel	34

The Sample List and Sample Results tables also contain a few unique toolbar buttons. Open the Sample List and you will see two buttons in the toolbar which facilitate the calculation of water types. The first button shown next to the '**Calculate water type**' field allows you to '**Calculate water type for selected samples**' [ ] (i.e. the samples highlighted in blue), whereas the second button allows you to '**Calculate water type for all the samples in the list**' [ ].

Click the second button now to calculate water types for ALL samples in the sample list, and you should see the 'WATERTYPE' column populated for all samples (samples associated with station 'MW-4' previously were empty):

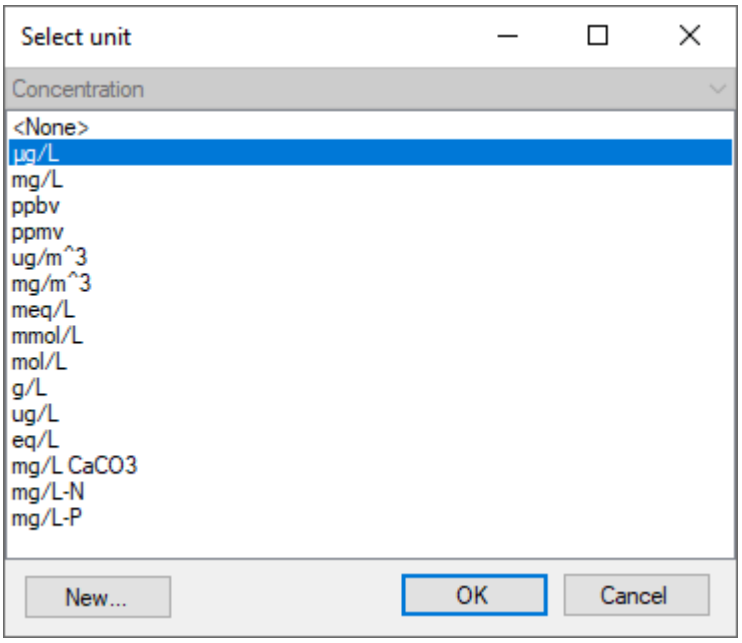


Id	Name	SampleDate	AnalysisDate	Symbol	Station	REP	Comment	WATERTYPE
18	OW-3-05	July 21, 2005 12		MW-3	MW-3	☐		Na-Ca-Cl-SO4
19	OW-3-06	July 24, 2006 12		MW-3	MW-3	☐		Na-Ca-Cl-SO4
20	OW-3-07	June 1, 2007 12		MW-3	MW-3	☐		Na-Ca-Cl-SO4
21	OW-3-08	July 24, 2008 12		MW-3	MW-3	☐		Na-Ca-Cl-SO4
22	OW-4-02	July 15, 2002 12		MW-4	MW-4	☐		Ca-SO4
23	OW-4-03	May 25, 2003 1		MW-4	MW-4	☐		Ca-SO4
24	OW-4-04	May 23, 2004 1		MW-4	MW-4	☐		Ca-SO4
25	OW-4-05	June 12, 2005 1		MW-4	MW-4	☑		Ca-SO4
26	OW-4-06	July 25, 2006 12		MW-4	MW-4	☐		Ca-SO4
27	OW-4-07	May 15, 2007 1		MW-4	MW-4	☐		Ca-SO4
28	OW-4-08-1	July 12, 2008 12		MW-4	MW-4	☐		Ca-SO4
29	OW-4-08-2	July 12, 2008 12		MW-4	MW-4	☐		Ca-SO4
30	OW-4-08-3	July 12, 2008 12		MW-4	MW-4	☐		CO3
70	OW-4-09	July 12, 2009 12	July 26, 2009 12:	MW-4	MW-4	☐		Ca-SO4
71	OW-4-10	June 21, 2010 1	July 5, 2010 12:0	MW-4	MW-4	☐		Ca-SO4
72	OW-4-11	May 27, 2011 1	June 10, 2011 1	MW-4	MW-4	☐		Ca-SO4
73	OW-4-12	July 10, 2012 12	July 28, 2012 12:	MW-4	MW-4	☐		Ca-SO4
74	OW-4-13	May 20, 2013 1	June 7, 2013 12:	MW-4	MW-4	☐		Ca-SO4
75	OW-4-14	May 18, 2014 1	June 5, 2014 12:	MW-4	MW-4	☐		Ca-SO4
76	OW-4-15	June 7, 2015 12	June 25, 2015 1	MW-4	MW-4	☐		Ca-SO4
77	OW-4-16	July 20, 2016 12	August 7, 2016 1	MW-4	MW-4	☐		Ca-SO4
78	OW-4-17	May 10, 2017 1	May 28, 2017 12	MW-4	MW-4	☐		Ca-SO4
79	OW-4-18	July 7, 2018 12:	July 25, 2018 12:	MW-4	MW-4	☐		Ca-SO4

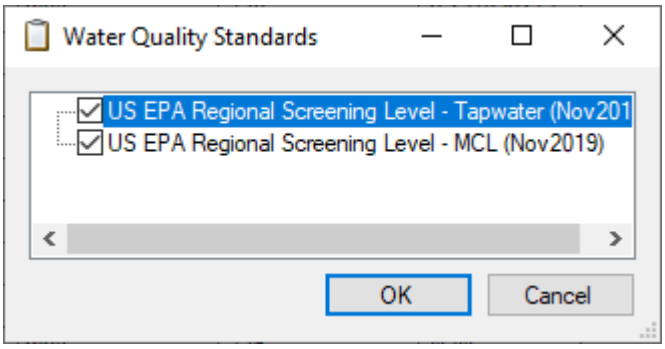
Sample set: All Stations **Rows:** 40 **Selected:** 1

The Sample Results tab is displayed to the right when the Sample List is active, and displays measured, calculated, and modeled parameter values for the currently selected sample. As you can see from the image below, parameter values which exceed active water quality standards are automatically highlighted with its associated color (more on water quality standards later). All three of the available tabs within the Sample Results frame (e.g. 'Measured', 'Calculated' and 'Modeled') provide a button to 'Add or remove secondary unit column' [], and the 'Measured' tab toolbar also includes an option to display 'Standards' [ ].

Click the 'Add or remove secondary unit column' [] button to open the 'Select unit' window, and select 'µg/L' (micrograms per liter) as a secondary unit, as shown below, then click the OK button:

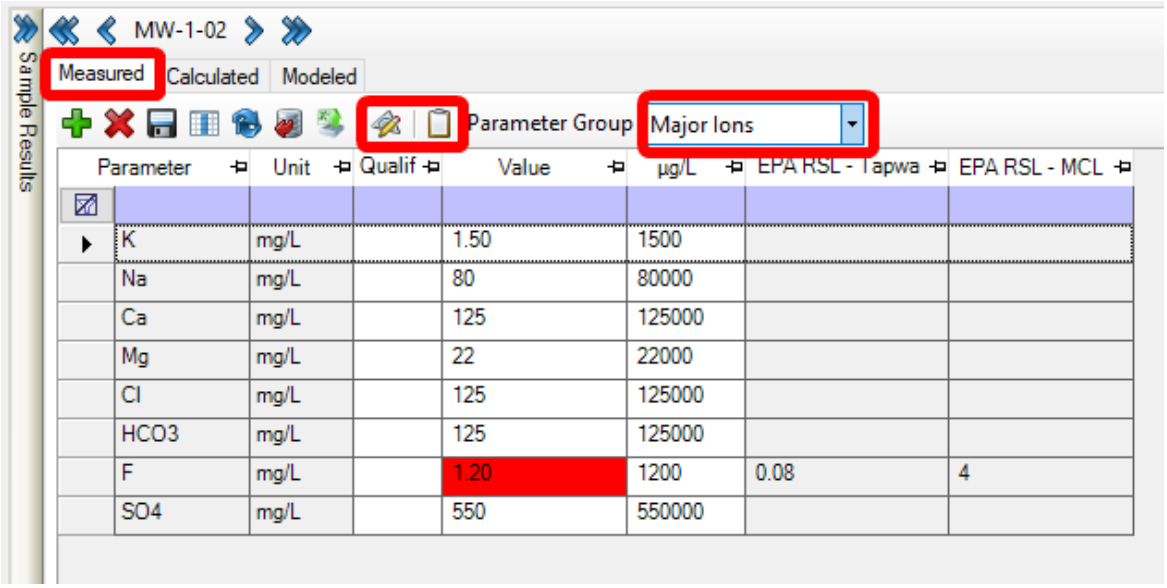


Now click the 'Standards' [] button to open the 'Water Quality Standards' window, and use the checkboxes to activate both available standards (US EPA Tapwater and US EPA MCL), as shown below:



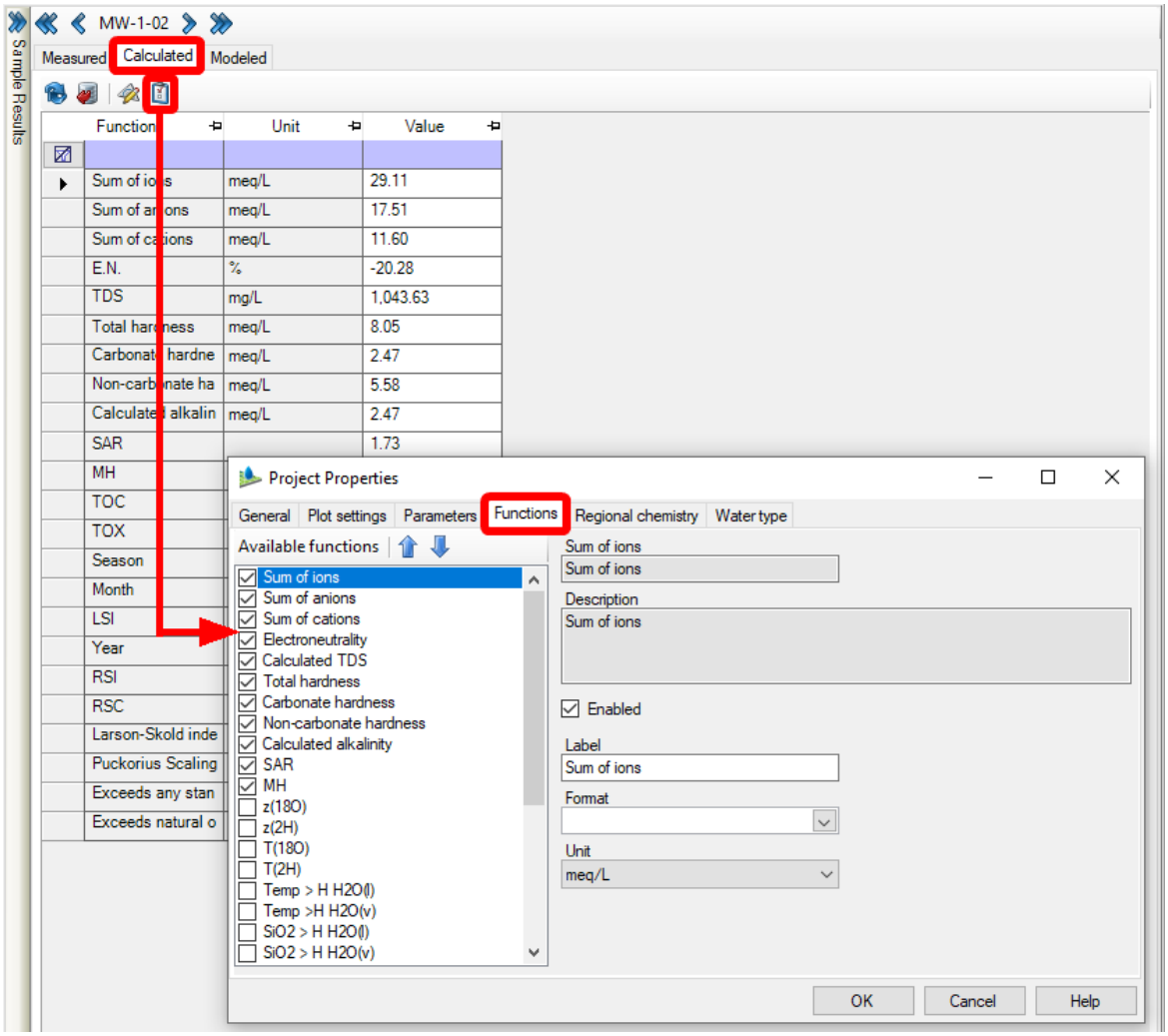
Also take note of the 'Parameter Group' menu shown in the 'Measured' tab toolbar. This menu allows you to quickly update the list of parameters displayed within the table below. A number of default parameter groups are included, and it's possible to create custom parameter groups of your own; which we will do later in the tutorial. For now, select the 'Major Ions' parameter group and you should see the list of parameters in the table below updated to only display the major groundwater ions.

Once these updates have been made, the Sample Results 'Measured' tab should look like the image below (for sample 'MW-1-02'). As you can see, the original unit is displayed in the 'Unit' column, the recorded value is displayed in the 'Value' column, and the recorded value is displayed in a secondary column labeled based on the secondary unit (µg/L in the example below). And finally, the associated water quality standards are displayed in their respective columns as well:

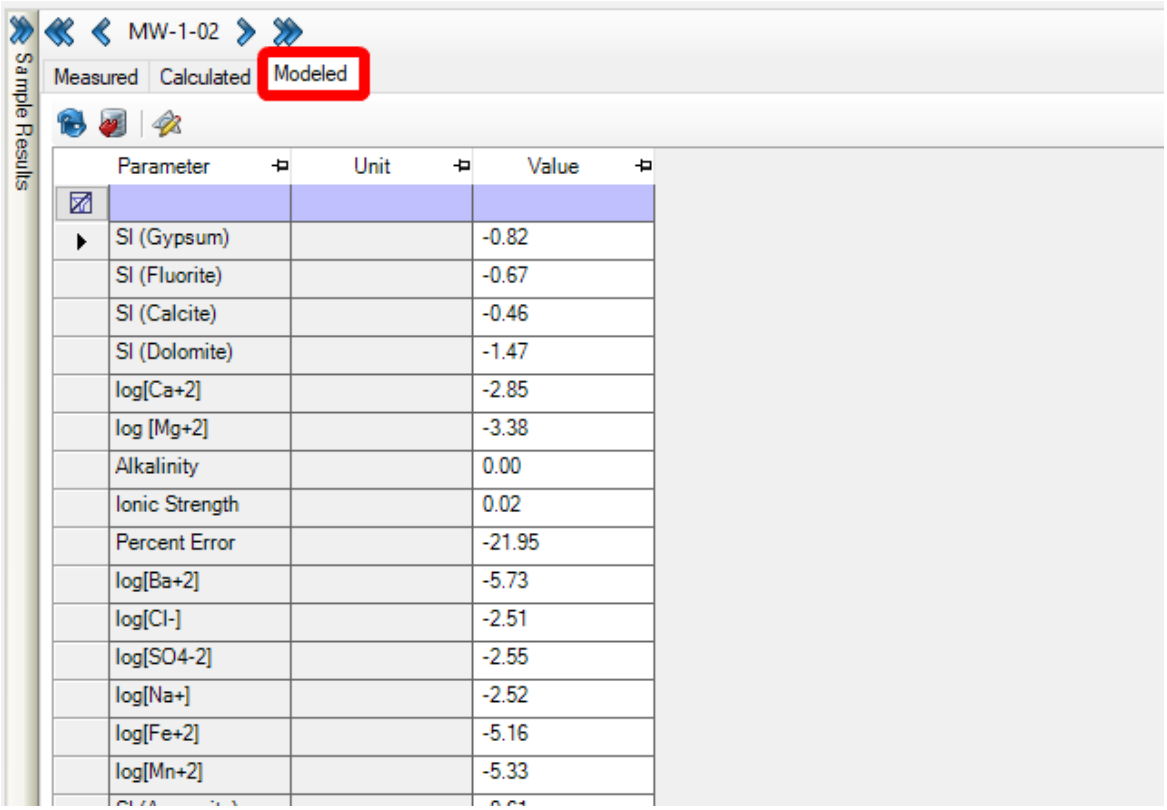


If you access the 'Calculated' data tab, you will be able to review the results of all calculated functions supported in AquaChem. For more detailed information regarding each function, review the Fundamental Concepts > Functions section of the user manual. Within the Calculated data tab, the results of each function are displayed in the 'Value' column, and the associated units are displayed in the 'Unit' column.

The Calculated tab does include one unique toolbar button, namely the 'Properties' button [ ]. Clicking this button will open the 'Functions' section of the Project Properties window (normally available from the main menu by clicking 'Project > Properties'). The Functions section of the Project Properties displays a simple description of each function, allows you to select the display format/units, and you can activate/deactivate the available functions using the checkboxes in the list of available functions:



Finally, the 'Modeled' data tab displays the results of PHREEQC geochemical speciation modeling performed in AquaChem 2014. Please note that PHREEQC modeling is not yet supported in AquaChem. In this tab, the results of each modeled parameter is stored in the 'Value' column:



Parameter	Unit	Value
SI (Gypsum)		-0.82
SI (Fluorite)		-0.67
SI (Calcite)		-0.46
SI (Dolomite)		-1.47
log[Ca+2]		-2.85
log [Mg+2]		-3.38
Alkalinity		0.00
Ionic Strength		0.02
Percent Error		-21.95
log[Ba+2]		-5.73
log[Cl-]		-2.51
log[SO4-2]		-2.55
log[Na+]		-2.52
log[Fe+2]		-5.16
log[Mn+2]		-5.33

This concludes your initial introduction to the primary components of the AquaChem interface which allow you to review station and sample data. In the next short sections, you will review some of the primary 'modules' available in AquaChem, which provide various features that facilitate analysis, visualization, and interpretation of your data.

Main Modules - Plot Collections, Sample Reports, R-Console

There are three important modules in AquaChem which allow you to analyze and interpret your data:

- The **Plot Collection Module** provides the ability to generate a wide range of water quality plot types, which can be organized into plot collections consisting of one or more individual plots. Plot collections can be saved and will persist on project close/reopen, saving you time when you need to review the same plots on a number of occasions. To learn more about the plot collection module you can skip ahead to the 'Creating Plot Collections' section of this tutorial.

- The **Sample Report Module** allows you to create custom tabulations of your samples and their results based on one or more criteria including: station/sample sets, specific parameters or groups, and/or exceedances of one or more active Water Quality Standards. The report can also evaluate general statistics for samples included in the report. To learn more about the sample report module you can skip ahead to the 'Creating Sample Report' section of this tutorial.

-  The **Map Viewer Module** allows you to create simple maps with thematic spatial information from specified stations and samples. Maps can include location-based proportionally sized/colored symbols, Stiff diagrams, radial plots, and/or pie charts. You can also add supplemental spatial information including imported shapefiles and basemaps. To learn more about the Map Viewer Module, you can skip ahead to the 'Creating Sample Report' section of this tutorial.

-  The **R-Console Module** allows you to run scripts in the R scripting language and leverage the thousands of available libraries that facilitate data analyses, visualization, categorization, and much more. To learn more about the R-console module you can skip ahead to the 'Basic Scripting with the R-Console' section of this tutorial.

Data Management Modules

There are several supporting modules in AquaChem which will help you to organize your data based on your specific project requirements:

-  The **Template Manager Module** is one of the most powerful tools provided with AquaChem 10.0, since it allows you to alter the structure of your database. This module provides tools for adding/removing database tables/fields, altering the properties of tables/fields, define relationships between tables, group tables into data categories, save database templates for future projects, and specify user-level table/field names, display units and data formats. The Template Manager is not covered in this tutorial, but you can review the 'Creating a New Project and Importing Data' tutorial for a brief introduction to this module.

-  The **Import Data Module** facilitates the process of importing data into AquaChem projects. The Import Data Module is not covered in this tutorial, but you can review the 'Creating a New Project and Importing Data' tutorial for a brief introduction to this module.

-  The **List Editor Module** provides the ability to create and customize lists for any field within the AquaChem project and facilitating efficient and effective data entry. A list in AquaChem may be considered as a lookup table - they become drop down lists within the interface (e.g. in the Sample List, Station List, Station Data tab, and Non Station Data tab). An example of a list is included in the Demo Project, specifically for the 'Geology' field within the 'Station' table.

-  The **Parameter Editor Module** allows you to modify the data structure of the current AquaChem database project by adding or deleting parameter fields from each of the four parameter categories. This option can also be used to modify the properties of analytical parameters (e.g. Display label, Internal name, Molecular weight, Charge,

Units, etc.) or to change the order in which the parameters are displayed in the Sample Details window.

-  The **Parameter Group Editor Module** allows you to group measured numerical parameters into user-defined groups, providing a quick and easy method of viewing specific sample data accessible in the Sample Details window and several other modules. The parameter group editor module is introduced in the Managing Data section of this tutorial.

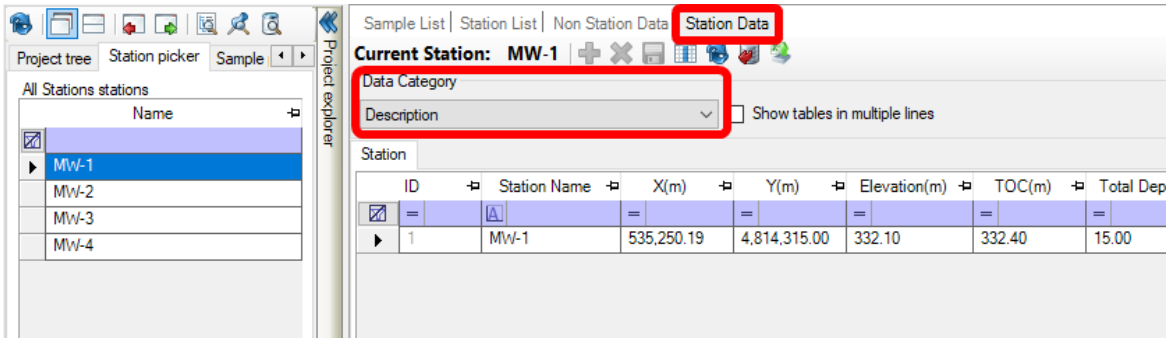
Additional Data Review Modules - Station and Non-Station Data Tabs

AquaChem 10.0 provides the user with much more flexibility compared to AquaChem 2014 in terms of the types of data which can be stored in the database. In this Demo Project, there aren't any additional user-defined data tables, but in your own projects, you may be interested in creating additional data categories/tables. The contents of these optional tables could then be managed using the 'Station Data' and 'Non Station Data' tabs. Both of these views can be accessed from the main menu by clicking 'View > Station Data/Non Station Data', or by clicking the following buttons from the main toolbar:

-  The **Station Data** tab provides a detailed view of the active Station's attributes. The Station Data tab displays available information about the currently selected station based on the active Data Category

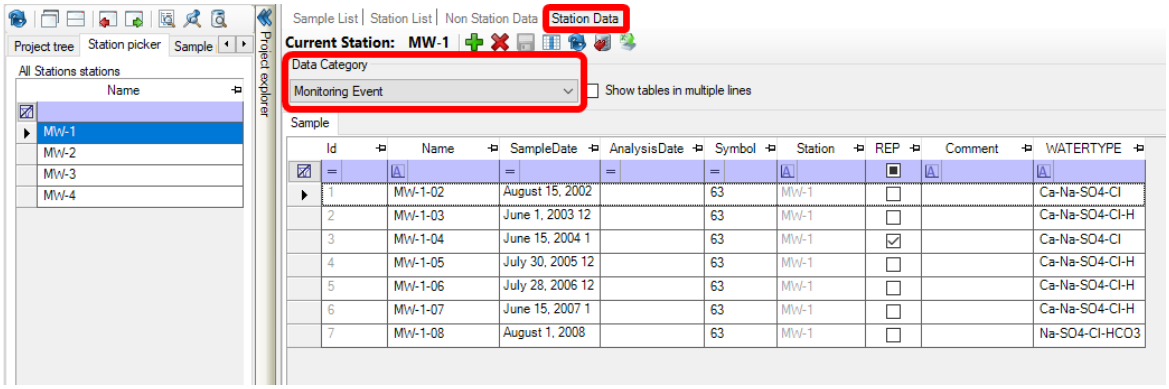
-  The **Non Station Data** tab provides you with the ability to view tables that are not directly associated with the Station Table (e.g. the Sample Analysis and Parameter tables). You can find out more information about how to add a Non Station Data table in your database in the Template Manager section.

Open both of these tabs now, and spend a moment reviewing the contents. When you open the Station Data tab the 'Description' data category will be displayed at first, and you will see the contents of the 'Station' table for the active station (based on the currently selected station in the Station Picker):

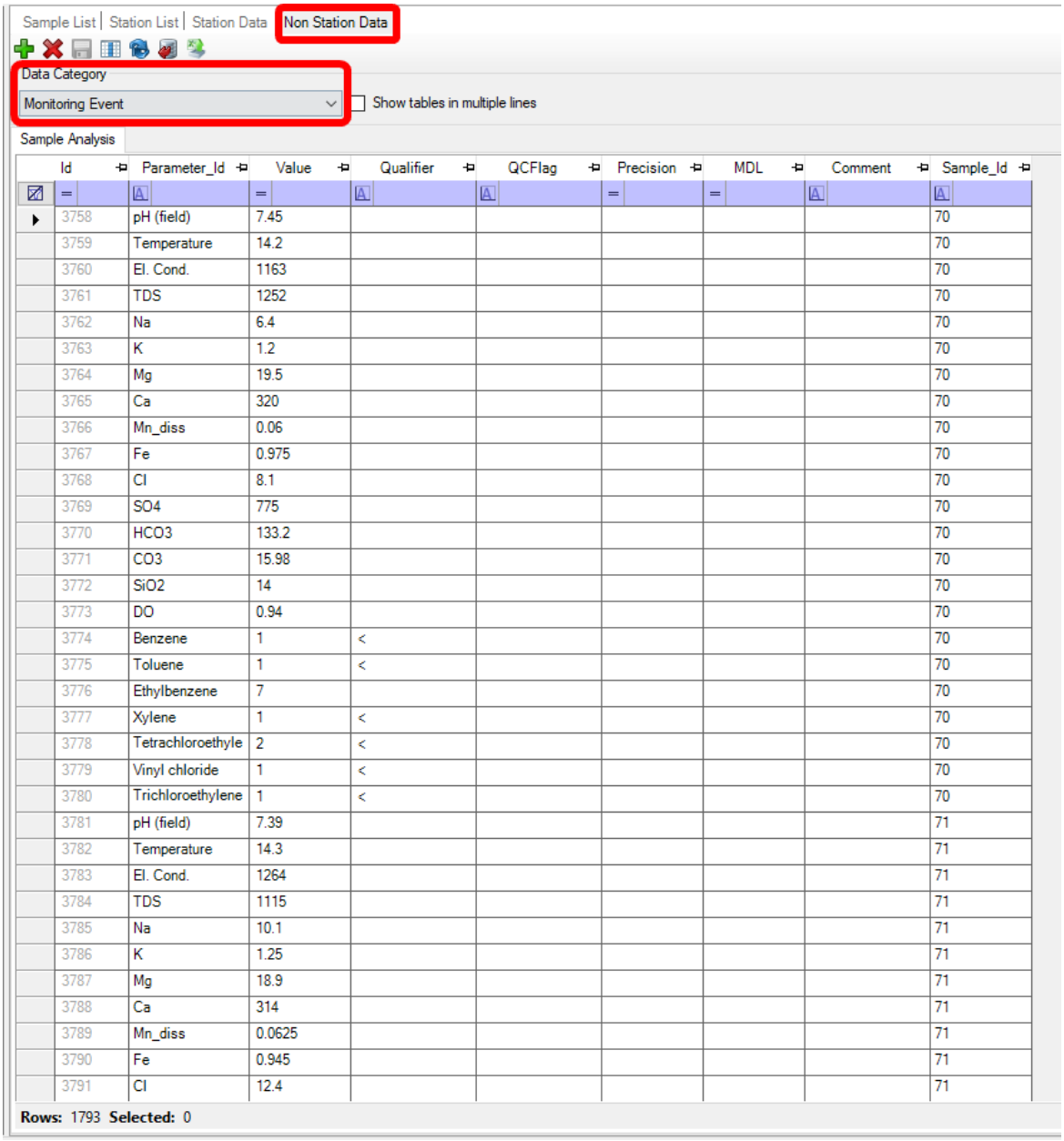


If you select the 'Monitoring Event' Data Category (using the menu highlighted in the image above), the Station Data tab will reflect the contents of the 'Sample' table for the active

station. As you can see from the image below, all seven samples associated with station MW-1 are displayed:



If you access the 'Non-Station Data' table the default Data Category will be 'Uncategorized', but if you update the Data Category to 'Monitoring Event' you will be able to view the individual parameters/result records associated with every available sample in a flat table:

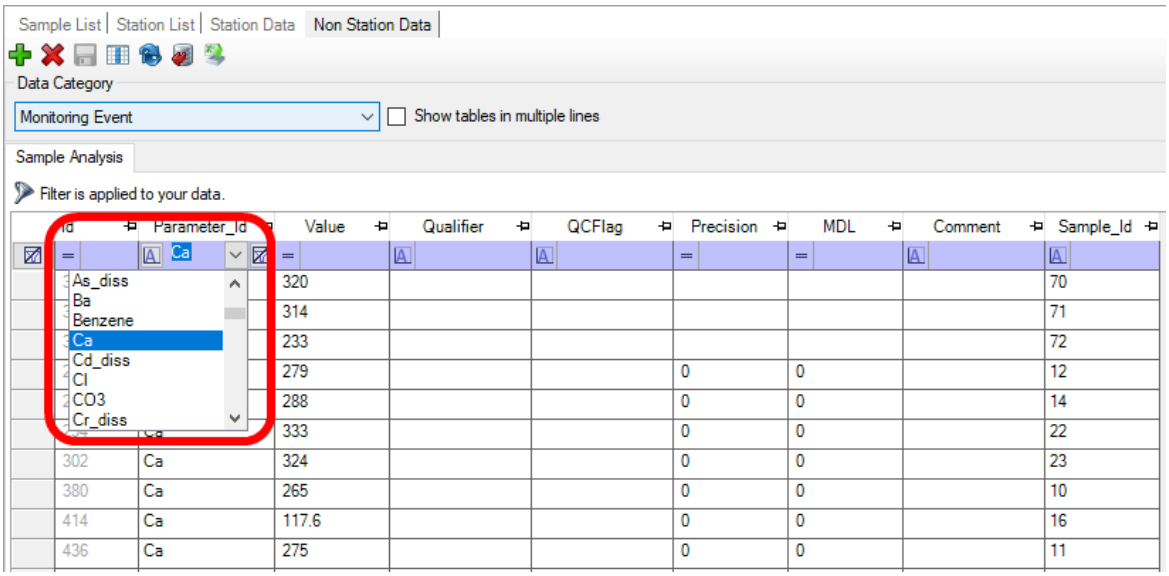


Id	Parameter_Id	Value	Qualifier	QCFlag	Precision	MDL	Comment	Sample_Id
3758	pH (field)	7.45						70
3759	Temperature	14.2						70
3760	El. Cond.	1163						70
3761	TDS	1252						70
3762	Na	6.4						70
3763	K	1.2						70
3764	Mg	19.5						70
3765	Ca	320						70
3766	Mn_diss	0.06						70
3767	Fe	0.975						70
3768	Cl	8.1						70
3769	SO4	775						70
3770	HCO3	133.2						70
3771	CO3	15.98						70
3772	SiO2	14						70
3773	DO	0.94						70
3774	Benzene	1	<					70
3775	Toluene	1	<					70
3776	Ethylbenzene	7						70
3777	Xylene	1	<					70
3778	Tetrachloroethyle	2	<					70
3779	Vinyl chloride	1	<					70
3780	Trichloroethylene	1	<					70
3781	pH (field)	7.39						71
3782	Temperature	14.3						71
3783	El. Cond.	1264						71
3784	TDS	1115						71
3785	Na	10.1						71
3786	K	1.25						71
3787	Mg	18.9						71
3788	Ca	314						71
3789	Mn_diss	0.0625						71
3790	Fe	0.945						71
3791	Cl	12.4						71

Rows: 1793 **Selected:** 0

Please Note: all data tables in AquaChem (i.e. Sample List, Station List. Sample Results tab, Station Data tab, Non-station Data tab) include the ability to perform data filtering, using the blue ( ) row at the top of each data table. To demonstrate, we will filter the 'Sample Analysis' table here in the Non-Station Data tab to display only calcium data.

To filter the data, simply hover your mouse pointer over first cell in the below the 'Parameter_Id' column and open the menu that appears. Select 'Ca' from the list of parameter IDs, and the table will be filtered so that only 'Ca' results are shown:



Now that you are familiar with the main and supporting modules available in AquaChem, let's review how you can manage and use data within an AquaChem project.

2.1.2 Managing Data

In this section of the tutorial, you will review the following functionality:

- Manual Data Entry
- Creating Sample Sets and Station Groups
- Create Parameter Groups

Other than the manual data entry portion, these functions will help you understand how data can be you can efficiently organize and access data within the AquaChem interface. The creation of station groups and sample sets (especially dynamic groups) facilitates and streamlines management, retrieval, and plotting of data stored in the database. For instance, you may wish to find all samples that:

- were collected within a certain period of time,
- exceed some water quality standard,
- belong to a certain group of stations, or
- a combination of the above

Similarly, station groups can be created based on any criteria. Common examples include:

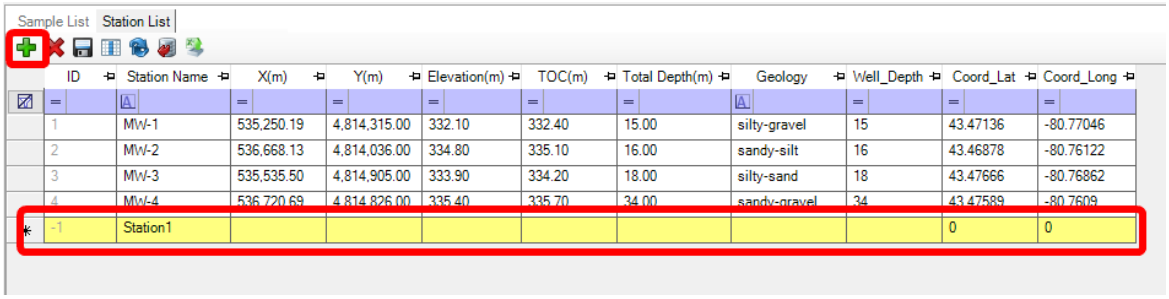
- Locations of the stations (e.g. locations categorized by City, Project Site, watershed, etc.)
- Station type (e.g. Monitoring Locations, Boreholes, etc.), or
- Purpose of Study (e.g. remediation, site monitoring, etc.)

And finally, creating parameter groups allows you to sort and categorize measured numerical parameters into user-defined groups, providing a quick and easy view of specific sample data.

2.1.2.1 Manual Data Entry

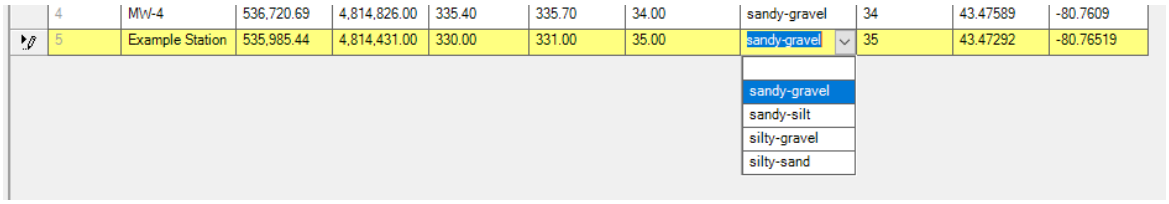
Please Note: In addition to this tutorial, you may want to review the 'Creating a New Project and Importing Data' tutorial for an introduction to the Import Data Module. This section only covers manual data entry, which can be a tedious and error-prone process if you have a large dataset.

Manual data entry is a very simple process. To review, access the Station List tab and click the 'Add new station' [+] button in the toolbar. A new row will appear in the Station List, and it will be highlighted yellow to indicate that this data has not been saved yet and committed to the database, as shown below:



ID	Station Name	X(m)	Y(m)	Elevation(m)	TOC(m)	Total Depth(m)	Geology	Well_Depth	Coord_Lat	Coord_Long
1	MW-1	535,250.19	4,814,315.00	332.10	332.40	15.00	silty-gravel	15	43.47136	-80.77046
2	MW-2	536,668.13	4,814,036.00	334.80	335.10	16.00	sandy-silt	16	43.46878	-80.76122
3	MW-3	535,535.50	4,814,905.00	333.90	334.20	18.00	silty-sand	18	43.47666	-80.76862
4	MW-4	536,720.69	4,814,826.00	335.40	335.70	34.00	sandy-gravel	34	43.47589	-80.7609
-1	Station1								0	0

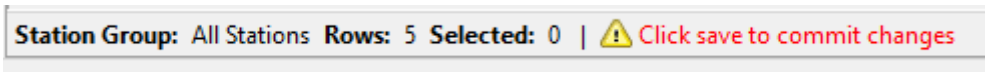
Now that a new record is available, you can simply click in each of the associated fields and manually specify values. Enter the following values, and also take note how the 'Geology' field includes the option to select values from a predefined list:



4	MW-4	536,720.69	4,814,826.00	335.40	335.70	34.00	sandy-gravel	34	43.47589	-80.7609
5	Example Station	535,985.44	4,814,431.00	330.00	331.00	35.00	sandy-gravel	35	43.47292	-80.76519

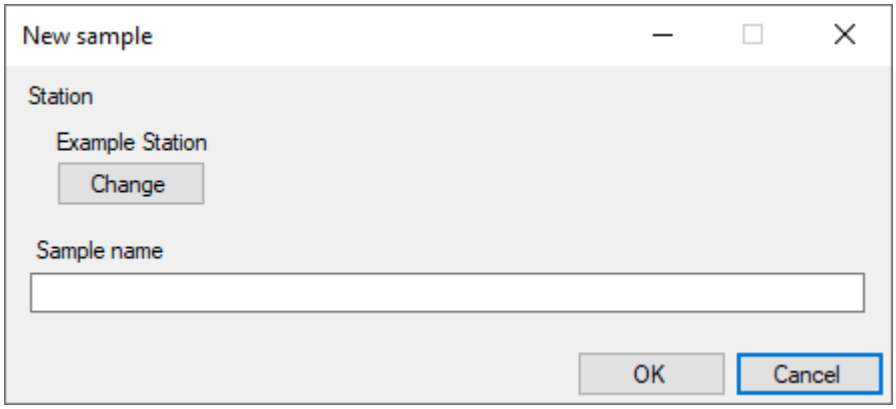
sandy-gravel
sandy-silt
silty-gravel
silty-sand

Once the data has been entered you have to click the 'Save station changes' [💾] button in the toolbar (or alternatively press 'CTRL+S') to save the record. Until the record has been saved the row will be highlighted yellow [ ], and the following message will be displayed in the status bar at the bottom of the interface:

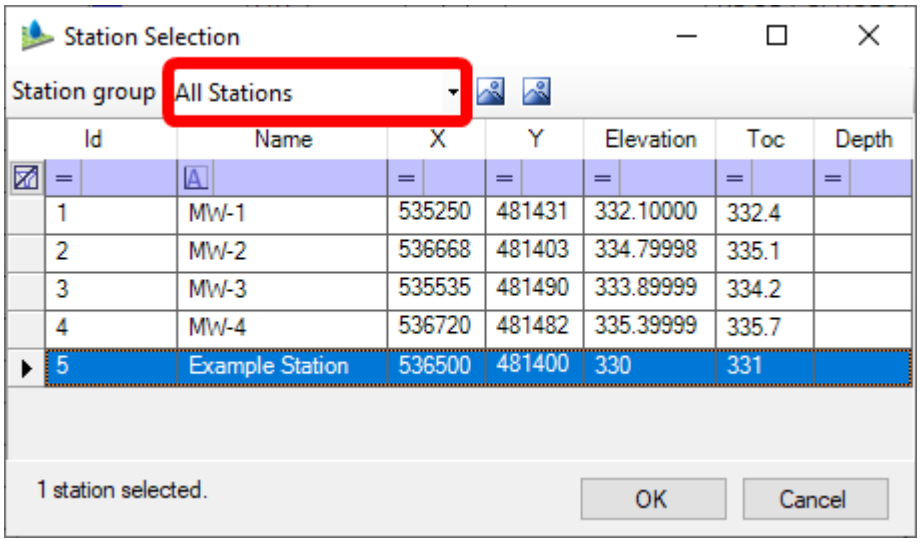


Click the 'Save station changes' [] button now to commit the new record to the database, and now you can proceed to the Sample List to manually add some data there.

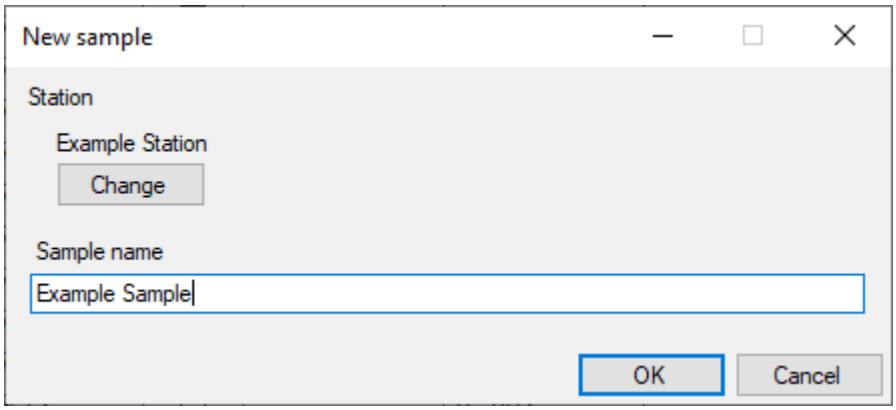
Access the Sample List and click the 'Add a new sample' [] button. Before the new row is added to the Sample List, the following 'New sample' window will appear:



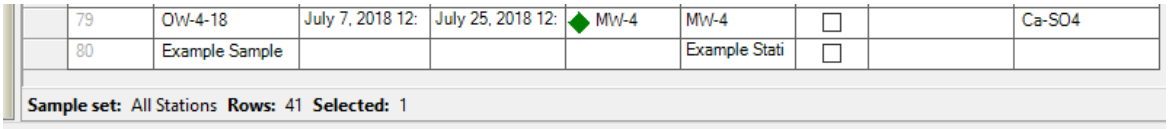
All samples added to the AquaChem relational database MUST be related to an existing station, which is why we see this window. Click the Change button to open the 'Station Selection' window as shown below, and select the 'Example Station' which we have just added to the project. You can use the highlighted menu to select from available station groups (more on station groups in the next sections), but by default all stations will be displayed:



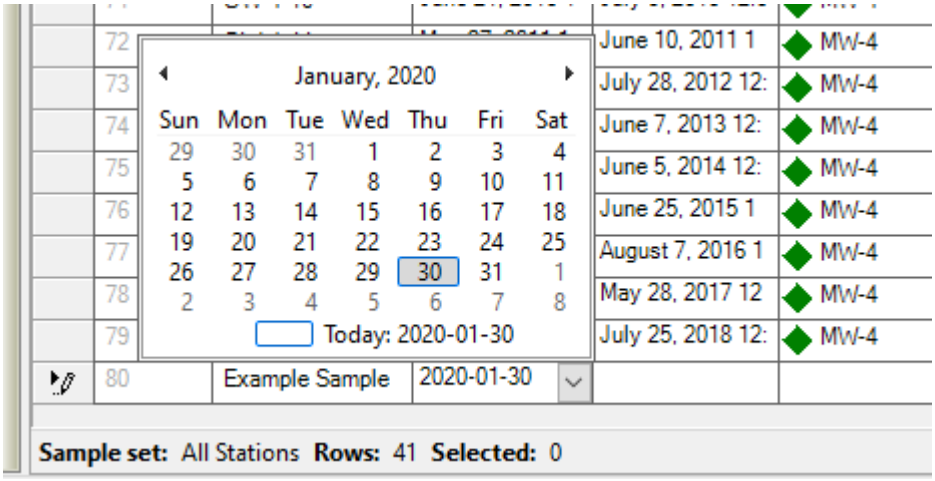
Once you have selected 'Example Station', click the OK button in the Station Selection window, and then type the sample name (e.g. 'Example Sample') in the New Sample window, as shown below:



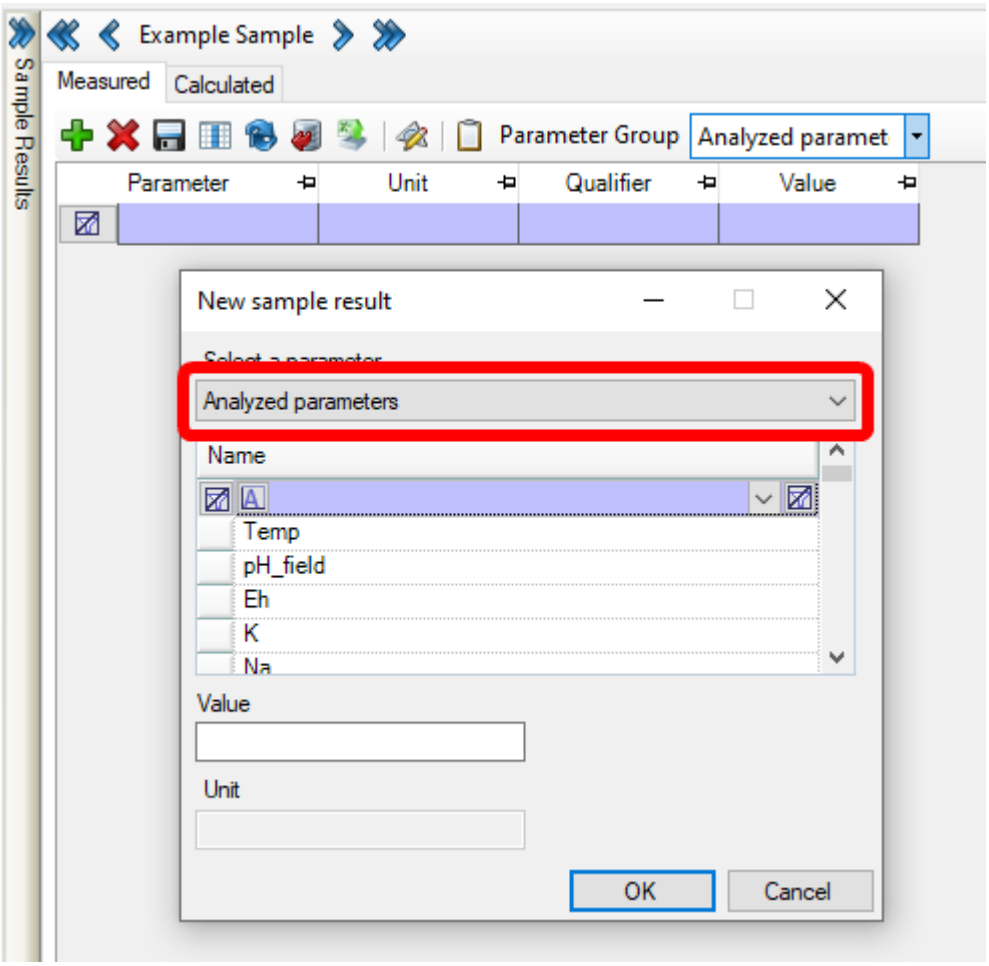
Click OK to create the sample, and you will see it added to the Sample List:



Now you can specify values for the Sample Date, Analysis Date, etc. Note again how values entered into these fields cause the row to be highlighted yellow [ ], and a message is displayed indicating that the changes must be saved in order to commit them to the database. Click the Sample Date field, and you can either type values into the field or you may click the menu button within the cell to open a small calendar. Select today's date:

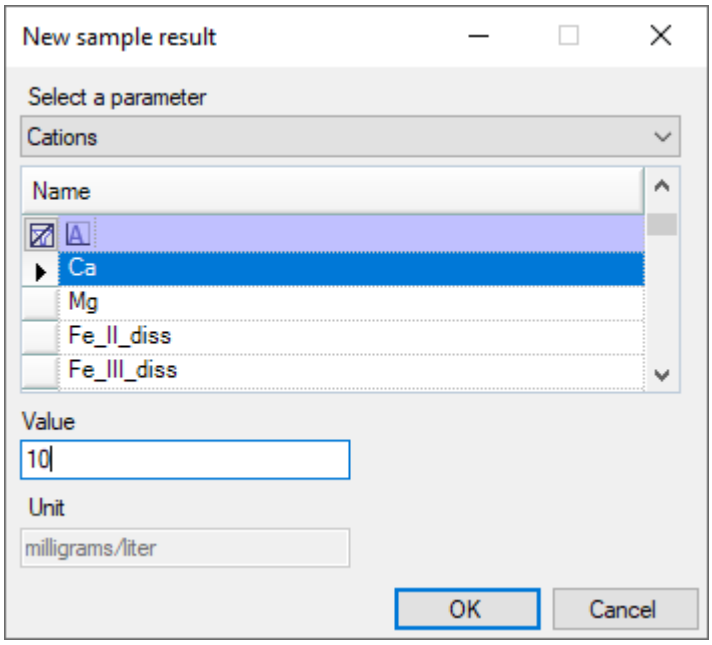


Finally, once the minimum data has been specified for the sample (and committed to the database by clicking the 'Save' [💾] button) you can turn your attention to the Sample Results tab, which should be empty at this time (since no data has been entered yet). In the Sample Results tab, click the 'Add measured values' [➕] button, and the 'New sample result' window will open, as shown below:

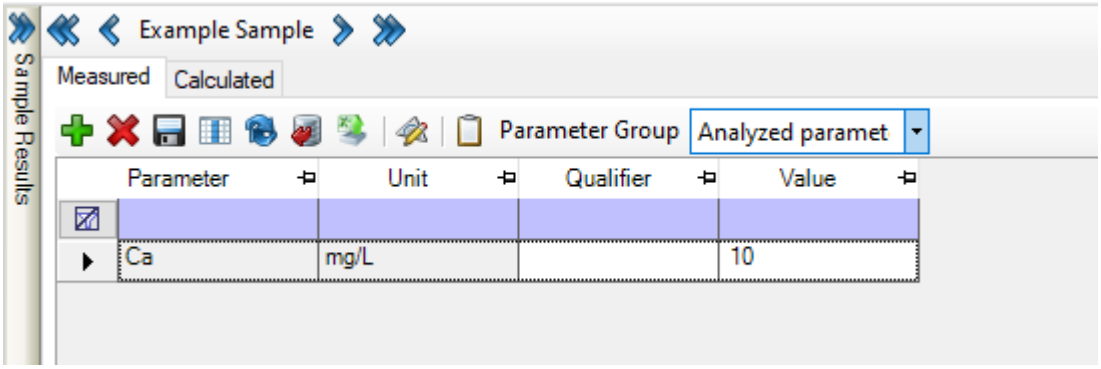


The 'New sample result' window provides a menu at the top (highlighted in the image above) which allows you to select from available parameter groups (more on parameter groups in the following sections). The most recently used parameter group should be selected by default.

Since this is simply an example sample for demonstration purposes, select 'Ca' (calcium) from the parameter list, and enter a value of 10. The unit is selected automatically based on the unit specified in the database structure (i.e. the unit specified within the Parameter Editor module). When you have entered this data, the 'New sample result' window should look like the image below:



Click OK to apply the new value to the Sample Result table, and then click the 'Save measured value changes' [] button to commit the new record to the database (once again, unsaved changed will be highlighted in yellow, and a message will be displayed in the status bar):



Feel free to add several other measured values for practice, but this is the essential process used to manually add data to the database. In the next section we'll discover how to review, edit and create new Sample Sets.

2.1.2.2 Creating Sample Sets and Station Groups

Sample sets are selections of samples which can be saved for rapid and consistent retrieval and use. There are two types of samples sets:

-  **Static sample sets**: a fixed list of specific samples that have been added to the static sample set

-  **Dynamic sample sets**: a variable list of samples that meet one or more conditions specified in the Sample Set Editor. The list of samples is dynamically built on demand by AquaChem.

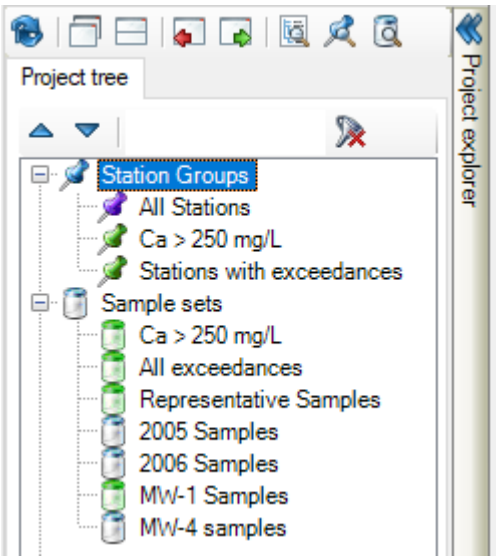
Dynamic sample sets are especially helpful, since they are automatically generated using one or more predefined criteria. As sample data are added to the project, the new data may be automatically added to relevant dynamic sample sets provided they meet the applicable criteria. This ensures that your sample sets will include relevant data as the project progresses without having to manually update sample sets. For instance, you way wish to find all samples that:

- were collected within a certain period of time,
- exceed some water quality standard,
- belong to a certain group of stations, or
- a combination of the above

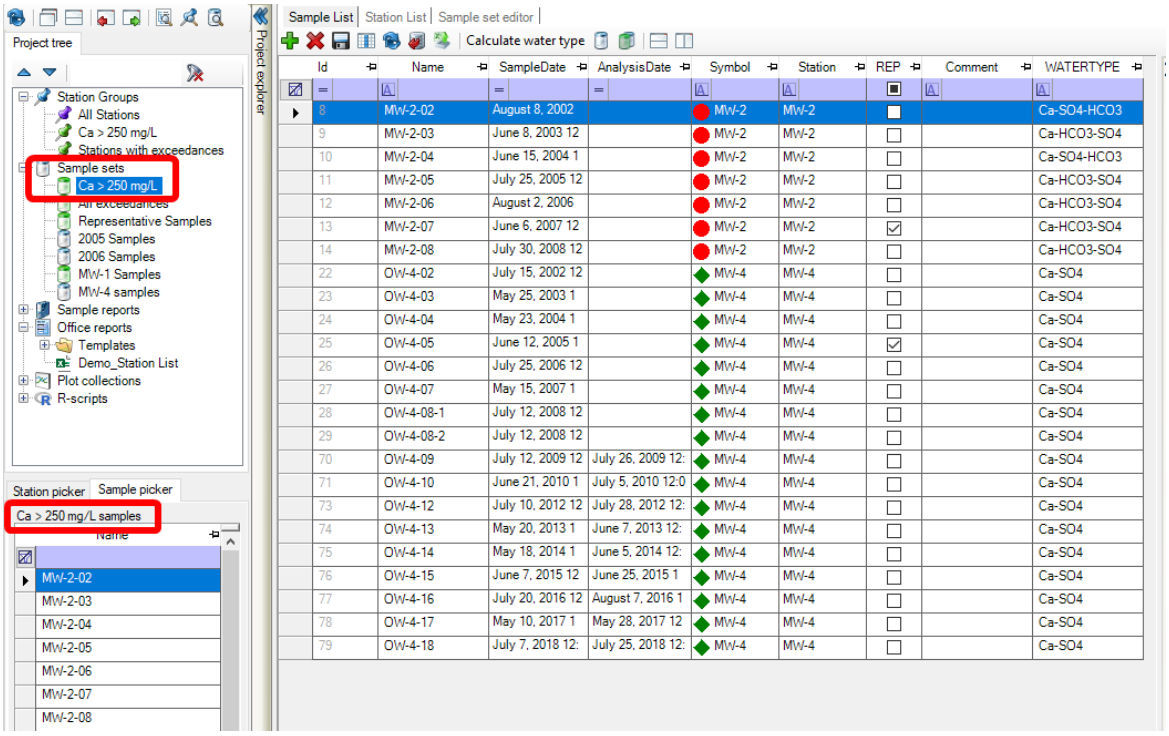
Similarly, static () and dynamic () station groups may be created in order to easily retrieve particular selections of stations. Station groups and sample sets are also dynamically linked to each other. Each station group in your project implicitly results in an associated sample set (i.e. all samples associated with the stations contained in the station group). Furthermore, dynamic station groups can be created based on the criteria of a dynamic sample set (i.e. a station group may be created from the stations associated with the dynamic sample set).

AquaChem projects always include a special station group called "All Stations" (denoted by ). This group contains all stations, and by definition, all samples.

The Demo Project includes some predefined static and dynamic sample sets/station groups. As with all sample sets and station groups, these are saved in the Project Tree, under the 'Sample Sets' and 'Station Groups' nodes, respectively:

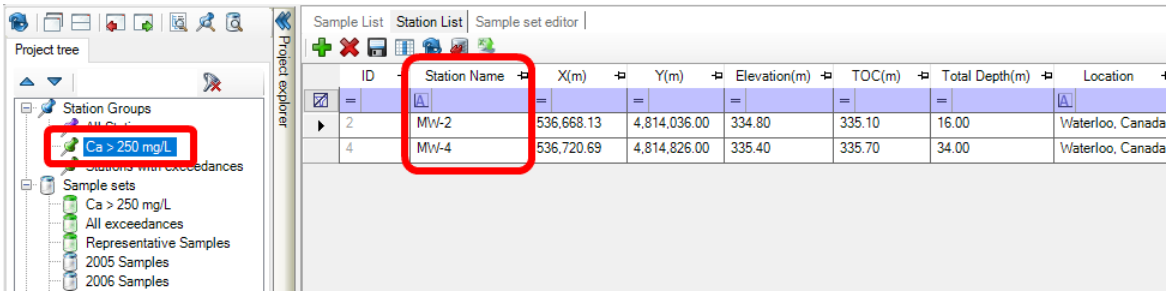


To activate any given station group or sample set, simply double-click them in the Project Tree. For example, if you double-click the 'Ca > 250 mg/L' sample set, the Sample List will be displayed and the associated samples will be displayed in the here and in the Sample picker:

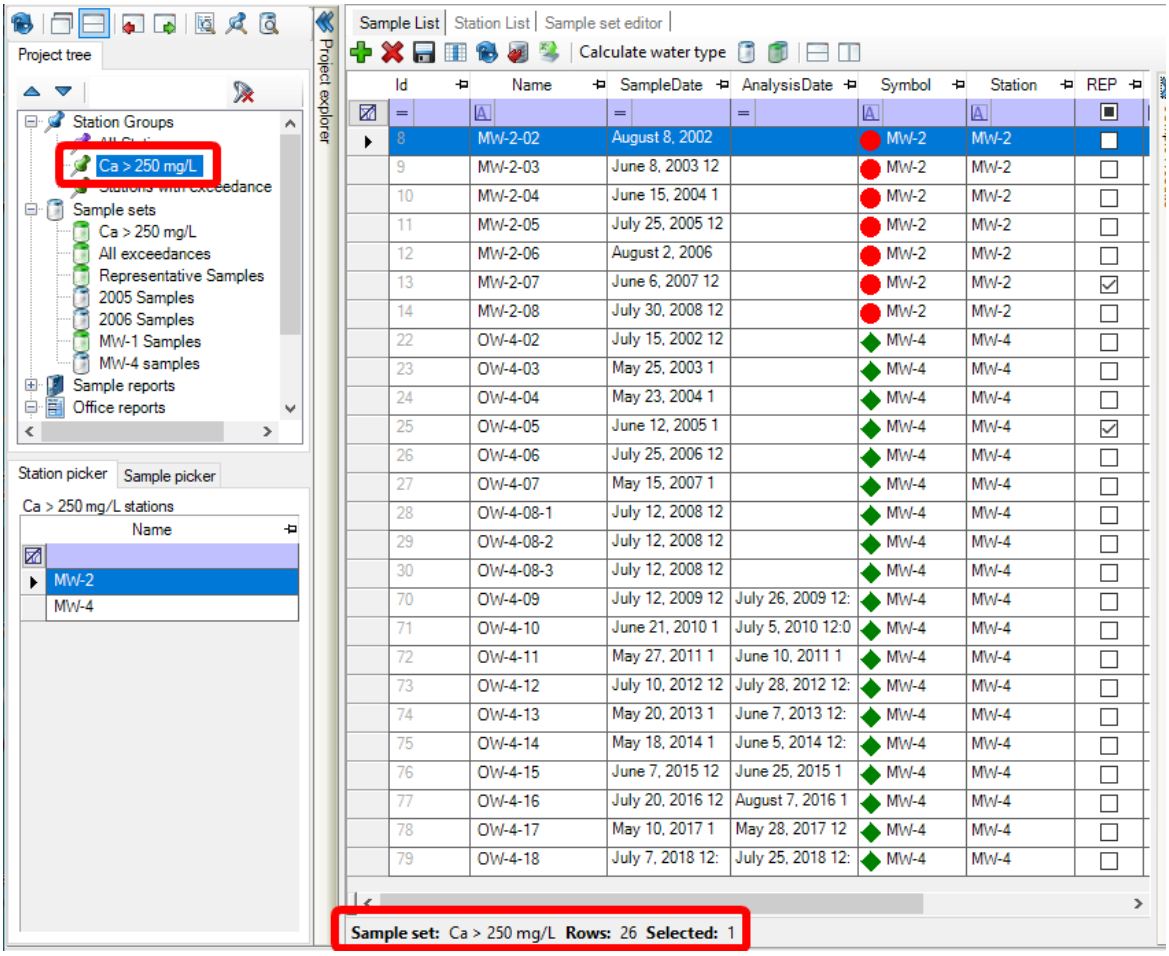


Please Note: the status bar at the bottom of the Sample List should indicate that there are 24 rows, i.e. 24 samples which meet the criteria for this sample set.

You may notice that all the samples in the list above are associated with station MW-2 and MW-4. A related station group is also available under the 'Station Groups' node of the Project Tree. Double-click the 'Ca > 250 mg/L' station group, and the Station List tab will be opened and should display stations MW-2 and MW-4:



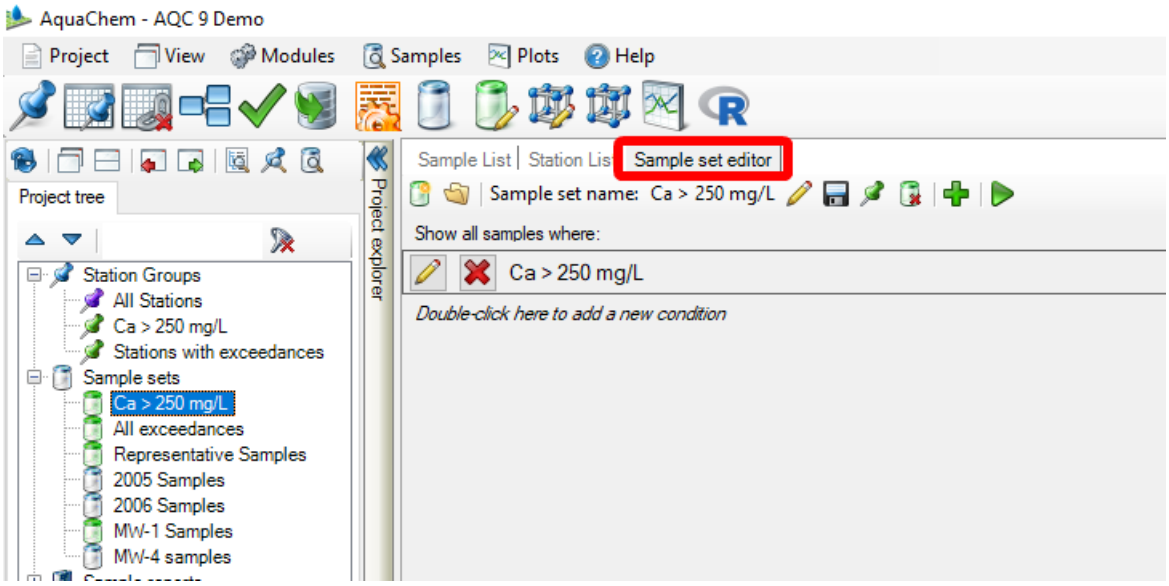
If you access the Sample List again you will see that ALL samples associated with the 'Ca > 250 mg/L' station group are displayed. A total of 26 rows will be displayed, which you may notice is 2 more than the number of samples associated with the ***'Ca > 250 mg/L'*** sample set:



This discrepancy (i.e. 24 samples in the sample set, 26 samples in the station group) illustrates the differences between sample sets and station groups.

A sample set consists ONLY of the samples which meet the criteria used to generate the sample set. A station group based on a dynamic sample set also implicitly results in a *station* sample set, but this *station* sample set includes ALL samples from the associated stations.

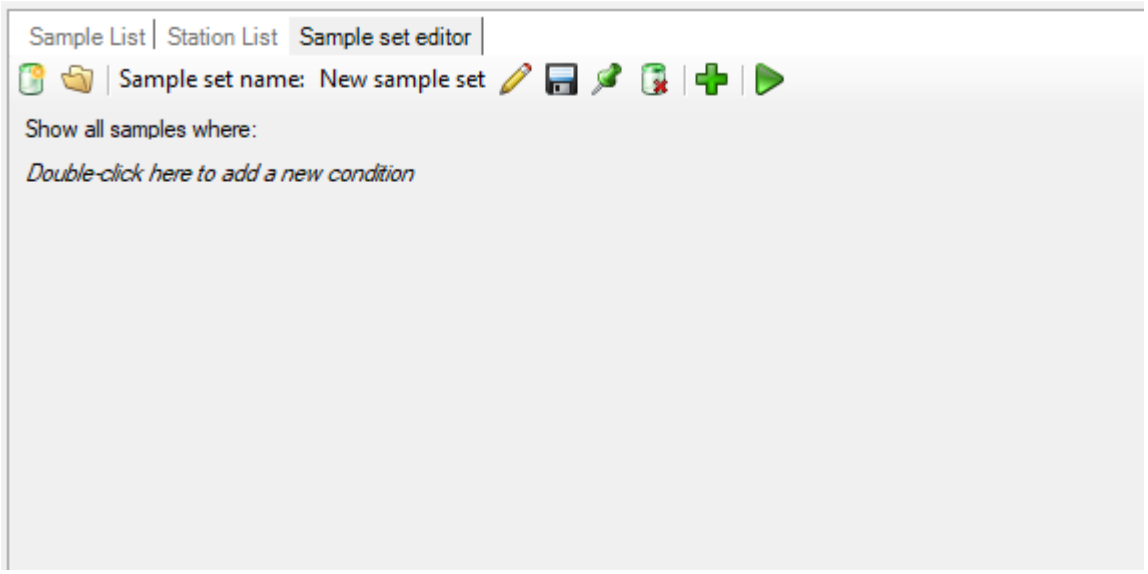
To review the criteria used to generate this sample set simply right-click the 'Ca > 250 mg/L' sample set in the Project Tree and select 'Edit'. The 'Sample Set Editor' module will then open (you can access the Sample Set Editor at any time by clicking 'Samples > Sample set editor' from the main menu), as shown below:



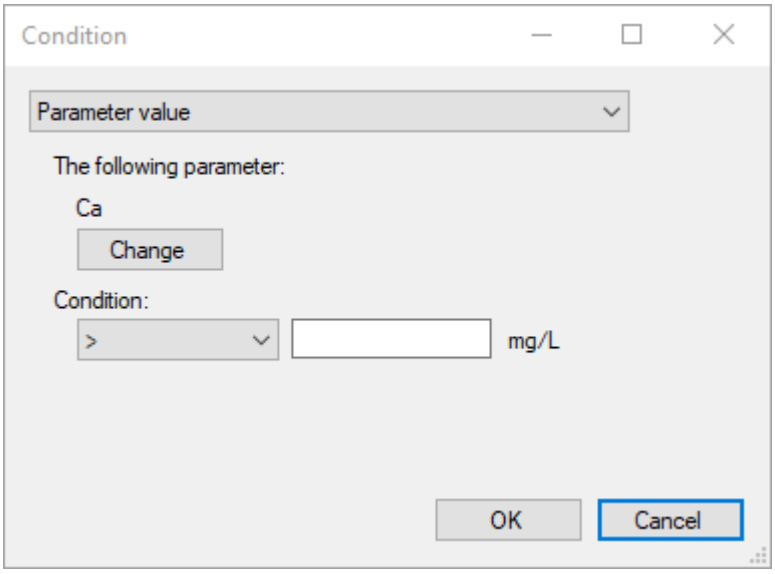
The Sample Set Editor contains a number of simple toolbar buttons, including options to create a 'New dynamic sample set' [], 'Open sample set' [], 'Rename' [] a sample set, 'Save' [] a sample set and 'Delete' [] a sample set. There are also a few buttons which are more unique to the Sample Set Editor in particular, including the options to 'Create a dynamic station group' [], which allows a new station group to be generated automatically based on the results of the current sample set. For example, the 'Ca > 250 mg/L' station group was created based on the 'Ca > 250 mg/L' sample set using this very button. The 'Add condition' [] button allows you to add new conditional criteria to the current sample set. Finally, the 'Test sample set' [] button allows you to test the sample set before saving it, and will display the results in a table on the right side of the Sample Set Editor module.

Let's test some of these features out. The aim of the new sample set will be to find all samples which have calcium concentrations greater than 250 mg/L AND magnesium concentrations greater than 20 mg/L.

First, click the 'New dynamic sample set' [.] button to create a new blank sample set

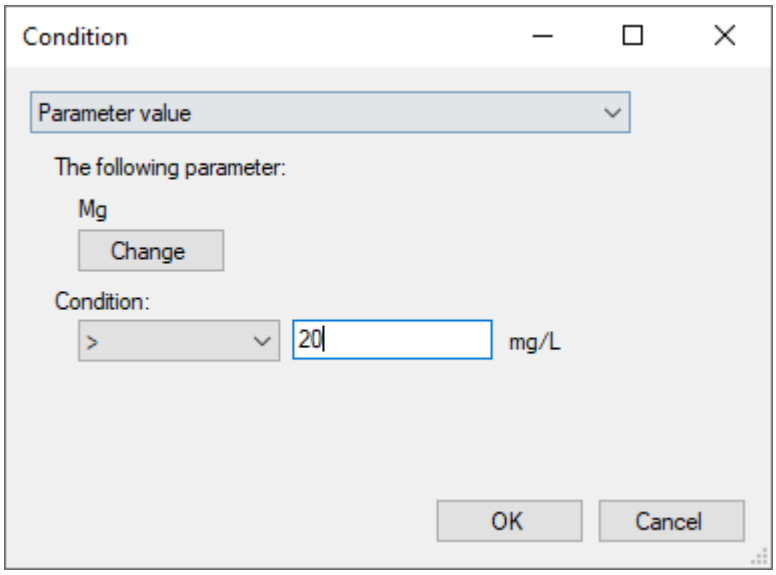


Now click the 'Add condition' [+] button to open the 'Condition' window, as shown below (note: you can also double-click anywhere below the existing condition to open this window):

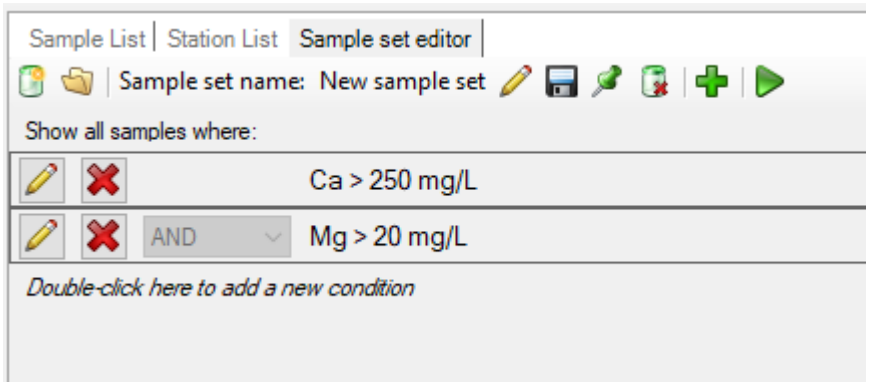


The first condition for the new sample set will still be Ca > 250 mg/L, so simply type 250 in the condition field, then click OK.

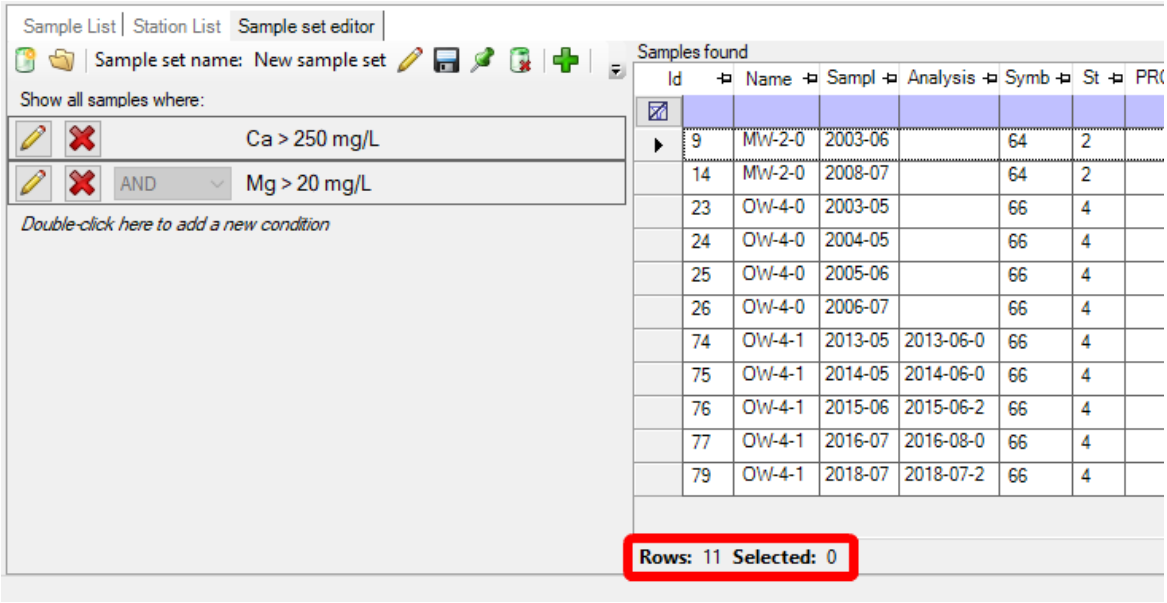
Now you'll add the second condition, so click the 'Add condition' [+] button again. The new condition (Mg > 20 mg/L) is also based on a parameter value, so click the the first menu can remain unchanged. But you will click the 'Change' button to open a 'Parameter Selector' window and update the parameter to 'Mg', and then enter a value of 20 in the condition field. The 'Condition' window should look like this:



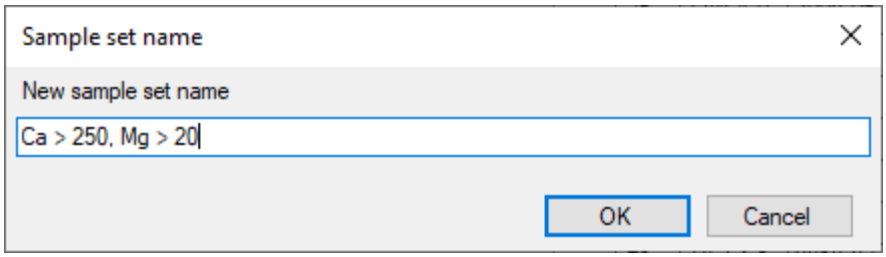
When the condition is defined simply click OK, and the new condition will be listed beneath the existing Ca > 250 mg/L condition:



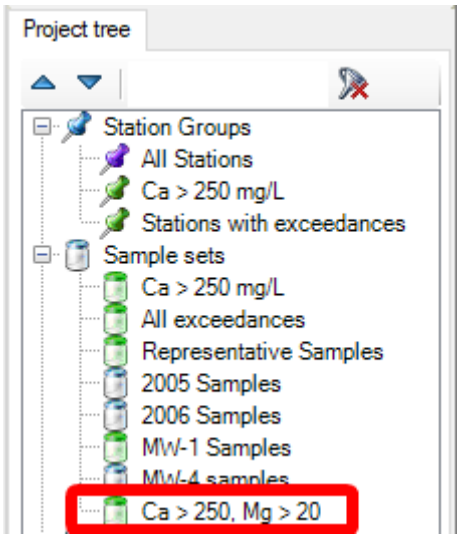
Clicking the 'Test sample set' [▶] button again should result in a total of 11 records:



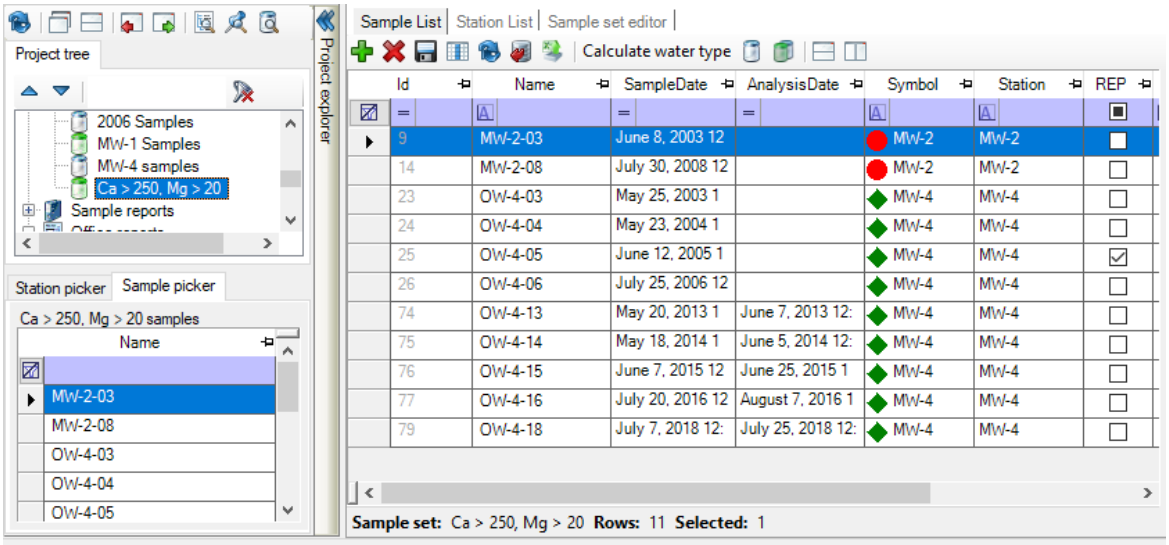
Now simply rename the sample set so that it does not overwrite our existing 'Ca > 250 mg/L' sample set, and then save it. Click the 'Rename' [✎] button and a window will open which allows you to enter a new sample set name, and type in 'Ca > 250, Mg > 20' and click OK.



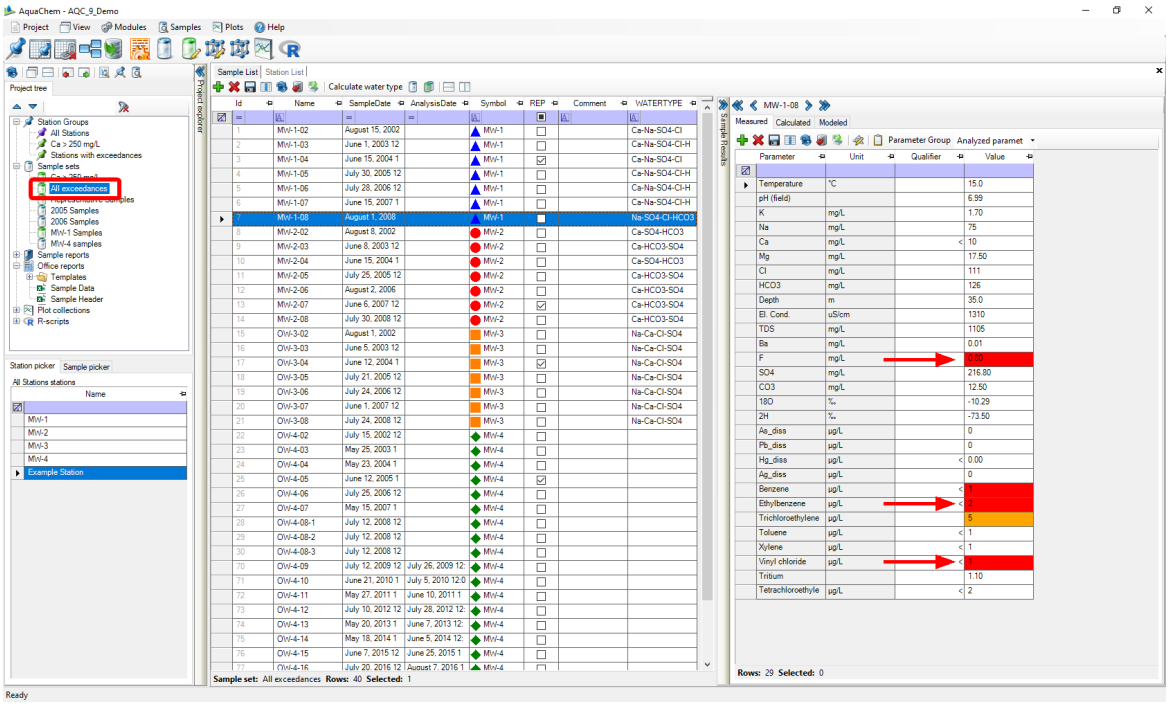
Finally, click the 'Save' [💾] button and the new dynamic sample set will appear in the Project Tree:



Now if you double-click the new sample set we will see the 11 samples identified earlier appear in the Sample List:

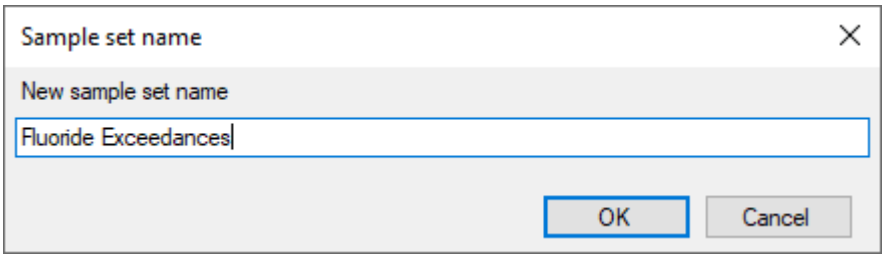


It's also possible to create sample sets based parameter exceedance, based on the active water quality standards. For example, you can double-click the 'All exceedances' sample set the Sample List will be updated, and if you review the sample results for any of those samples you will notice that at least one analyzed value contains an exceedance (i.e. the parameter values which are highlighted in orange or red):

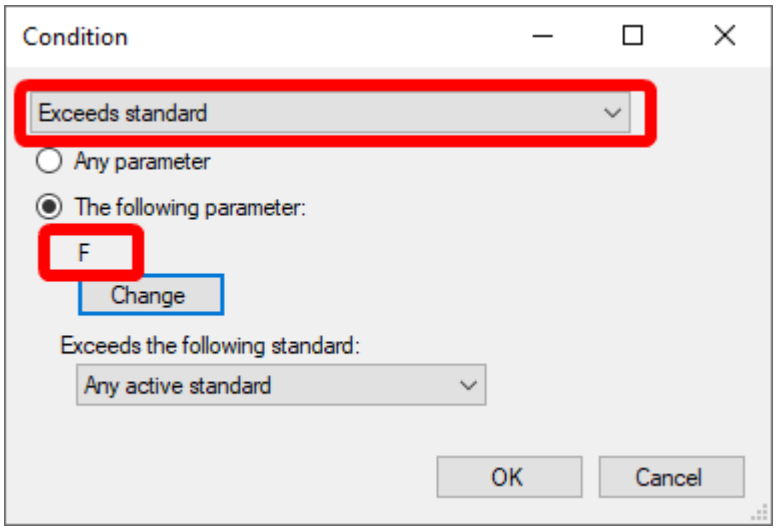


Let's test the ability to create a sample set based on exceedances. A review of the 'All exceedances' sample set indicates that a subset of these samples have exceedances for fluoride, barium and lithium, so let's create a set of samples based on fluoride and barium as examples.

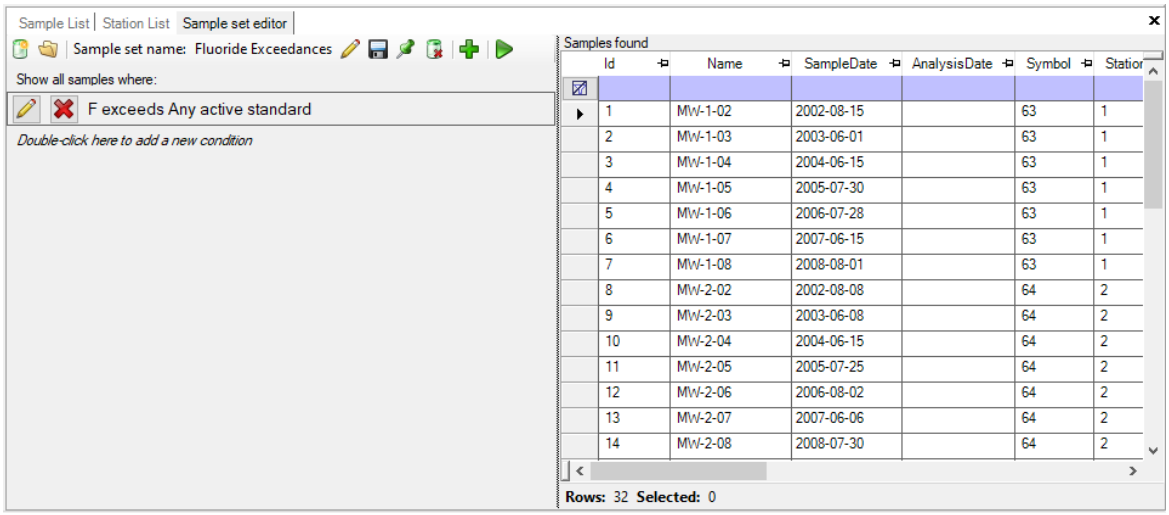
Return to the Sample Set Editor module, and click the 'New dynamic sample set' [] button. Click the 'Rename' [] button and enter the name 'Fluoride Exceedances':



Click OK to apply the sample set name, and then click the 'Add condition' [] button. This time change the first menu to 'Exceeds standard', then select 'The following parameter', and use the parameter selector menu to select 'F'. The Condition window should look like the image below:



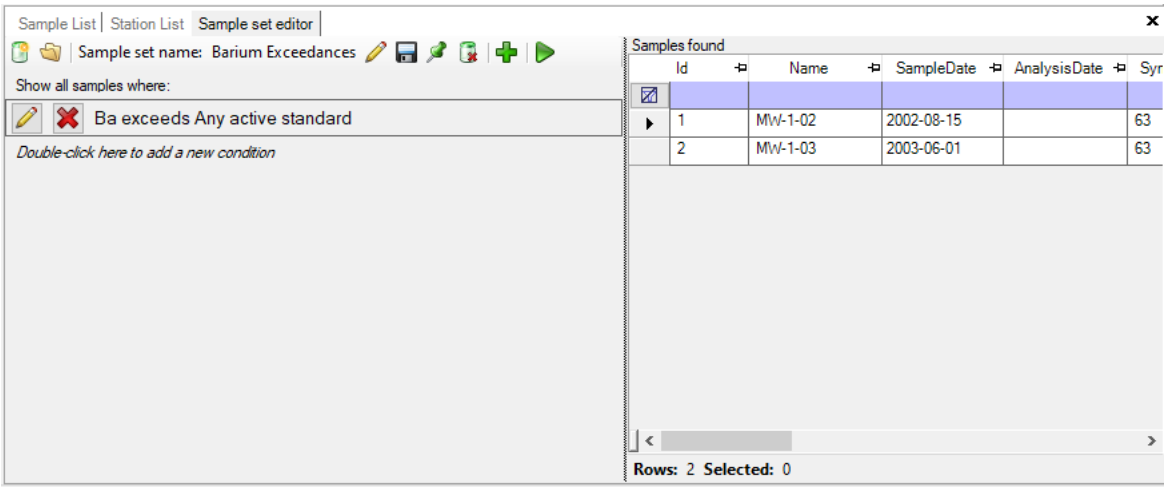
If you test the sample set [▶] now you should see a total of 32 samples with fluoride exceedances:



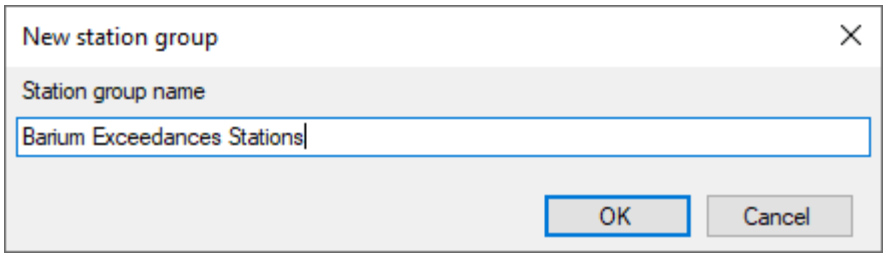
Id	Name	SampleDate	AnalysisDate	Symbol	Station
1	MW-1-02	2002-08-15		63	1
2	MW-1-03	2003-06-01		63	1
3	MW-1-04	2004-06-15		63	1
4	MW-1-05	2005-07-30		63	1
5	MW-1-06	2006-07-28		63	1
6	MW-1-07	2007-06-15		63	1
7	MW-1-08	2008-08-01		63	1
8	MW-2-02	2002-08-08		64	2
9	MW-2-03	2003-06-08		64	2
10	MW-2-04	2004-06-15		64	2
11	MW-2-05	2005-07-25		64	2
12	MW-2-06	2006-08-02		64	2
13	MW-2-07	2007-06-06		64	2
14	MW-2-08	2008-07-30		64	2

Don't forget to save the 'Fluoride Exceedances' sample set by clicking the 'Save' [💾] button.

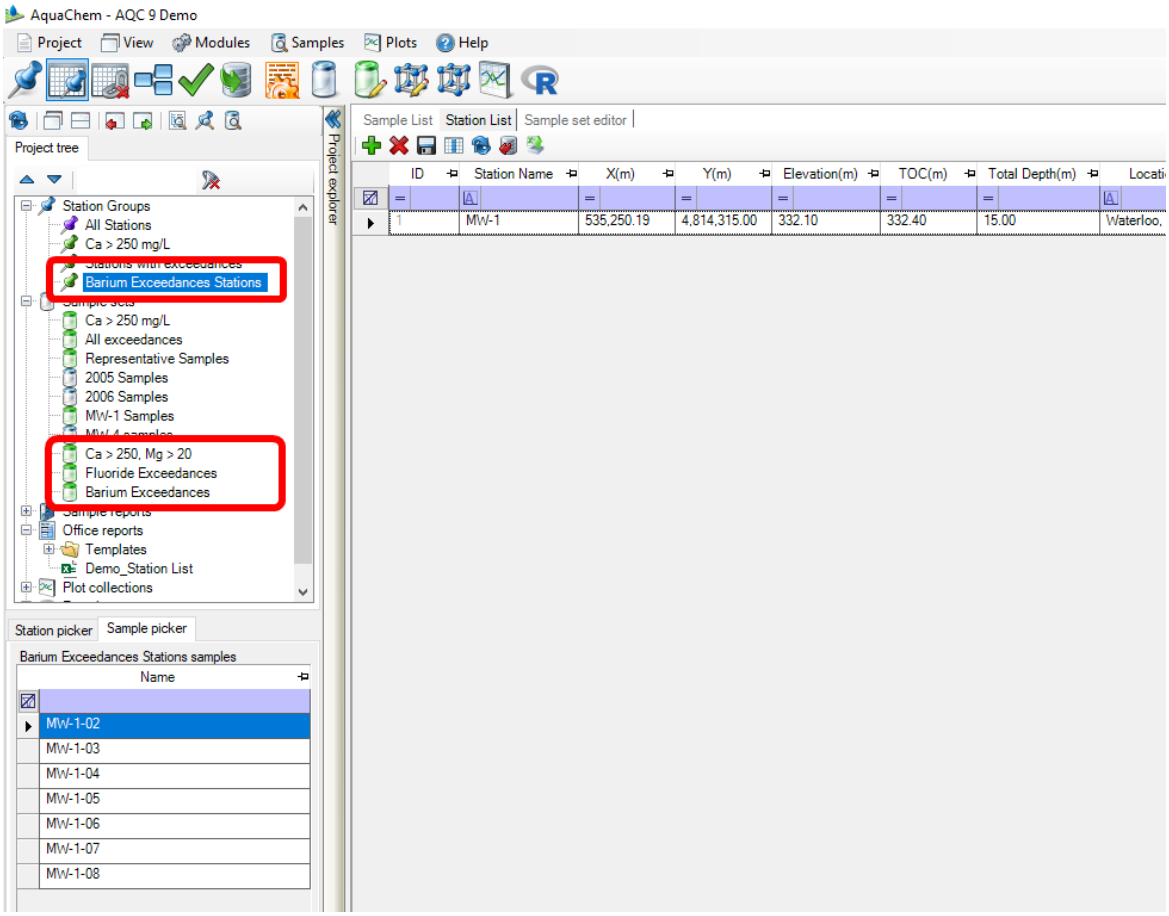
If we repeat this process for barium ('Ba') we should see a total of two exceedances, both at station MW-1:



Finally, let's create a dynamic station group based on the 'Barium Exceedances' sample set. Click the 'Create a dynamic station group' [ ] button in the toolbar and you will be prompted to name the new station group. Specify the name 'Barium Exceedances Stations', and then click OK:



At this point we should see all the new sample sets and station group in the Project Tree, and if we activate the 'Barium Exceedances Stations' station group, the Station List will be updated to show only station MW-1:



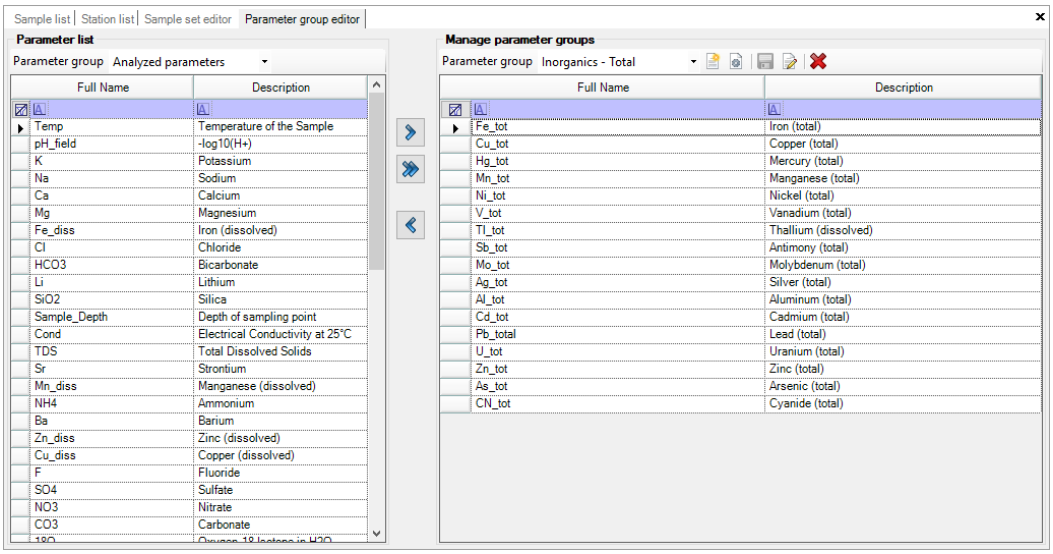
Please Note: that it is also possible to create 'Static' station groups and sample sets by simply selecting multiple stations/samples from the station/sample list, right-clicking them and selecting 'Add to new sample set' or 'Add to new station group', as the case may be. But please be aware that the contents of static station groups and sample sets are simply that, a static snapshot. These will not be updated unless you manually add new stations or samples, respectively.

This concludes the section on creating sample sets and station groups. In the next section we will discover how to create parameter groups using the Parameter Group Editor module.

2.1.2.3 Creating Parameter Groups

In this section, we will create a new parameter group for organic constituents, since there are lots of organic constituent exceedances of water quality standards within this project and having a defined parameter group will allow us to display/select these specific parameters more easily throughout the AquaChem interface.

To create a parameter group, first access the Parameter Group Editor module from the main menu ('**Modules > Parameter Group Editor**') or from the button on the Main Toolbar. When the Parameter Group Editor opens you should see the following window:

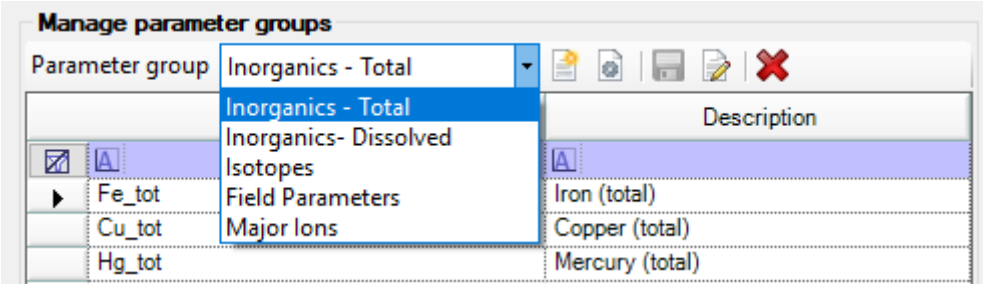


On the left side of the Parameter Group Editor module (under '**Parameter List**'), you will see a list of the parameters which are included in a number of default parameter groups which are part of every AquaChem project, along with any other user-defined parameter groups. If you open the 'Parameter group' menu item under '**Parameters List**', you should see the following groups:

- **Analyzed parameters** - a default parameter group which includes all project parameters which have records associated with them
- **Cations** - a default group including all parameters with a positive valency (defined in the Parameter Editor)
- **Anions** - a default group including all parameters with a negative valency (defined in the Parameter Editor)
- **Ions** - a default group including all parameters with any valency (as defined in the Parameter Editor)
- **Required** - a default group including all parameters required in calculated functions (e.g. sum of anions/cations, electroneutrality balance, etc.)
- **Used in standard** - a default group including all parameters listed in the active water quality standards
- **All measured parameters** - a default parameter group which includes all active project parameters (even if they do not have records associated with them)
- **Inorganics (total)** - a user-defined parameter group which includes all active total metal parameters
- **Inorganics (dissolved)** - a user-defined parameter group which includes all active dissolved metal parameters
- **Isotopes** - a user-defined parameter group which includes available isotopes (18O, 2H and 14C)
- **Field parameters** - a user-defined group including parameters commonly measured on-site/in the field (temperature, pH, Eh, conductivity, dissolved oxygen)

- **Major Ions** - a user-defined parameter group containing the major groundwater ions (K, Na, Ca, Mg, Cl, HCO3, F, SO4)

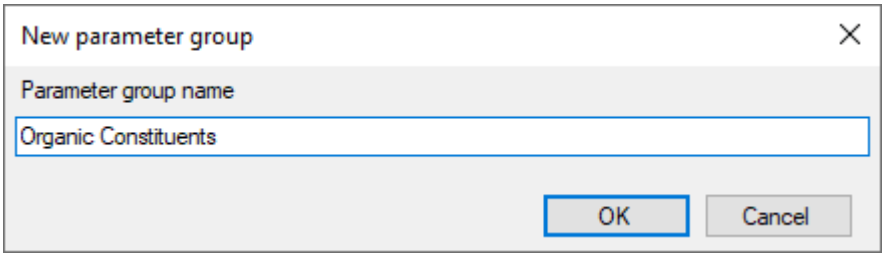
Please note that the **user-defined** parameter groups mentioned above are also listed on the right side of the Parameter Group Editor module, under the '**Manage parameter groups**' section:

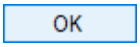


These user-defined parameter groups have been included specifically in the Demo Project for the purposes of demonstration, and will not be included automatically when a new project is created. However, as they are user-defined, it is quite easy to recreate them yourself. Let's review how user-defined groups can be created by creating one for the organic constituents included in this project. The new group will contain the following parameters:

- Benzene
- Ethylbenzene
- Trichloroethylene (TCE)
- Tetrachloroethylene (PCE)
- Toluene
- Xylene
- Vinyl Chloride

First, click the 'Create a new parameter group' [] button in the toolbar under the Manage parameter groups section. A window will appear allowing us to name the new parameter group; type 'Organic Constituents' into this window as shown below:

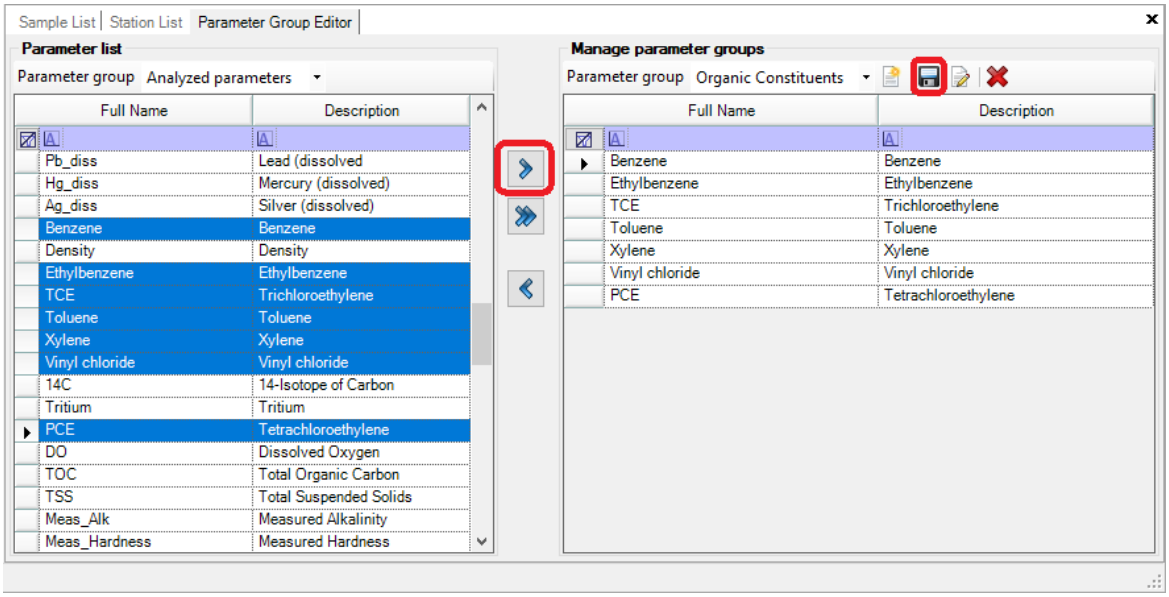


Click 

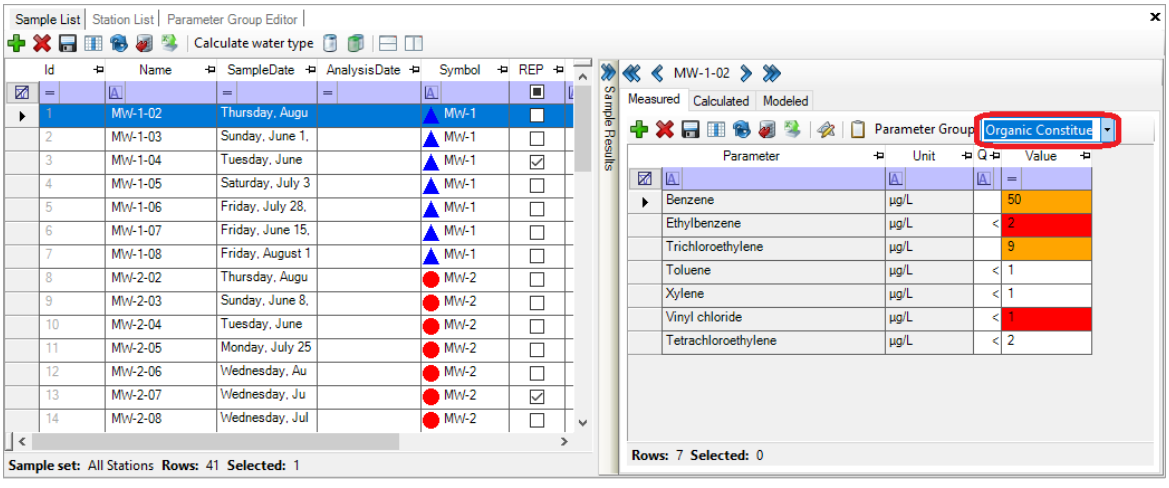
and the new parameter group will officially be created. However, the Organic Constituents group is currently empty and must be populated using parameters from the existing/default parameter groups.

Under the '**Parameter List**' section of the Parameter Group Editor module, select the 'Analyzed Parameters' group and scroll through the list until you find the necessary parameters. You can select them one at a time and then click the 'right' blue arrow button [ ] to add them to the 'Manage parameter groups' side of the interface. It's also possible to select several parameters at once by holding the <CTRL> button and selecting them, and these can all be added to the user defined parameter group at once using the blue arrow button. If you accidentally move any undesired parameters into the new Organic Constituents group, they can simply be removed by clicking the 'left' blue arrow button [ ].

Once all the organic constituents have been added to the new 'Organic Constituents' group, the Parameter Group Editor module should look like this:



To make this new parameter group available throughout the rest of the AquaChem interface you simply have to click the 'Save' [ ] button (highlighted above). Now you can return to the Sample Results tab and select the new parameter group using the menu in the Sample Results toolbar, and the results table will be updated to only display the associated parameters:



User-defined parameter groups can be used with many other features throughout AquaChem to more quickly and easily find and display parameters that you are interested in.

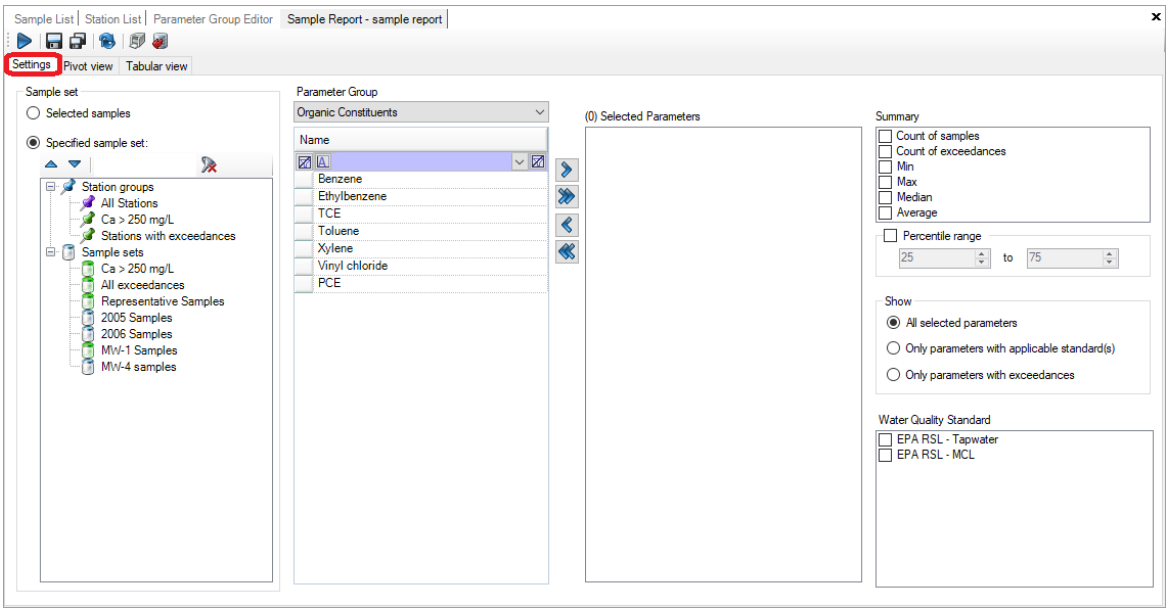
For example, in the next section of the tutorial, we will explore the Sample Reports module and we can make use of this newly defined parameter group to efficiently build the report specifically for these organic constituents.

2.1.3 Creating Sample Reports

The Sample Report Module allows you to create custom tabulations of your samples and their results based on one or more criteria including: station/sample sets, specific parameters or groups, and/or exceedances of one or more active Water Quality Standards. The report can also produce general statistics for samples included in the report.

To demonstrate the power of the Sample Report module, you can build a simple report based on the Organic Constituents parameter group which was created in the previous section. Please note that if you have skipped ahead to this section and have not created the Organic Constituents parameter group you can still build this report by selecting the desired parameters from the Analyzed Parameters group.

To begin, open the Sample Report module by clicking '**Samples > Sample reports**' from the main menu. The Sample Report module will open, specifically on the settings tab as shown below:



As you might expect, the Sample Report module includes a number of toolbar buttons which allow you to 'Execute' [▶] or create a report based on the current settings, 'Save' [💾] the existing report to the Project Tree , 'Save as...' [💾] which allows you to create a new sample

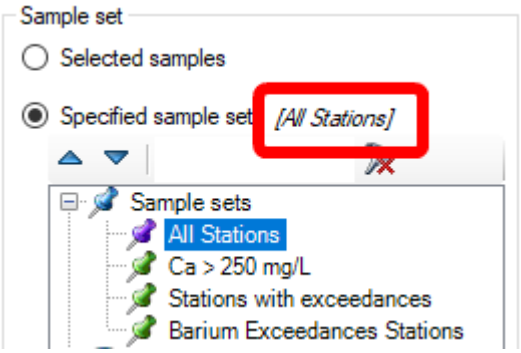
report based on the current settings, 'Refresh' [] the module, 'Print preview' [] and of course 'Export' [] the resulting sample reports.

The initial tab which is displayed in the Sample Report module is the 'Settings' tab, which allows you to specify the building blocks of the desired report. At this stage you can select which samples or sample sets and parameters will form the basis for the report. You can also specify if any summary statistics should be included in the report, and whether the report should display all results or whether the results should be limited to records with applicable standards and/or exceedances.

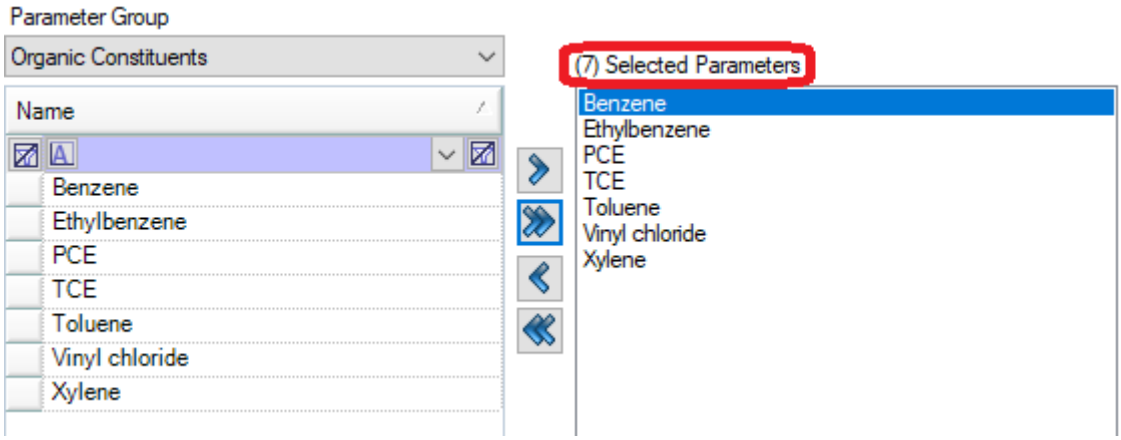
The first step in defining the sample report is to specify which samples or sample sets will be included in the report. This information is specified in the 'Sample set' frame on the left side of the Sample Report module. Two options are available:

1. **Selected samples** - this option will restrict the sample report to the samples which are currently selected in the Sample picker tab
2. **Specified sample set** - this option will restrict the sample report to the specific sample set or station group/set selected in the available table

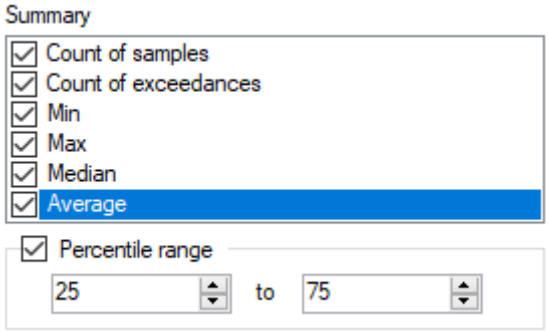
In this example, we would like to create a sample report for organic constituents across the entire project, therefore you should click the 'All Stations' sample set in the table. Once this group is selected it will be listed next to the 'Specified sample set' radial button, as shown below:



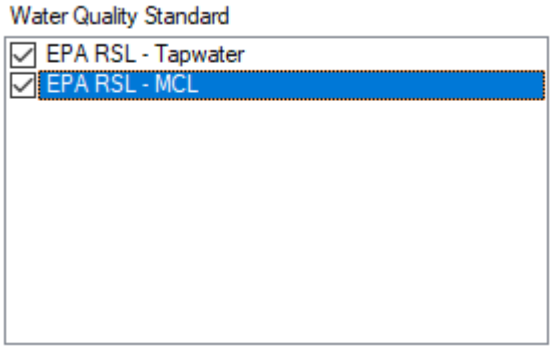
The second step in defining the sample report is to specify which parameters will be included in the report. Since the 'Organic Constituents' parameter group was the last parameter group which was used within this project, it has already been selected in the Parameter Group menu. To select all seven parameters in this group simply click the double-right arrow button [], or you can select them all individually using the single arrow buttons. Once the parameters have been selected they should all appear in the menu to the right of the arrows, and it should list '(7) Selected Parameters' as shown below:



The third step in defining the sample report is to select which summary statistics should be included. For this example simply activate all the available statistics, and also activate the percentile range option as shown below:

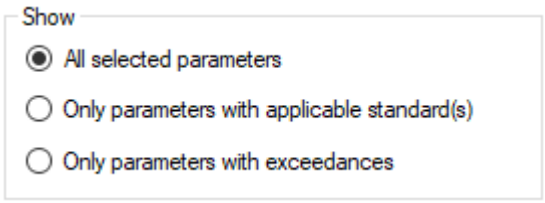


Since the 'Count of exceedances' option is active, it is also necessary to specify which water quality standards will be used for this comparison. Use the checkboxes in the 'Water Quality Standard' frame to activate both 'EPA RSL - Tapwater' and 'EPA RSL - MCL', as shown below:

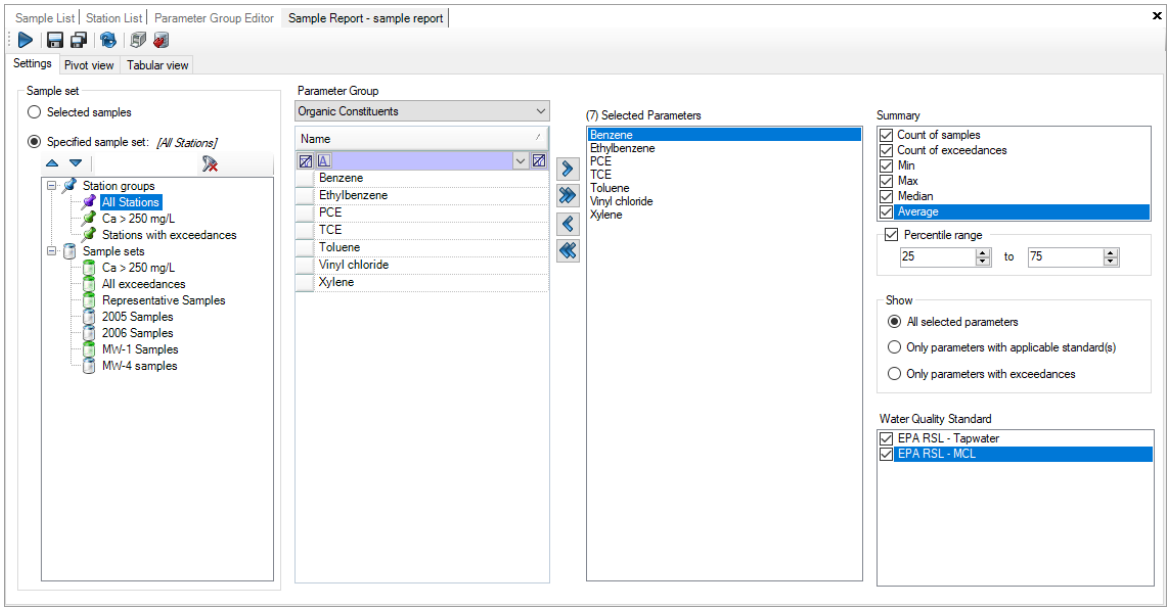


In some cases, you may be interested particularly in parameter records which represent exceedances, or specific parameters which have applicable standards. These options can

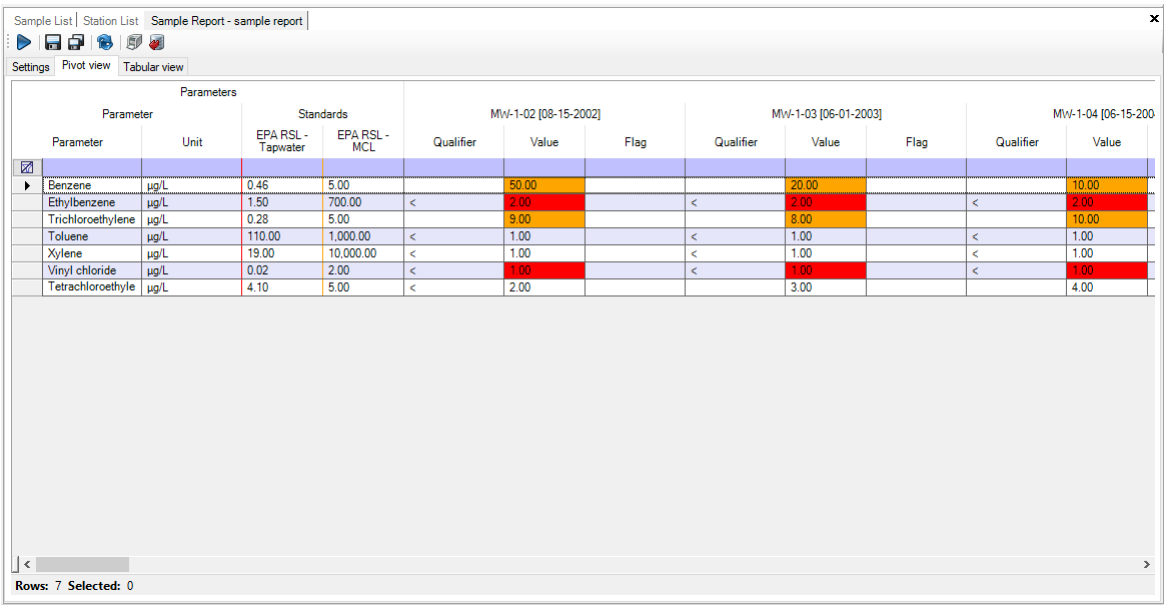
be selected using the radial buttons in the 'Show' frame, but in this case you can simply leave the default 'All selected parameters' option, as shown below:



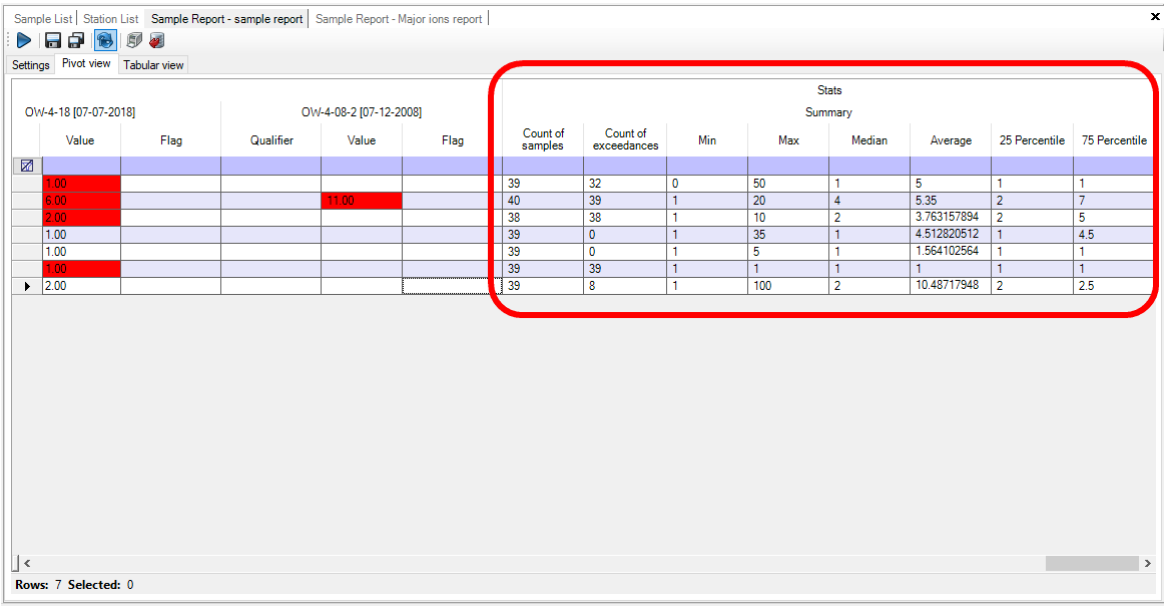
Once all these report settings have been specified, the settings tab should look like this:



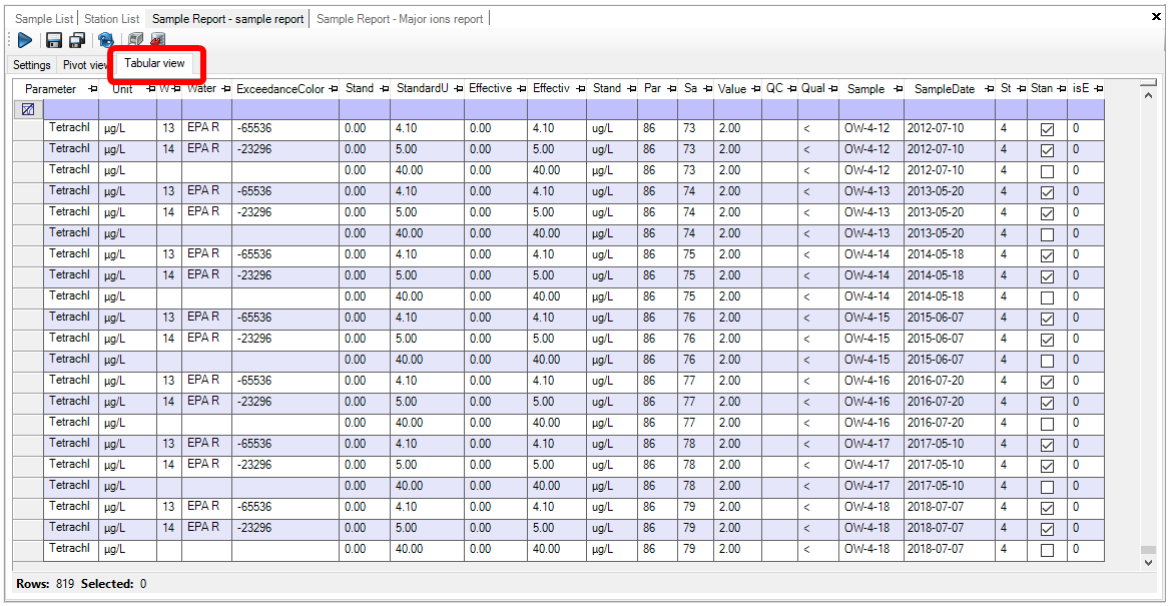
Click the **'Execute'** [▶] button to generate the report, which should be displayed automatically in the 'Pivot view' tab. Note how exceedances are highlighted automatically using the color associated with each water quality standard (these colors - and other water quality standard settings - can be customized in the Water Quality Standard module, available through the 'Samples' menu):



If you scroll to the far right side of the report you will be able to review the summary statistics:



If you access the 'Tabular View' tab you will be able to review the results as a 'flat' table, where each individual record is presented in its own row with additional metadata. However, the tabular view tab does not include summary statistics:



Parameter	Unit	W-B	Water	ExceedanceColor	Stand	StandardU	Effective	Effectiv	Stand	Par	Sa	Value	QC	Qual	Sample	SampleDate	St	Stan	isE
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	73	2.00		<	OW-4-12	2012-07-10	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	73	2.00		<	OW-4-12	2012-07-10	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	73	2.00		<	OW-4-12	2012-07-10	4	☐	0
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	74	2.00		<	OW-4-13	2013-05-20	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	74	2.00		<	OW-4-13	2013-05-20	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	74	2.00		<	OW-4-13	2013-05-20	4	☐	0
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	75	2.00		<	OW-4-14	2014-05-18	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	75	2.00		<	OW-4-14	2014-05-18	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	75	2.00		<	OW-4-14	2014-05-18	4	☐	0
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	76	2.00		<	OW-4-15	2015-06-07	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	76	2.00		<	OW-4-15	2015-06-07	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	76	2.00		<	OW-4-15	2015-06-07	4	☐	0
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	77	2.00		<	OW-4-16	2016-07-20	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	77	2.00		<	OW-4-16	2016-07-20	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	77	2.00		<	OW-4-16	2016-07-20	4	☐	0
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	78	2.00		<	OW-4-17	2017-05-10	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	78	2.00		<	OW-4-17	2017-05-10	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	78	2.00		<	OW-4-17	2017-05-10	4	☐	0
Tetrachl	µg/L	13	EPA R	-65536	0.00	4.10	0.00	4.10	ug/L	86	79	2.00		<	OW-4-18	2018-07-07	4	☑	0
Tetrachl	µg/L	14	EPA R	-23296	0.00	5.00	0.00	5.00	ug/L	86	79	2.00		<	OW-4-18	2018-07-07	4	☑	0
Tetrachl	µg/L				0.00	40.00	0.00	40.00	µg/L	86	79	2.00		<	OW-4-18	2018-07-07	4	☐	0

Both of these tabs can be exported to Microsoft Excel using the 'Export' [ ] button. Be sure to save the sample report by clicking the 'Save' [ ] button. A window will appear allowing you to name the new report (e.g. 'Organic Exceedance Report'). Once the report is saved, you will be prompted if you would like to open the report.

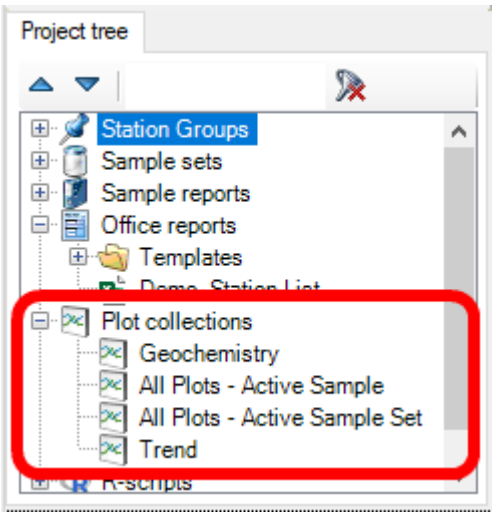
This concludes the introduction to sample reports. In the next section of the tutorial, you will review how to access, edit, and create new plot collections.

2.1.4 Creating Plot Collections

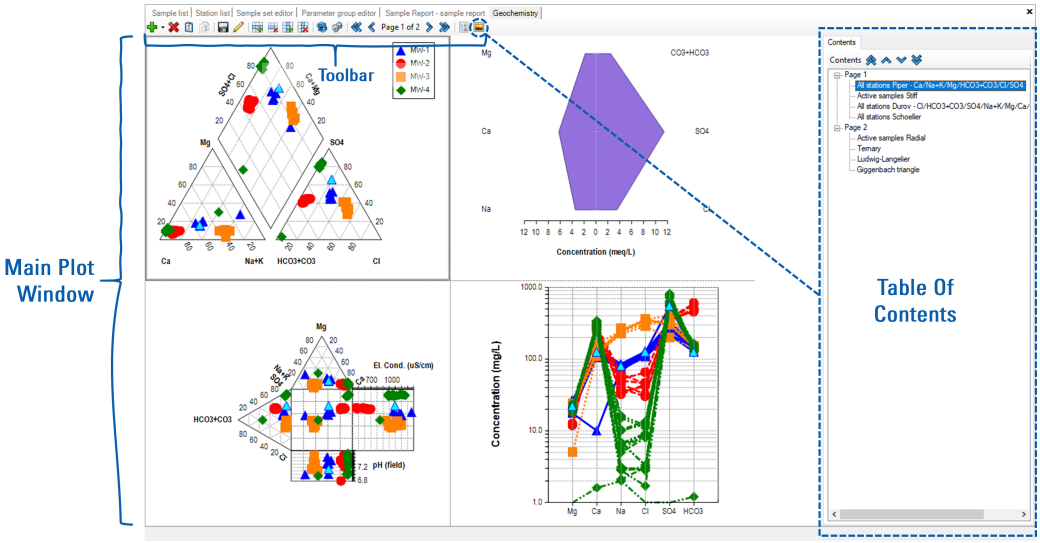
The Plot Collection Module provides the ability to generate a wide range of water quality plot types, which can be organized into plot collections consisting of one or more individual plots. In all, there are nineteen plot types supported in AquaChem. Plot collections can be configured and saved in the Project Tree so that you can quickly build and reproduce standard reports.

In this section, you will first review an existing plot collection which is already built into the Demo Project and explore how to edit/customize the plot collection. In the final section you will review the use of symbol groups within an AquaChem project, and create a new symbol group based on the 'Watertype' sample data field.

The AquaChem Demo Project comes with several pre-existing plot collections which you can easily review by simply double-clicking them from the Project Tree:



Double-click the 'Geochemistry' plot collection, and it will open in a new tab within the main workspace, as shown below:



Please Note: to see the same results as the image above, make sure to reactivate the 'All Stations' station group, which corresponds to the 'All Stations samples' sample group. Most of the plots within the Geochemistry plot collection are based on the active sample group, and in the images above are based on 'All Stations'.

The plot collection interface has three main components:

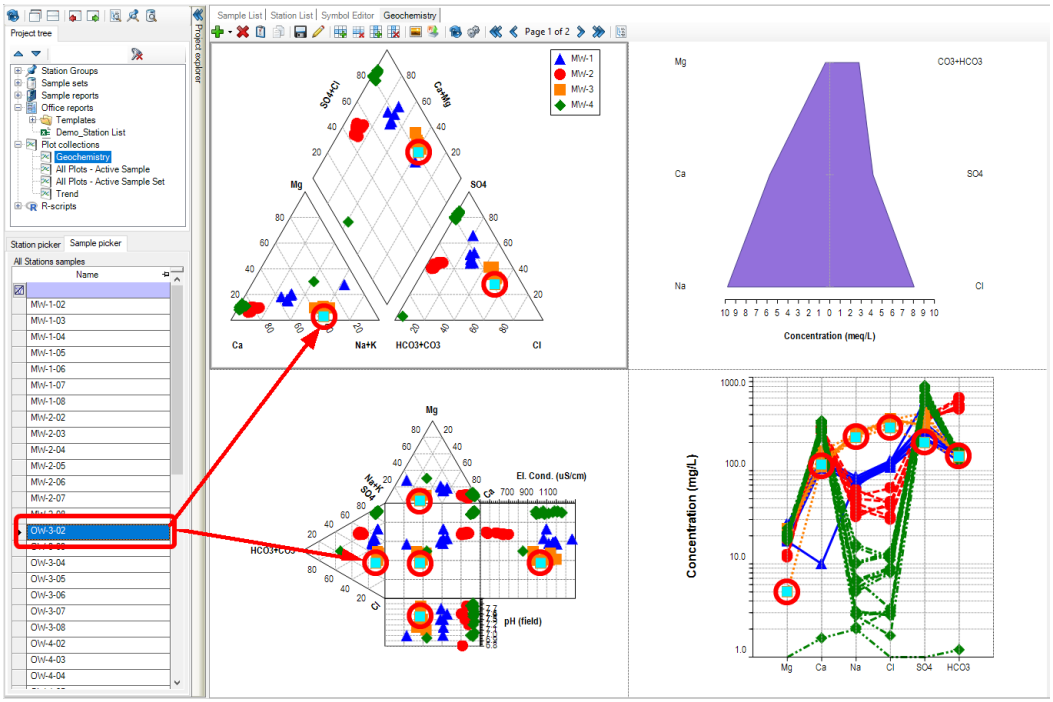
1. **A toolbar** which includes buttons to add/delete plots, save/rename plot collections, add/remove rows/columns for displaying plots, export options, and navigation arrows which allow you to move to different plot collection pages. All plot collection toolbar buttons are explained in further detail in the Plot Collections section of the user manual.

2. **The main plot window** which displays plots which have been added to the current plot collection. Page 1 of the Geochemistry plot collection displays a Piper, Stiff, Durov, and Schoeller plots, while page 2 includes a Radial, Ternary, Ludwig-Langelier, and Giggenbach triangle plots.
3. **A table of contents** which displays a list of the plots that belong to the collection. The functionality of the table of contents is outlined in detail in the Plot Collections section of the user manual.

As you can see, the 'Geochemistry' plot collections contains eight individual plots distributed over two pages (i.e. four plots per page). All of the plots contained within plot collections are dynamically linked to each other and the Sample Picker tab. In the image above you may notice that some of the symbols are highlighted with a light-blue color (■). These highlighted symbols represent the currently selected sample from the Sample Picker (i.e. sample 'MW-1-02'). If you click a different sample within the Sample Picker, the associated sample point in each plot will be highlighted. In a similar manner, the Stiff plot will be updated to reflect the results of the currently selected sample.

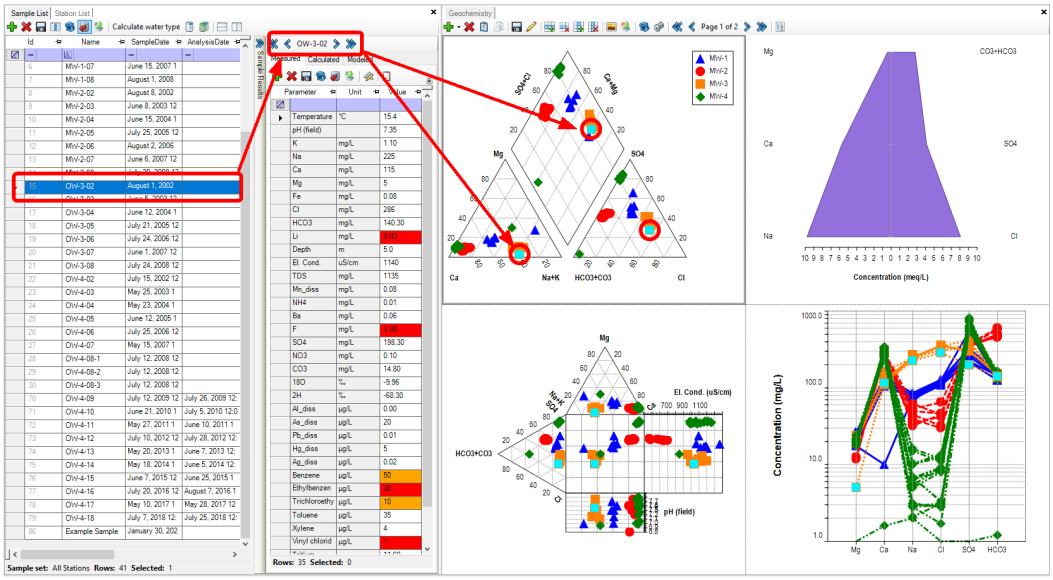
To illustrate, use the Sample picker to select sample 'OW-3-02', which is a sample from station 'MW-3'. You should see the associated symbol (i.e. one of the orange squares) highlighted in the light-blue color and the Stiff plot will be updated to reflect the composition of sample OW-3-02. This is an extremely handy feature which allows you to easily interpret your water quality data by dynamically highlighting selected samples.

Please Note: you can customize the style of selected samples by clicking the project plot settings [⚙] button in the toolbar.

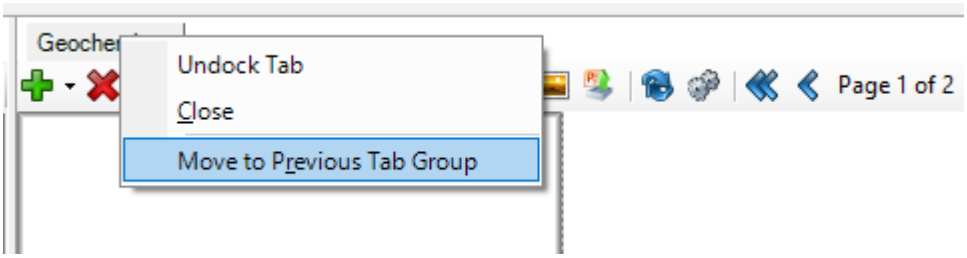


These dynamic links also extend to other portions of the AquaChem interface, such as the Sample Picker, Sample List, and Sample Details tabs. In the image below, the Geochemistry

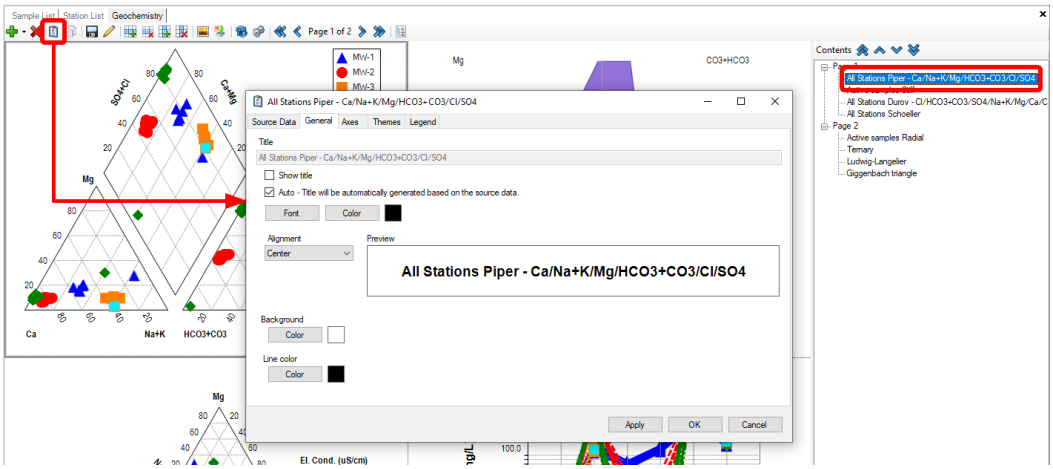
plot collection has been displayed in a new vertical tab group (by right-clicking the 'Geochemistry' tab and selecting 'New Vertical Tab Group'), which allows you to review individual sample results alongside the geochemistry plot collection. If you have multiple monitors, you can also click and drag the Geochemistry plot collection tab to another monitor. Note that the Table of Contents and Project Tree have been hidden in this image so that it isn't too cluttered:



You can return the Geochemistry plot collection to the original tab group by right-clicking and selecting 'Move to Previous Tab Group', as shown below:

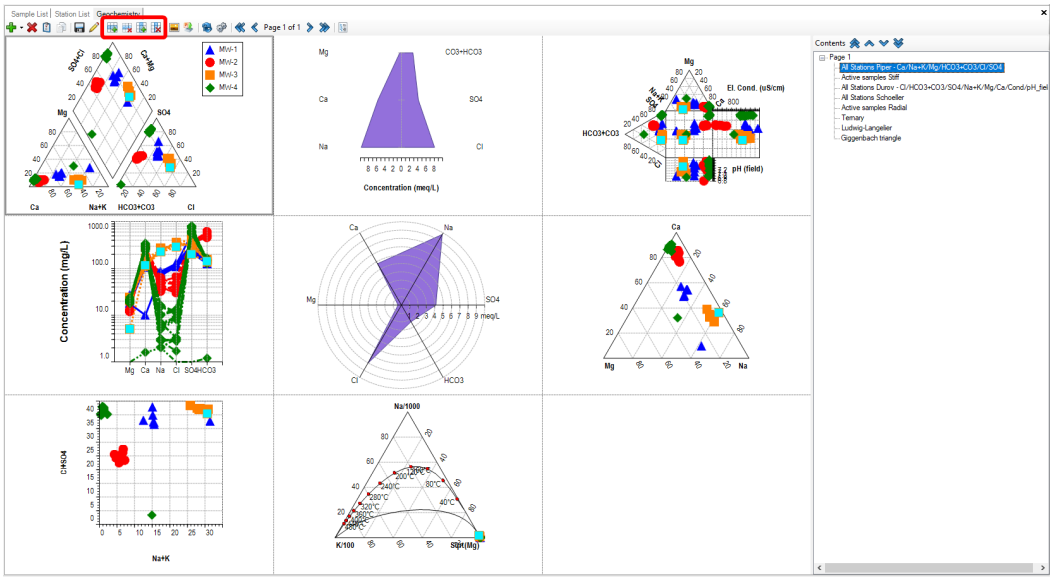


When reviewing plot collections, you can access the settings for individual plots by right-clicking anywhere in the desired plot frame, or you can select the desired plot by left-clicking, and then click the **'Plot Settings'** [] button in the toolbar (Note: the currently selected plot will be highlighted in the Table of Contents, and the frame/window around the selected plot will have a grey outline). The plot settings window will then appear as shown below, allowing you to customize all aspects of the selected plot:



Plot settings vary depending on the individual plot type and won't be covered in detail within this tutorial, but you can find more information in the Plot Module section of this user manual. There you can find information on common plot features, as well as information regarding plot settings which are unique to specific plot types.

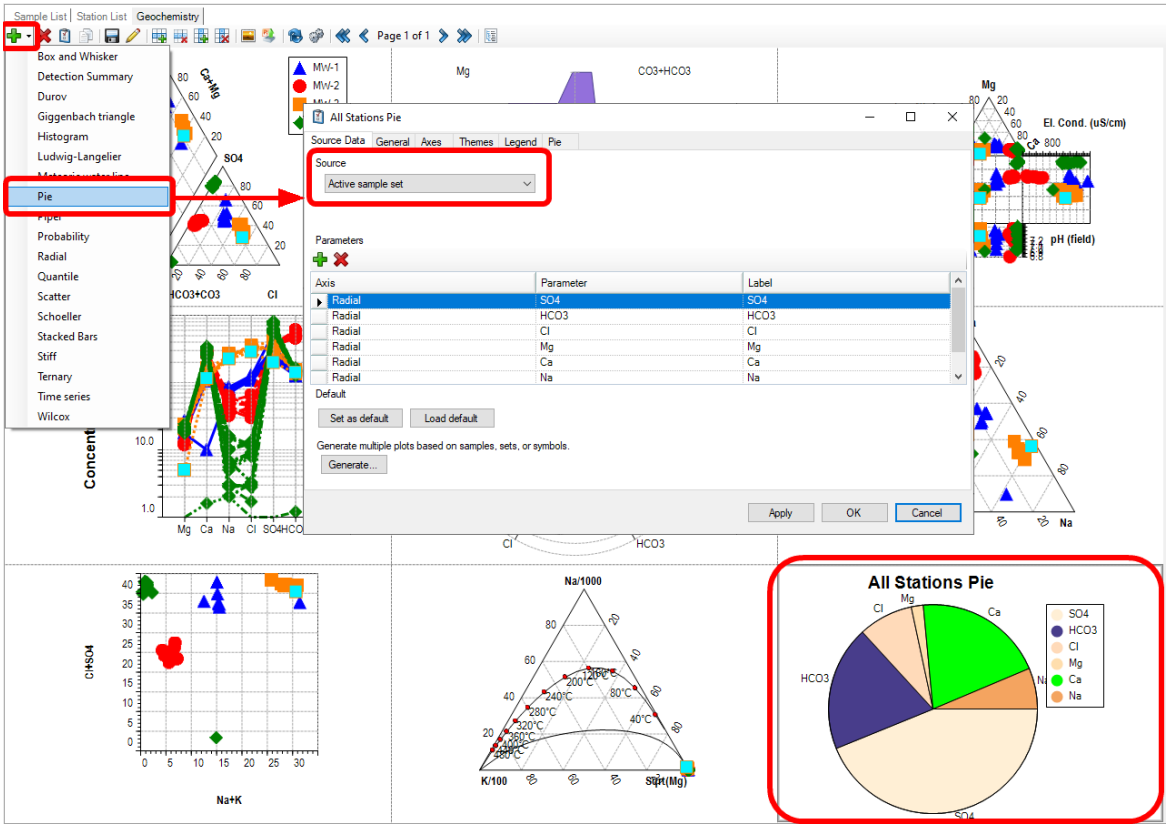
The overall structure of the plot collection can be customized using the **'Add/Remove Row/Column'** buttons in the toolbar []. If you add a new row [] and a new column [] you should see a 3x3 plot collection, which leaves us space for one additional plot:



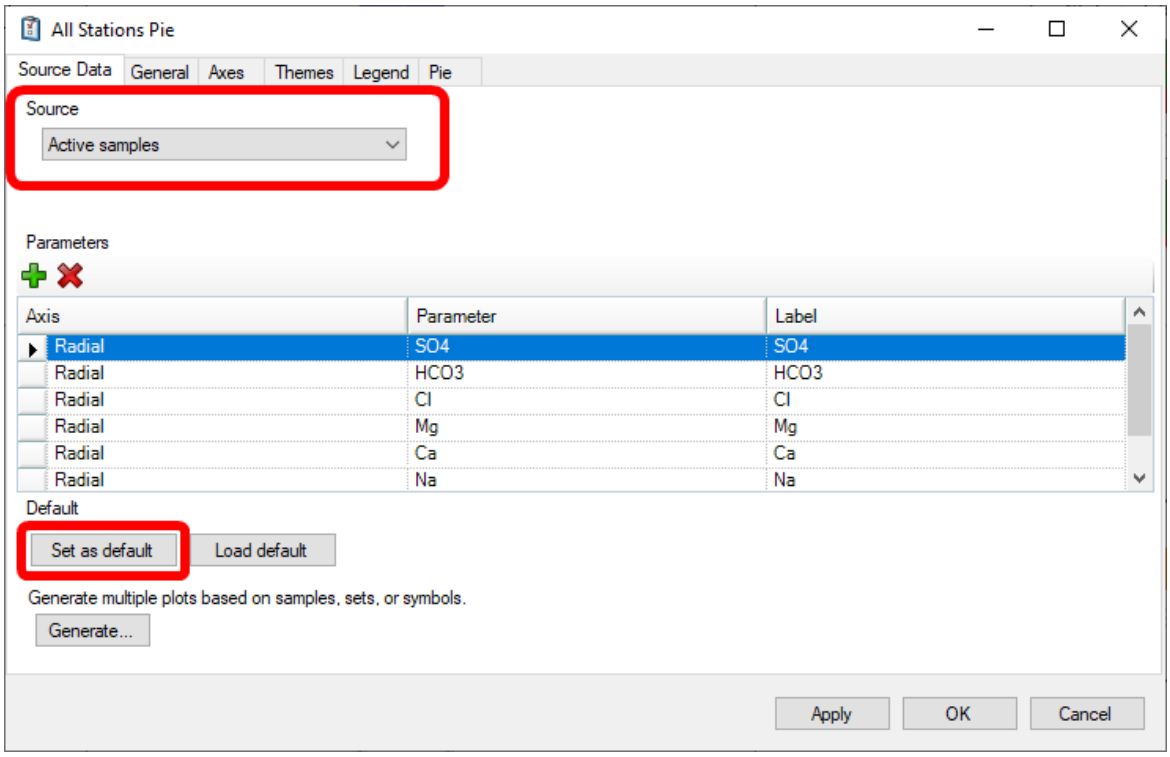
Individual plots can be added and removed from the plot collection using the **'Add plot'** [] and **'Remove plot'** [] buttons. Let's add a pie chart to this plot collection, with the source data based on the current active sample. Most of the plots within the 'Geochemistry' plot collection are based on the active sample group (i.e. the 'All Stations samples' group), but

some plot types (e.g. Stiff, Radial and Pie charts) should typically be based on a single sample.

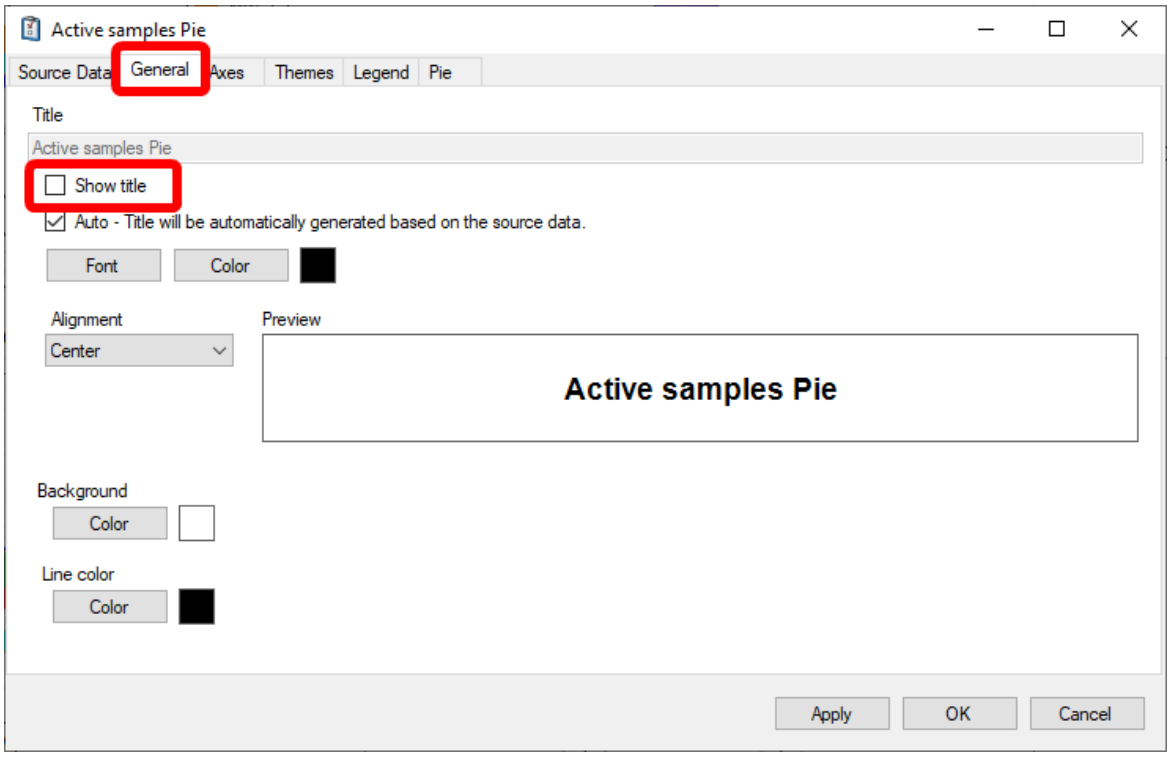
When you click the **'Add plot'** [ ] button, a menu will appear which displays all the available plot types. Select **'Pie'** as shown below, and the Pie chart will be added to the plot collection and the associated plot settings window will appear:



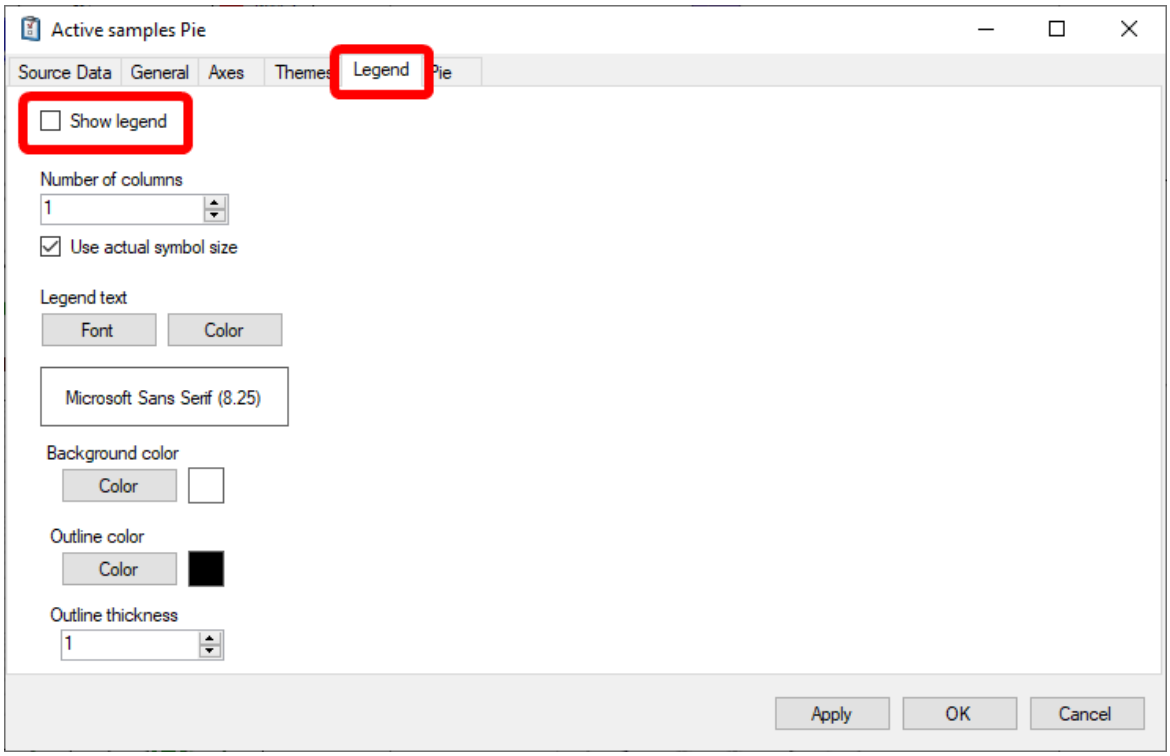
By default the 'Source Data' setting for the new plot will be based on the 'Active sample set', as highlighted in the image above. Change the 'Source' to 'Active Samples', click 'Apply', and then click the 'Set as default' button. This ensures that future pie charts will be automatically based on the 'Active samples' source data, instead of the 'Active sample set' (note: you will be making additional changes, so it would be ideal to return to the 'Source Data' tab and click the 'Set as default' button once again after all the desired changes have been applied):



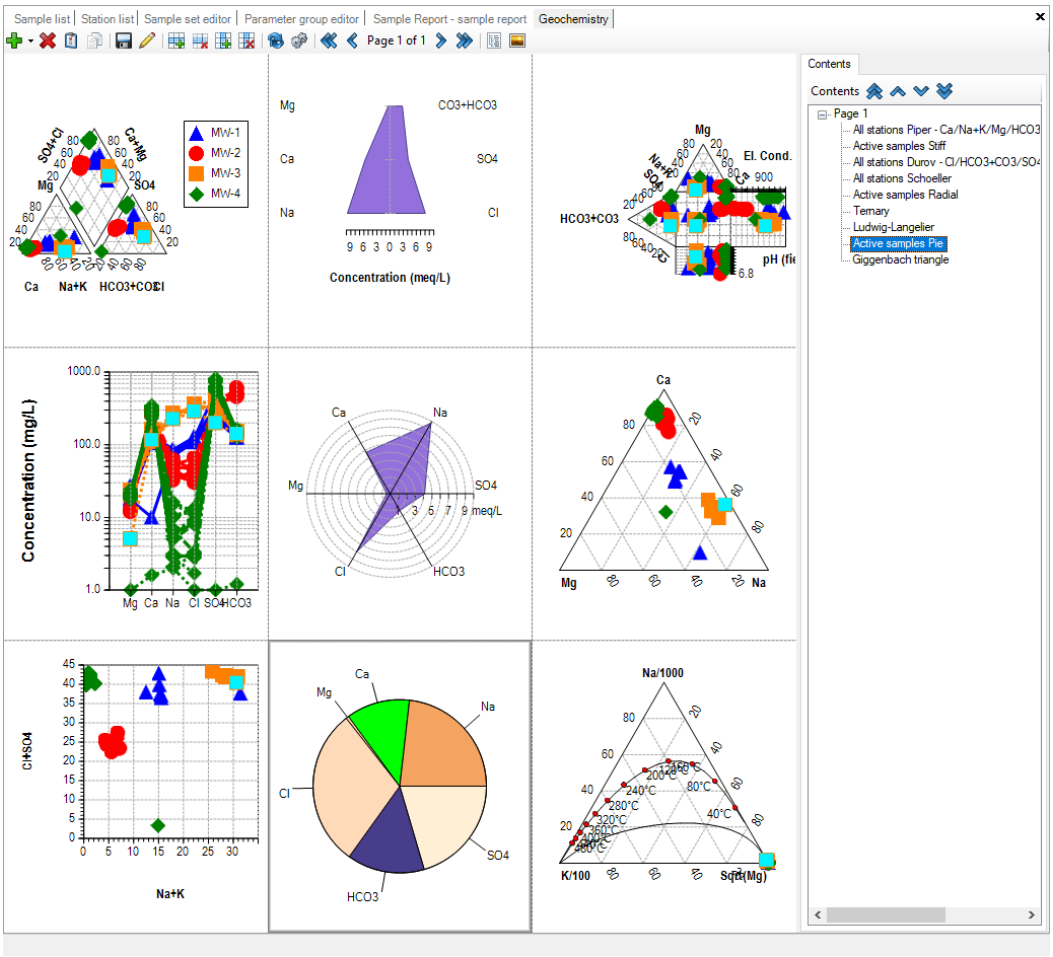
After updating the source data for the pie chart you may want to update some of the other settings to better match the rest of the plot collection. For this example you will remove the plot title by accessing the 'General' tab and unchecking the 'Show title' checkbox:



You can also remove the legend (since each slice is already labeled) by accessing the 'Legends' tab and and unchecking the 'Show legend' checkbox:



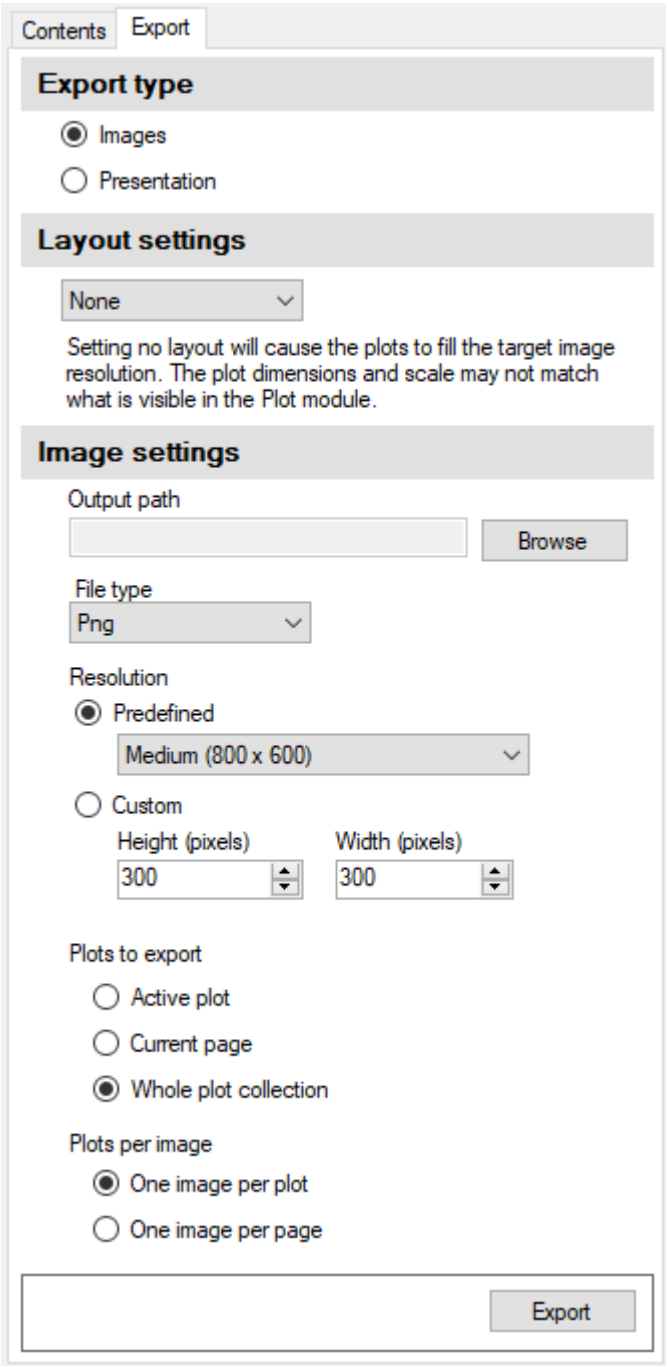
When these changes have been made simply click the OK button to apply the changes. You may also be interested in changing the order that these plots appear within the plot collection. You can rearrange the order of the plots using the up/down arrow buttons in the Table of Contents tab (highlighted in the image below). Assuming that the 'Active samples pie' chart is currently selected, click the 'Move plot up' [^] button to swap the pie chart and Giggenbach triangle. The updated plot collection should now look like the image below (assuming that sample OW-3-02 is still selected):



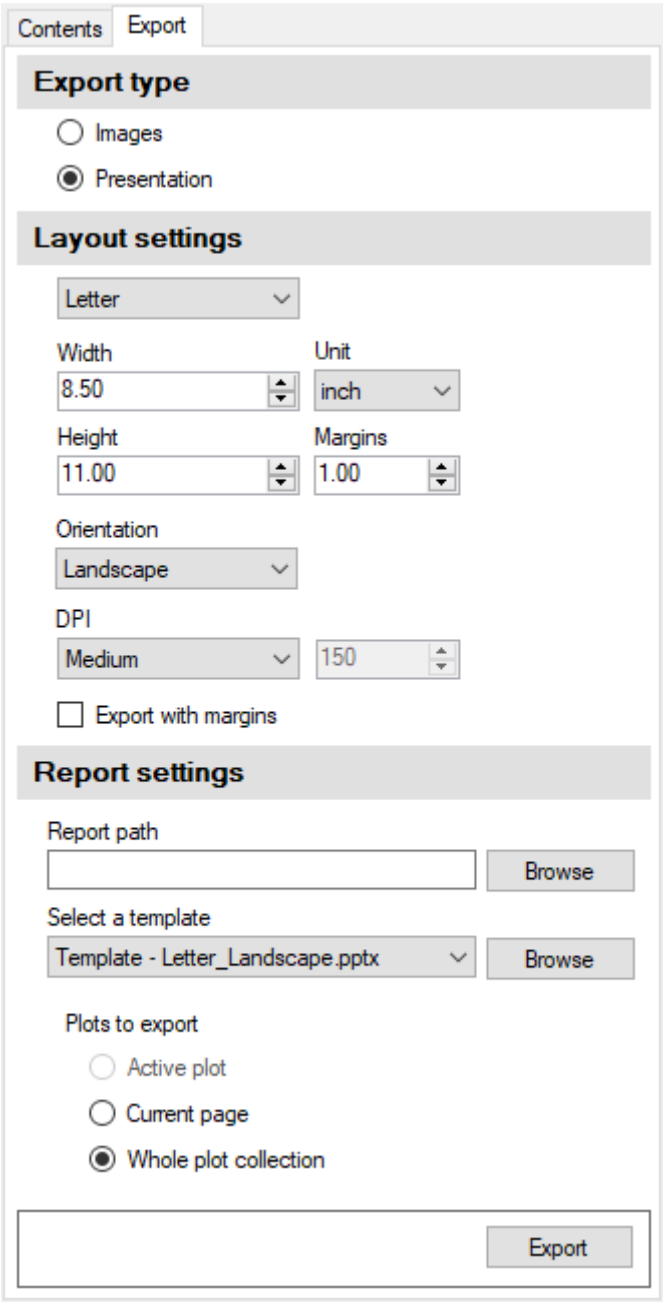
Now that you have made the desired changes you can click the **'Save plot configuration'** [ ] button in the toolbar. When you close/reopen the plot collection or project all these changes will be retained.

You may want to test exporting the plot collection as images or to a print-ready Microsoft PowerPoint template (using the **'Print to PowerPoint...'** [ ] button). This opens the Export Tab, which also includes a scaled preview of the plots based on a selected layout.

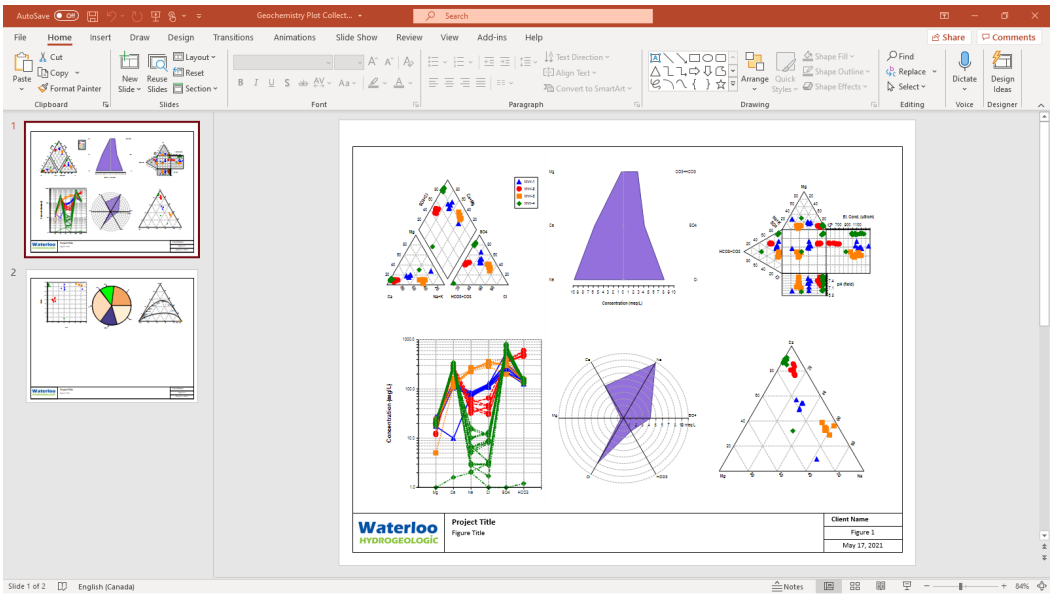
If you select the Images option, the Export tab will provide options that allow you to select a layout size and export any or all plots in a 'One image per plot' or 'One image per page' format. You can also select from *.PNG, *.BMP, *.JPG or *.EMF file formats, and specify the desired resolution. Select the "Letter" layout with a "Landscape" orientation. Click the Browse... button to select the output location, and then click Export and all the plots will be exported as images.



If you select Presentation, the following Export Tab will allows you to export any or all plots in a 'One image per plot' or 'One image per page' format. You can select from a number of print-ready templates using the 'Select a template' menu (note: you can customize the print-ready templates by double-clicking them in the Project Tree, making the desired changes within the applicable Microsoft application and then saving. Any changes you make within the template will be applied to the printed reports/plot collections/etc.). To export the plot collection to a PowerPoint template simply select from the available templates, click the 'Browse' button to save an output location and click Export.



After exporting the plot collection to PowerPoint (using the 'Whole plot collection' setting), PowerPoint will open with a presentation similar to the following:

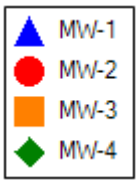


At this point, you may be interested in creating a plot collection of your own. To do so, simply click **'Plots > New plot collection'** from the main menu. A new plot collection tab will open which at first will be empty. Simply add as many new plots to the collection as desired and organize it however you like using the same techniques that we have just discussed.

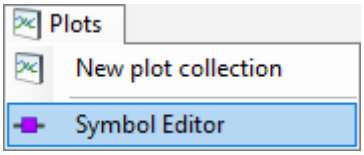
In the next section, we'll discover how to work with Symbol Groups.

2.1.4.1 Create Symbol Groups

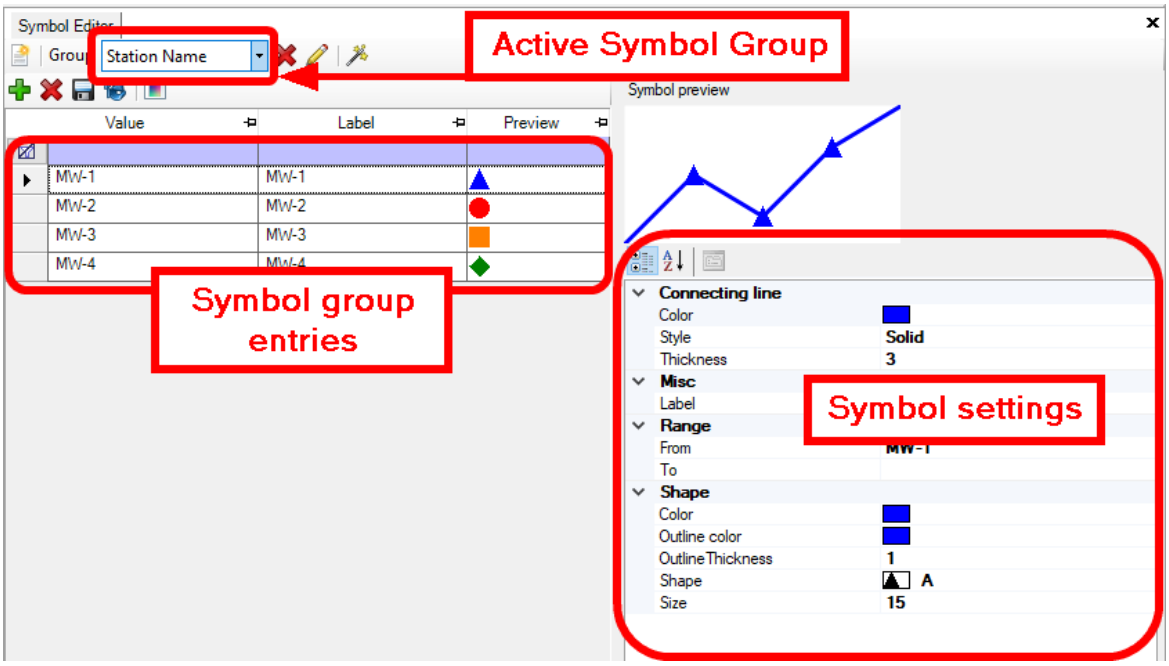
In the AquaChem Demo Project, the default symbols used in plot collections reflect the station ID (i.e. there is a unique symbol for each station). This is shown within the Geochemistry plot collection, you should notice the following legend appear next to the Piper plot:



You can update and customize the symbols used within your projects using the [ ] Symbol Editor Module, which can be accessed by clicking **'Plots > Symbol Editor'** from the main menu:

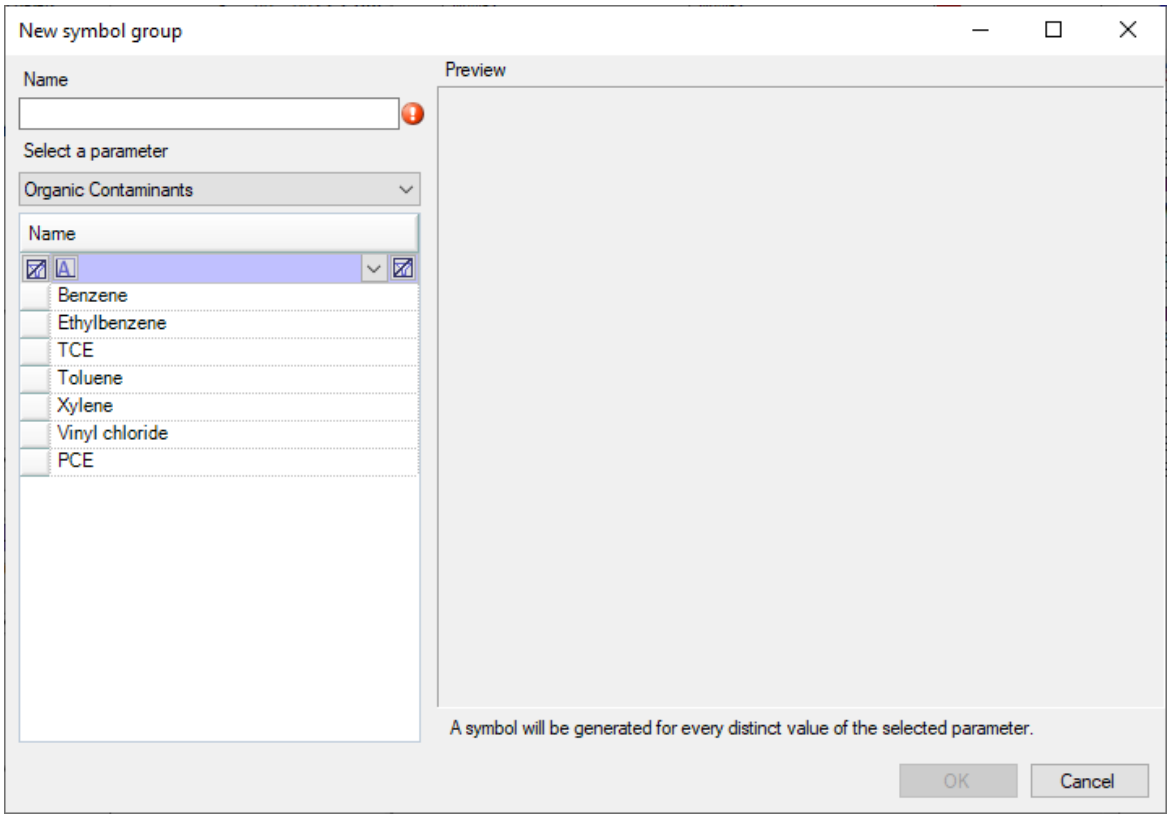


When the Symbol Editor module opens, it will initially display the currently selected/active symbol group, which in the case of the AquaChem Demo Project would be the 'Station Name' symbol group. The entries associated with this group are displayed in the table on the left, and the display settings for the currently selected symbol (MW-1 in the image below) are displayed on the right:

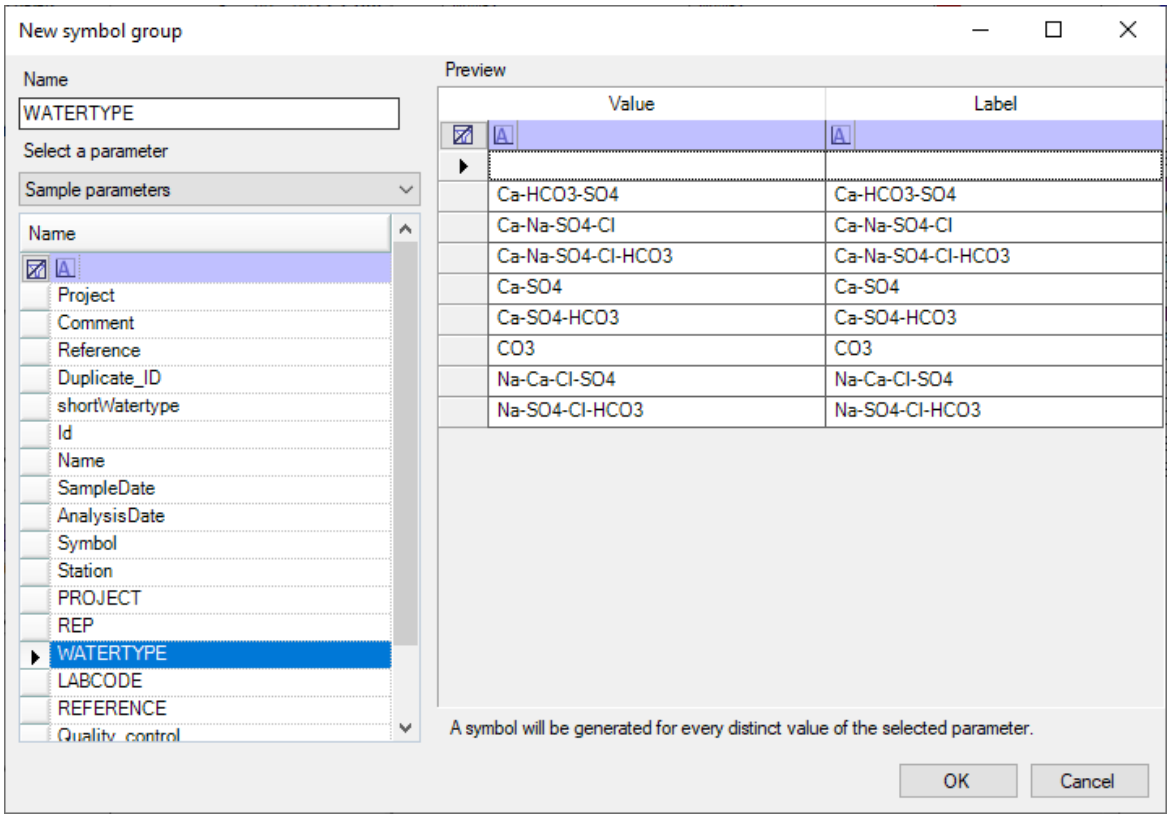


Let's test out creating a new symbol group based on the 'Watertype' data field.

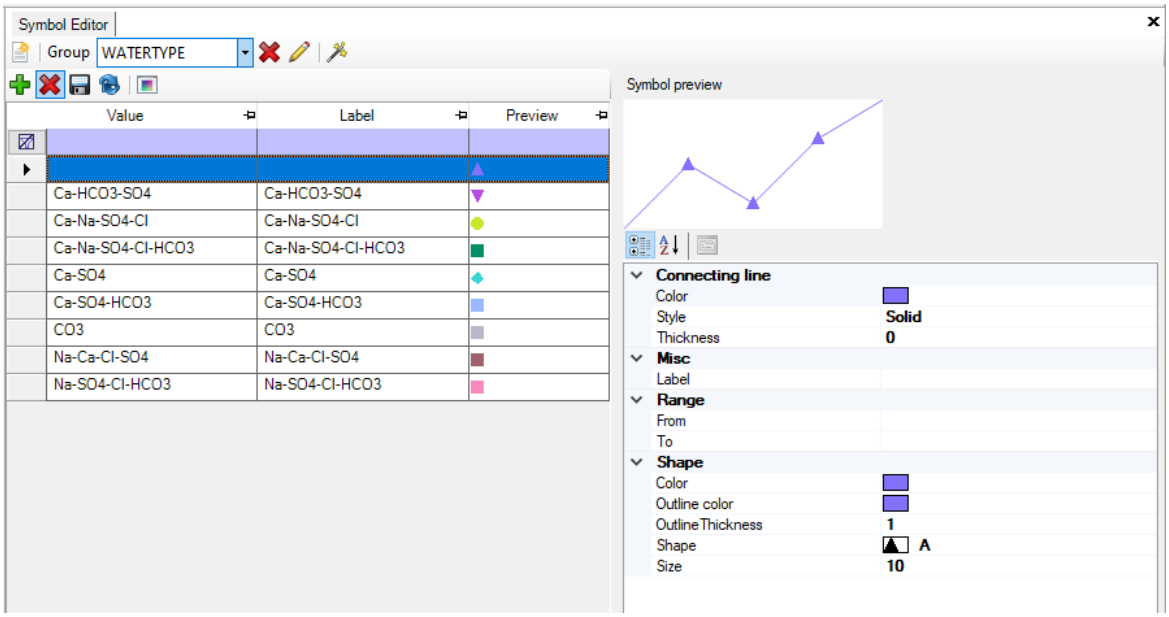
To create a new symbol group click the **'New group'** [] button in the toolbar and the **'New symbol group'** window will open, as shown below:



The first thing to do in the 'New symbol group' window is to select from the available database fields. Entries for the new symbol group will be generated automatically for all unique values within the selected database field. To do this, first use the menu under 'Select a parameter' to choose the 'Sample parameters' group, and then select 'WATERTYPE' from the list of parameters. You should see the 'Name' of the symbol group updated automatically to 'WATERTYPE' and a list of values for each distinct value within the selected database field, as shown below:



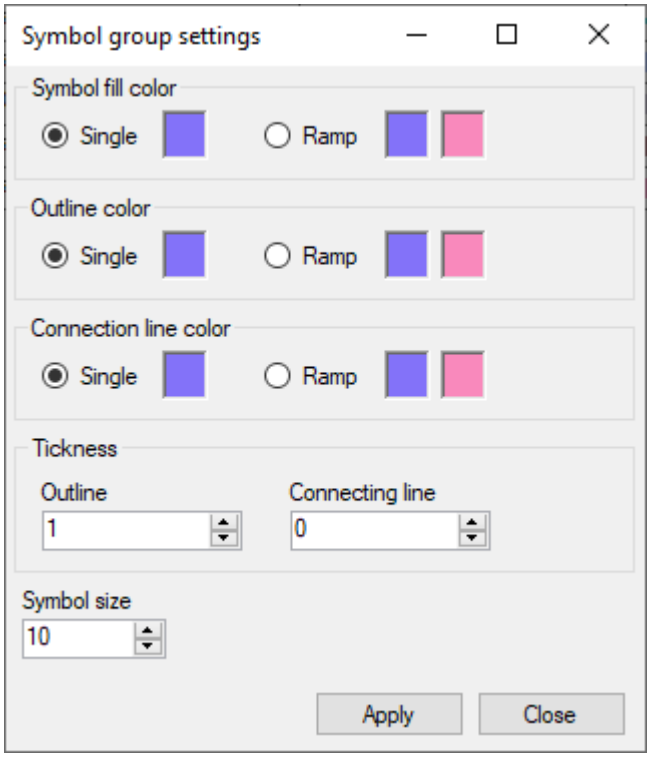
Click OK and this list of symbols will be added into the symbol editor module with default symbol settings (note that your symbols will look different as the symbols are randomly generated):



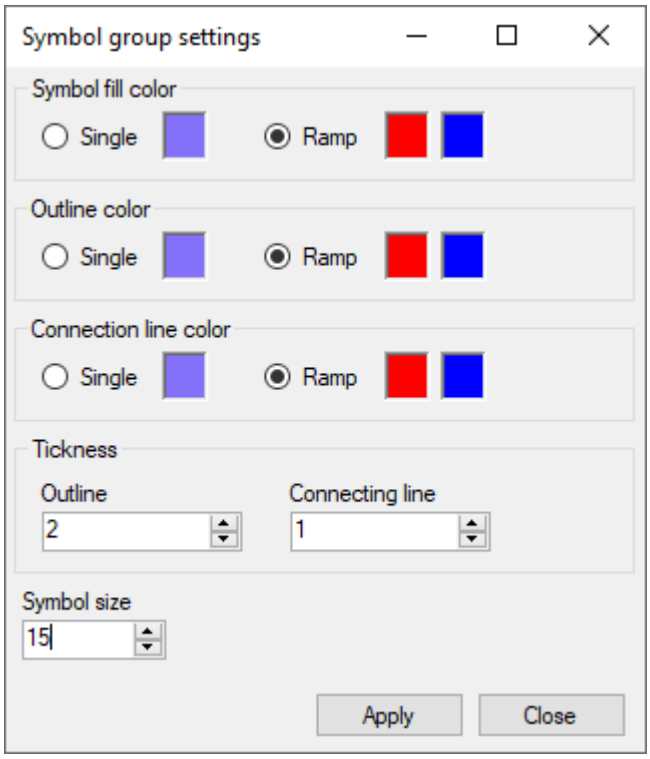
Please Note: there is also a symbol group with an 'empty' value, since earlier we manually added an 'Example Sample' without any actual calculated water type. You **must** delete this empty symbol by clicking the 'Delete Symbol' [] button in the toolbar.

Click the 'Save changes' [] button.

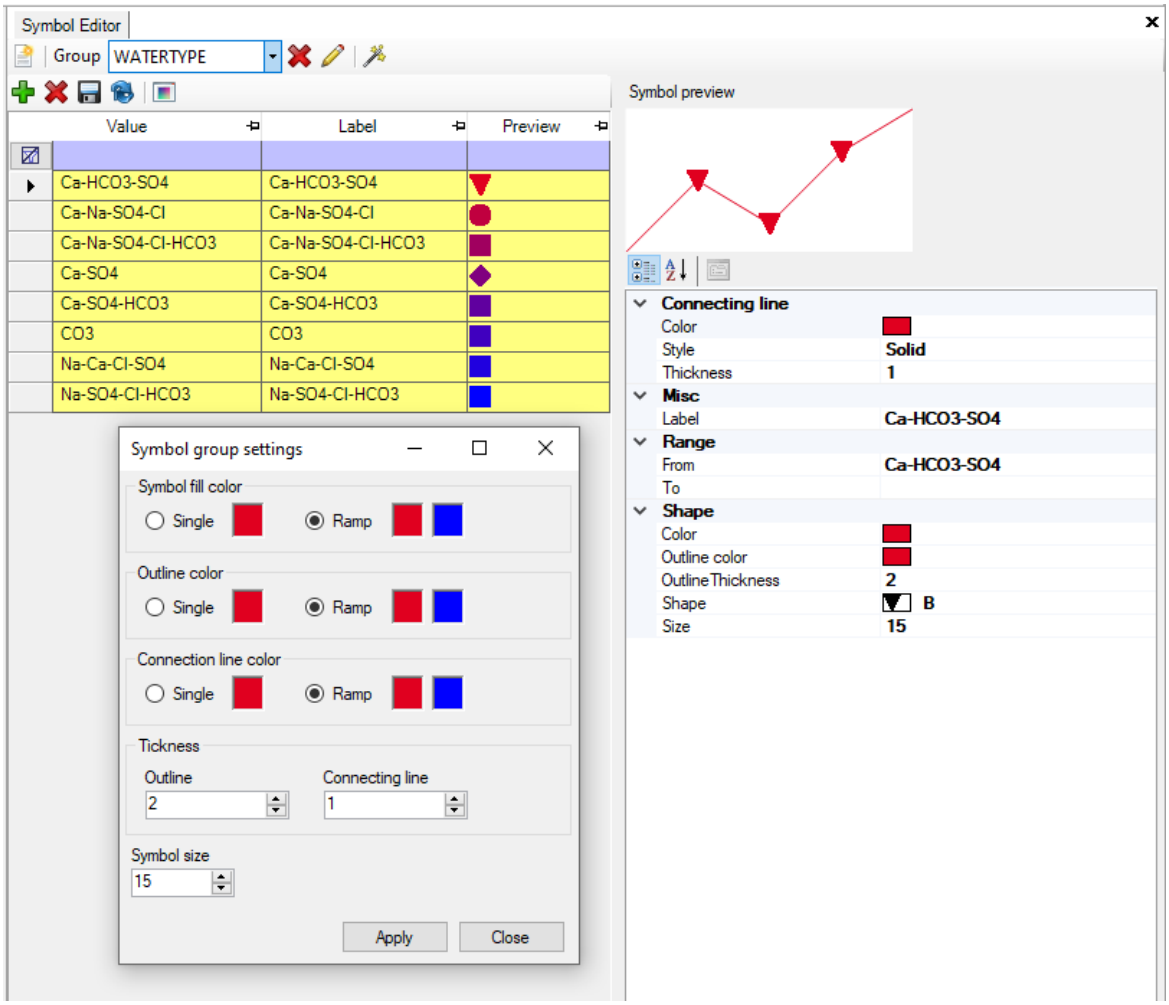
You can spend some time customizing symbol display settings individually by selecting the symbol and making changes to the settings listed below the 'Symbol preview' area. It is also possible to make changes to the entire symbol group by clicking the **'Group colors'** [] button. Click the **'Group colors'** [] button to open the following window:



Using this window you can specify a 'ramp' of colors for the symbols (fill color, outline color and connecting line color), and change the thickness and size of the entire group of symbols (both symbols and connecting lines). Select the 'Ramp' option for all three settings (Symbol fill color, Outline color and Connection line color) and change the two colors to RED and BLUE. You can also update the outline thickness to '2', connecting line thickness to '1' and the symbol size to '15'. When you're finished the 'Symbol group settings' window should look like this:

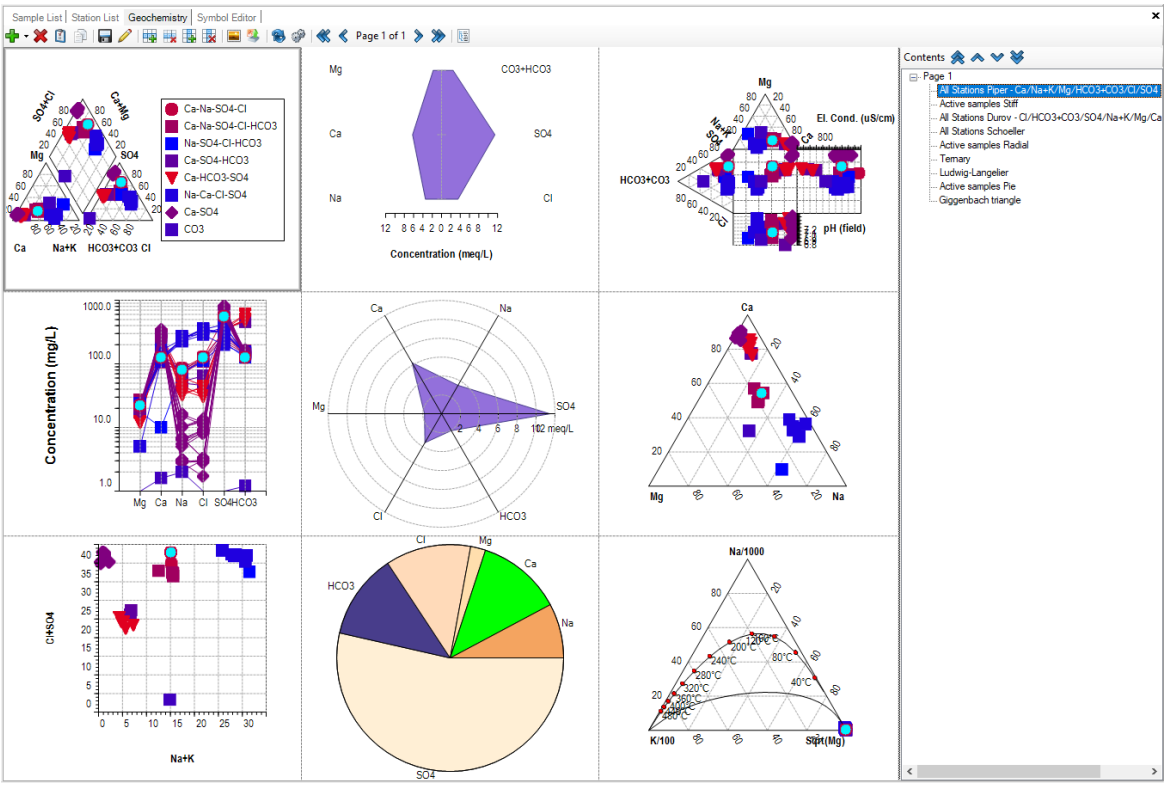


Click Apply to apply the changes to the symbol colors/settings, and the list of symbols should be updated as shown below:



Click Close in the 'Symbol group settings' window to dismiss it, and then click the **'Save changes'** [] button to save these updated settings. To use this symbol set throughout AquaChem, click the **Apply []** button.

Now that this is the active symbol group, if you return to one of the available plot collections (e.g. the 'Geochemistry' plot collection) you should see that all the plots have been updated with the new symbol group:



To revert back to the Station-based symbols, select "Station Name" from the dropdown and click the **Apply [ ]** button.

This concludes the introduction to plot collection. In the next section of the tutorial, you will create thematic maps.

2.1.5 Creating Maps

The Map Viewer Module provides the ability to generate thematic maps. Maps can be generated by adding station and sample data layers directly from the AquaChem database and supplemented by adding external layers (shapefiles and base map images). Layers from the database based on stations or samples can be presented using a variety of options that we will explore in this section of the tutorial.

Please Note: While you can complete this section of the tutorial on its own; previous sections and their relevance are discussed. If you have not completed these sections or are unfamiliar with their related modules. You may benefit from starting the tutorial from the beginning or reviewing specific sections as they are mentioned. Links are provided where appropriate.

To open the Map Viewer:

- select the **Map Viewer button** [ ] from the main toolbar
  or

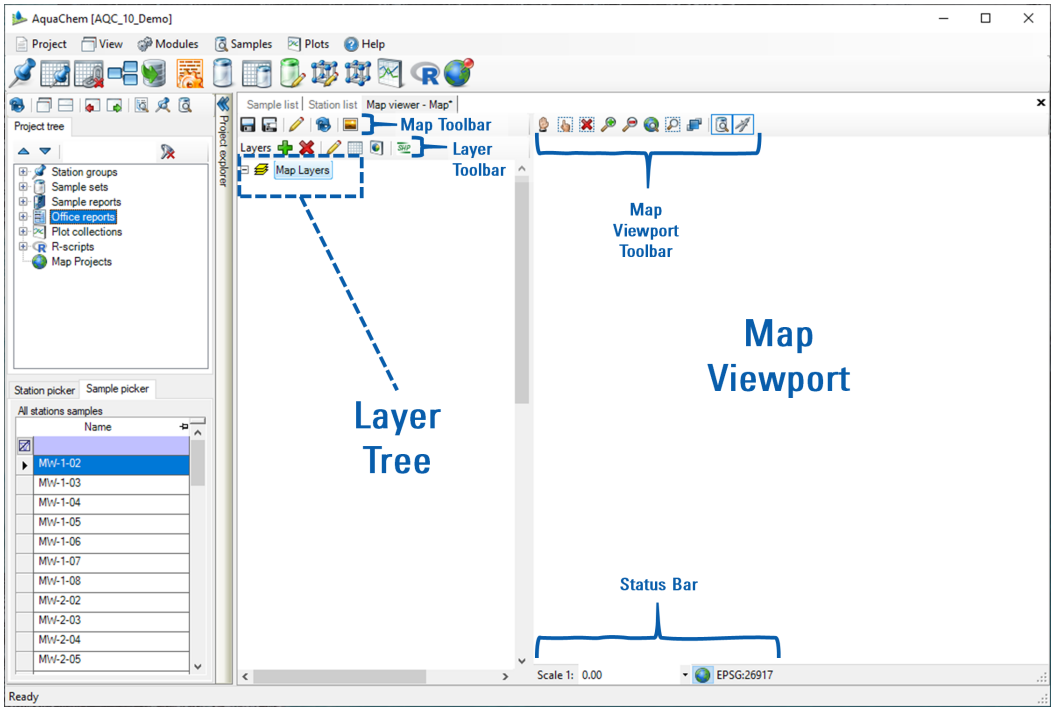
- select **Modules > Map Viewer** from the main menu.

General Layout

When first opening the Map Viewer Module, you will notice two main components and related controls:

1. **A Layer Tree** which lists map layers that have been added to the map. Layers include a label, a visibility checkbox, and a collapsible legend. The Layer Tree also inlcudes:
   - the **Map Toolbar** provides controls for the map including buttons to save the map, change the map name, refresh the map, and export the map to a PowerPoint template.
   - the **Layer Toolbar** provides controls for the map layers, including buttons to add/remove layers, customize labels, view the attribute table, edit the layer symbology, and export a layer as a shapefile.

2. **A Map Viewport** which displays the visible map layers drawn based on the order in the Layer Tree (layers at the bottom will be drawn first)
   - the **Map Viewport Toolbar** provides controls for the map viewport including pan, zoom, and selection tools.
   - the **Status Bar** provides controls for the map layers, including buttons to add/remove layers, edit labels, view the attribute table, alter the layer symbology, and export a layer as a shapefile.



The Map Viewer controls are described in more detail in the Map Viewer section of the documentation.

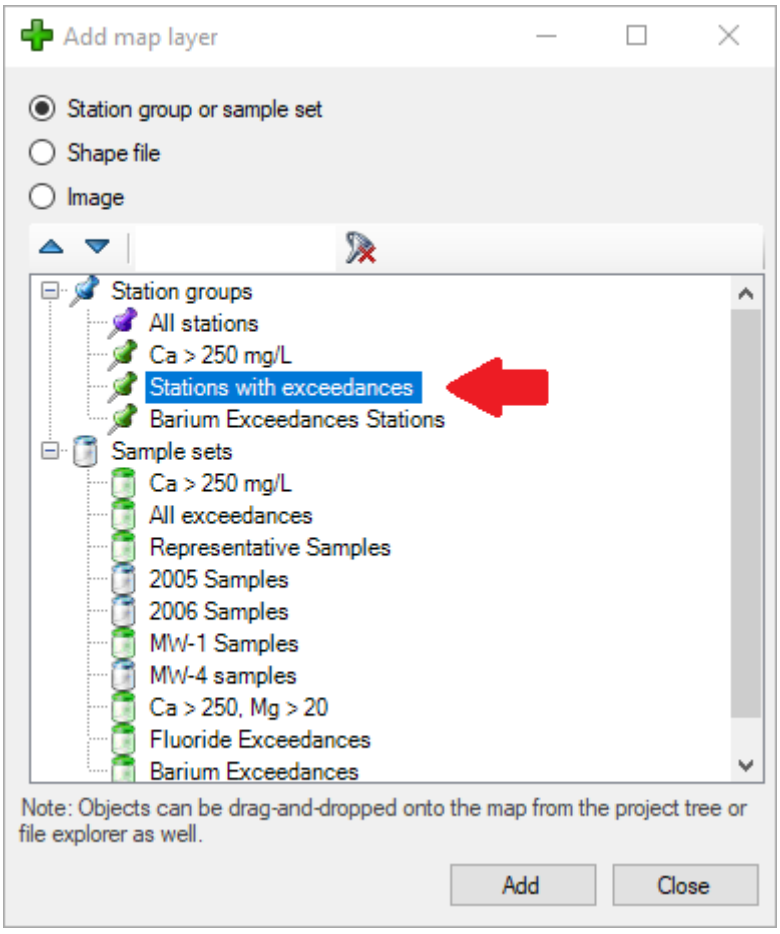
Adding Layers

As part of the tutorial, we will develop a map that contains several layers including:

- Station locations with labels and symbols from the station
- Samples with Stiff diagrams, and
- A Basemap

To begin:

- Click the **Add layer** button [] in the **Map Layers** toolbar to open the Add map layer dialog:



- Select the **Stations with exceedances** station group and click **Add** to add the layer to the map and close the dialog.

There is more than one way to add layers to the map: you can also simply drag-and-drop any station group or sample set from the project tree onto the Map Viewer to add it.

Furthermore, we can also add external data to the map in the form of shapefiles (.shp) and basemap images.

The shapefiles data format is an open source vector-based Geographic Information Systems (GIS) data format developed by ESRI (1998) that may include a set of points, polylines, *or* polygons. Shapefiles consist of a set of files with the same file name — four of these are required for use in the Map Viewer Module: .shp (spatial data), .shx (spatial index), .dbf (attribute data), and .prj (coordinate reference definition).

You can also add basemaps to the Map Viewer module, using the following supported image formats and associated world files:

Format	File Extension	World File
Bitmap	.BMP	.BPW
Tagged Image Format	.TIF	.TFW
JPEG	.JPG	.JPW

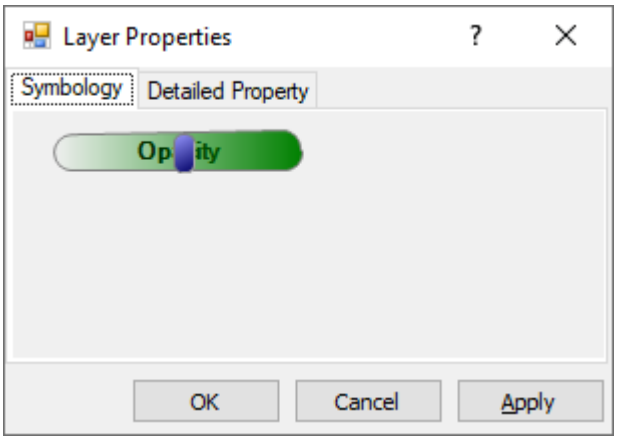
Note that basemaps *must* match the project coordinate system to be displayed correctly on the map. Images are not currently reprojected.

Let's add an image basemap to enhance the map:

- Click the **Add layer** button [] in the **Map Layers** toolbar to open the Add map layer dialog
- Select **Image** and Click **Add**
- Navigate to the location of the Demo Project and select the GeoSpatial folder
- Select Basemap.tif and click Open
- Click Close to close the Add Map Layer window

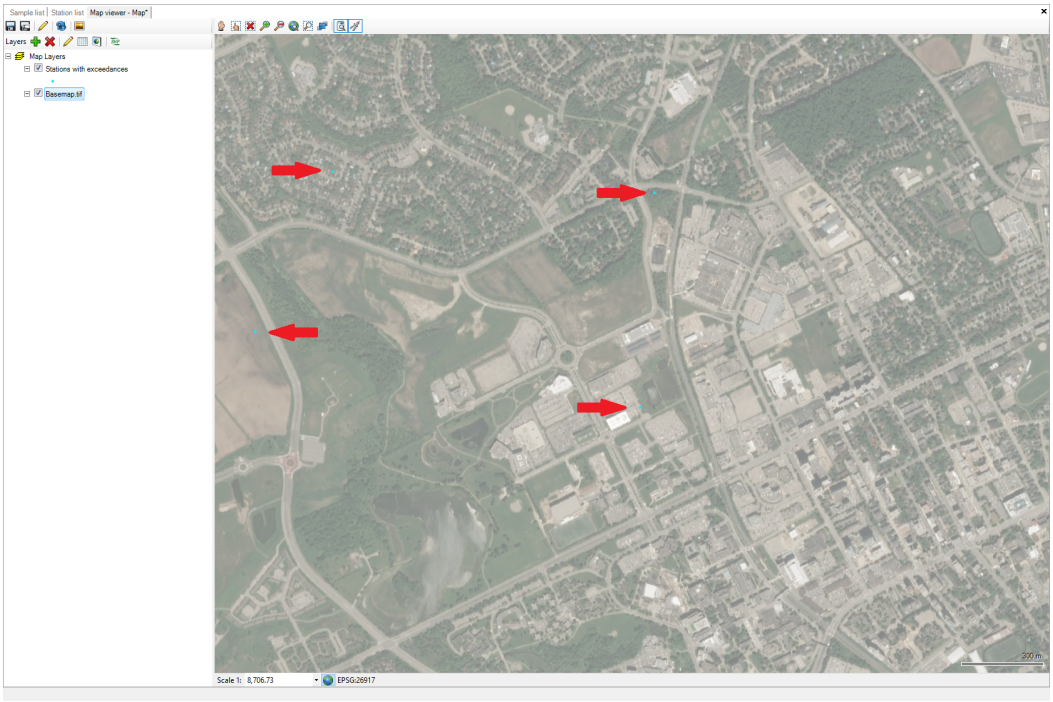
Your basemap should be added to the map, but you may notice that the points from the Station group we added are no longer visible. This is because they are below the basemap in the rendering order and the basemap is quite prominent in the view. Let's adjust the map to make the map easier to look at:

- Drag and drop the **Basemap.tif** layer in Map Layer tree so that it is below the **Stations with exceedances** layer
- Right-click on Basemap.tif and select Properties
- Change the Opacity slider to approximately 50%:



- Click OK

Your map should look similar to the following:

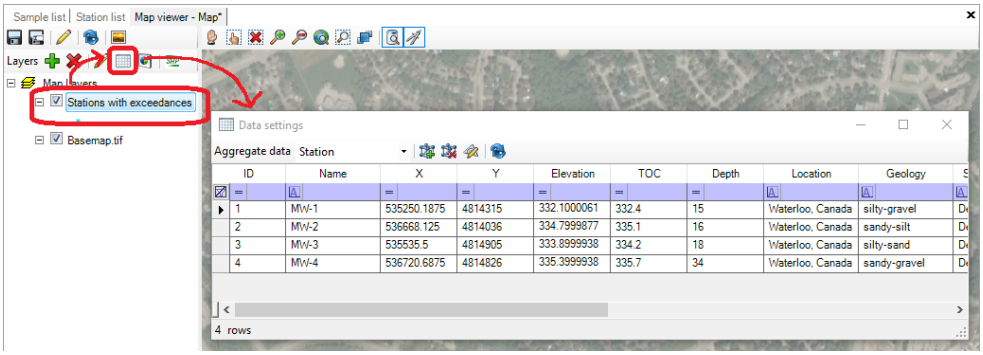


The datapoints are now visible on the map, but depending on your screen settings, they are likely very small and not at all easy to see (the red arrows point to these locations). We will adjust their style settings later in this tutorial, but first we will explore some of the data settings.

Data Settings and Layer Attributes

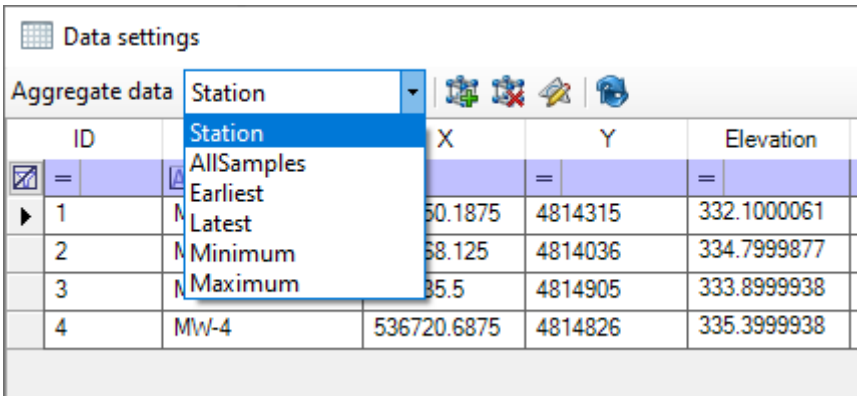
An important point about adding and working with project data-driven layers in the the Map Viewer is that you can access information about stations and samples from both types (i.e. station groups and samples sets). By default, added station groups contain one record per station with attribute data from the station table and sample sets contain one record per sample with attribute data from the sample table. Because of the relational data structure underpinning AquaChem, you can quickly switch back and forth between these two data tables for an added layer. To do this:

- Select the **Stations with exceedances** layer in the Map Layers Tree so that it is highlighted
- Click the Attributes [ ] button to open the layer's Data Settings window:



As described above, one record has been added per station from the **Stations with exceedances** station group along with their inherited attributes (i.e. fields) from the station table. Note that the Example Station that we included in the Manual Data Entry section is not included in this station group since it only has one result for Calcium which does not have an active standard in this project. This further highlights the utility of dynamic station groups and sample sets that we explored earlier in this tutorial.

The **Aggregate data** dropdown in the Data Settings (Attribute table) viewer allows you to define the scope of the data. Currently, the data are based on the Station table. However, we can redefine what data are included by selecting the dropdown:



Note that there are several options that redefine the scope of the attribute table for the current layer as follows:

- **Station**: Station List data for all related stations
- **All Samples**: Sample List data for all related samples
- **Earliest**: Sample List data for the oldest Sample Date at each station in the sample set/station group
- **Latest**: Sample List data for the most recent Sample Date at each station in the sample set/station group
- **Minimum**: Sample List data for each station in the sample set/station group with lowest value of a specified numeric parameter
- **Maximum**: Sample List data for each station in the sample set/station group with highest value of a specified numeric parameter

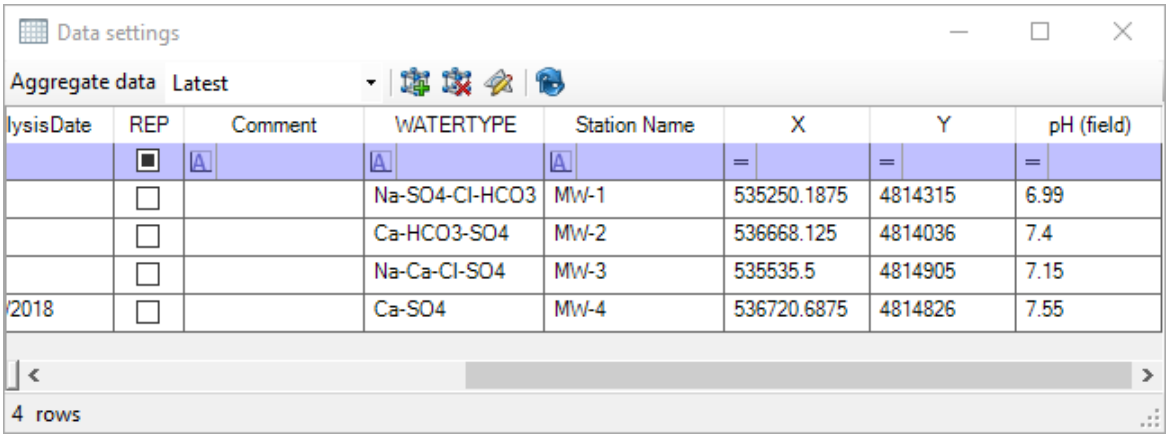
Since we want to create a simple layer based on the "Station Name" symbology from the Symbol Editor that we reviewed in the previous section, we can choose the Latest Sample to streamline the data table:

- Select the **Aggregate data** dropdown and select "**Latest**"
- Click the refresh [ ] button to apply the change and update the attribute data table

Let's also add a pH as a parameter to the table. To add a parameter:

- Click the **Add parameter** [ ] button
- Select "pH_field" and click OK to add the parameter

At this point, the attribute table will include data from each of the fields in the Sample List and pH results for the samples most recently collected at each of the four stations in the station group. Scroll the far right of the Data Setting table to confirm that the data for the pH (field) parameter has been added to the table:



lysisDate	REP	Comment	WATERTYPE	Station Name	X	Y	pH (field)
	☐		Na-SO4-Cl-HCO3	MW-1	535250.1875	4814315	6.99
	☐		Ca-HCO3-SO4	MW-2	536668.125	4814036	7.4
	☐		Na-Ca-Cl-SO4	MW-3	535535.5	4814905	7.15
/2018	☐		Ca-SO4	MW-4	536720.6875	4814826	7.55

4 rows

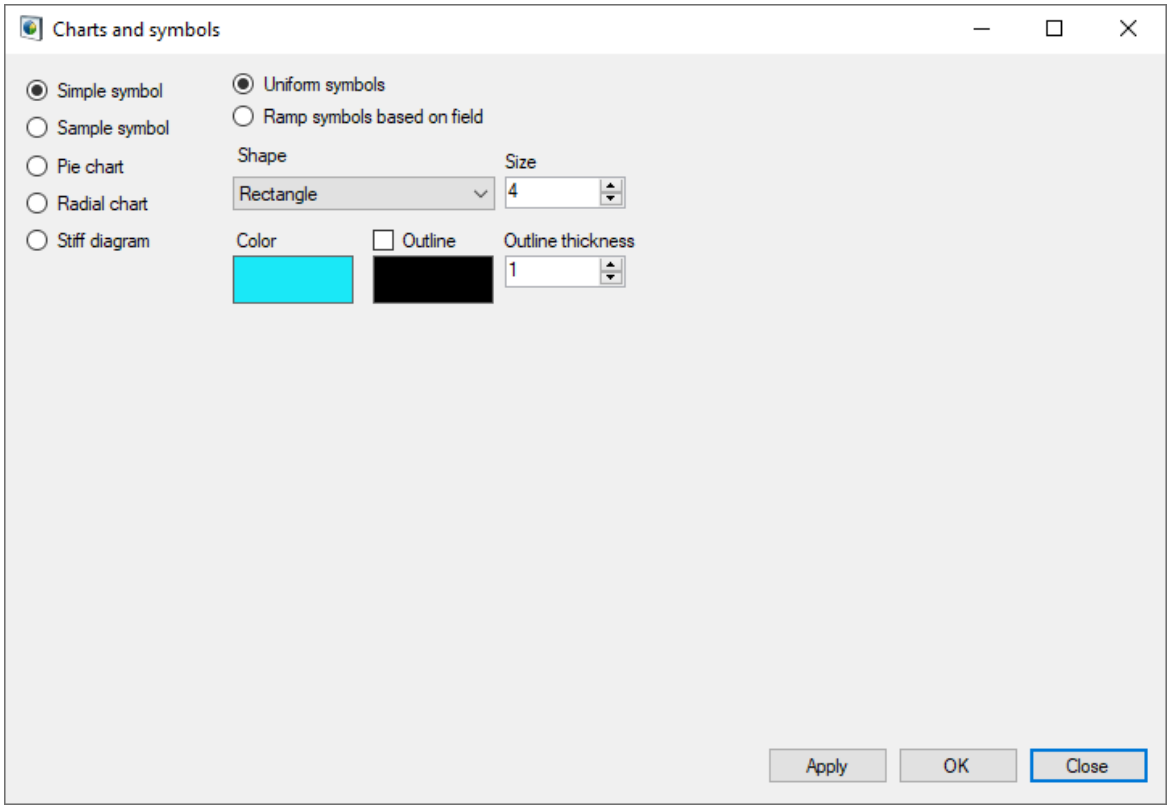
- Click the [×] in the upper right corner of the Data Settings window to close it

Next we will explore how to edit the layer style settings in the map.

Layer Settings for Charts and Symbols

The Map Viewer allows you to render project data-driven layers using several thematic options that we will now explore:

- Click the Chart Setup [ ] button to open the Charts and Symbols dialog:



You will note that there are five options on the left:

- **Simple Symbol:** allows you to define uniform symbols or ramped symbols with sizes/colors proportional to a selected field
- **Sample Symbol:** allows you to use the symbols defined in the Sample List using the Symbol Editor.
- **Pie Chart:** allows you to define two or more parameters to create one pie chart per sample
- **Radial Chart:** allows you define three or more parameters to create one radial chart per sample
- **Stiff Diagram**: allows you to define six parameters to create one Stiff Diagram per sample

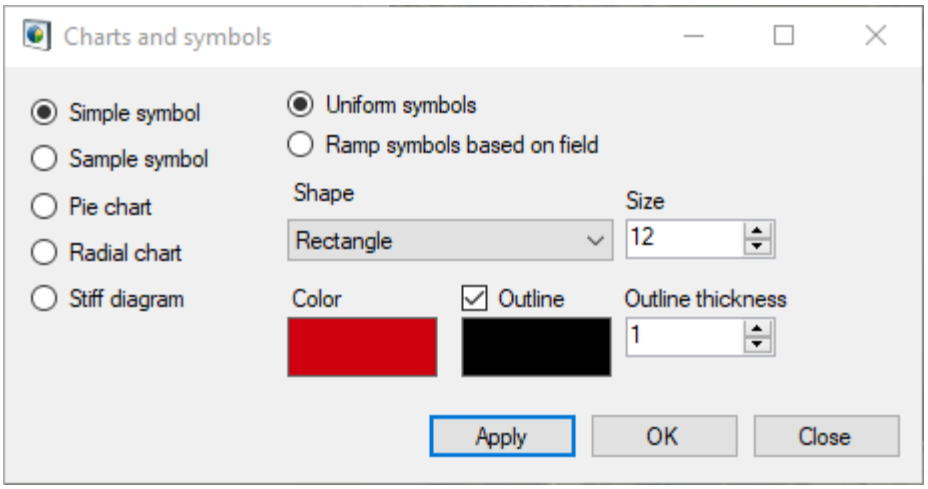
All of these options will render one symbol per record in the Attribute table as defined by the Aggregate data setting. This has several implications:

- The Sample Symbol option is not available if the aggregate data is set to the Station option, since there may be more than one symbol defined at each station
- The plot-based symbols (i.e. Pie, Radial, and Stiff) may render more than one overlapping symbol at a given station if the attribute table includes more than one sample per station (e.g. if the aggregate data option is Station or AllSamples and there is more than one sample per station in the station group/sample set)

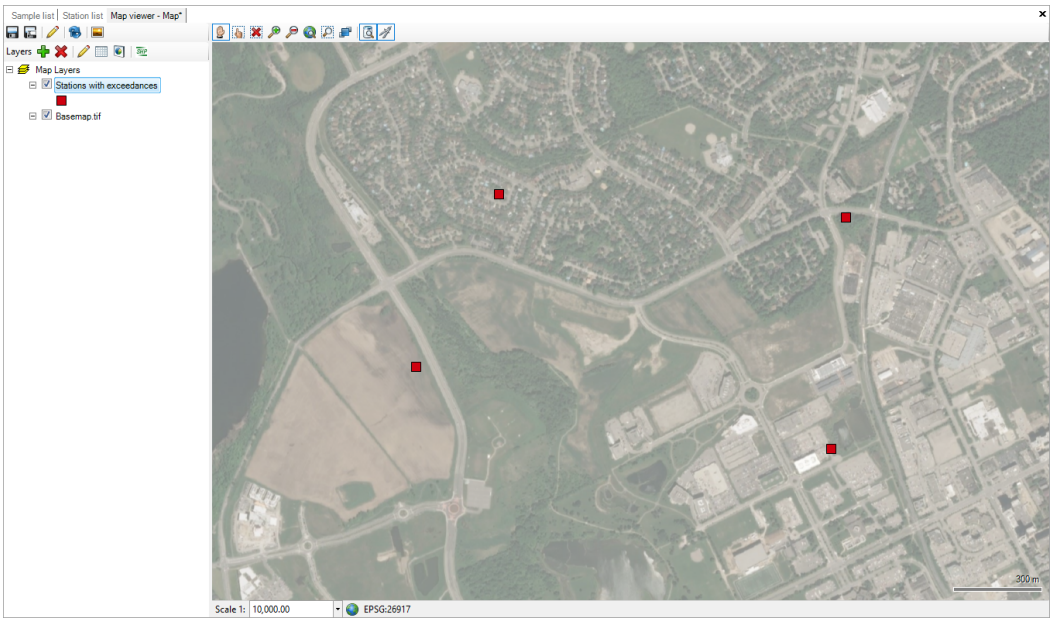
Uniform Symbols

For now let's define uniform symbols with the following settings to increase visibility on the map:

- Set the following settings on the dialog:
  - Size = 12
  - Color = Red (*#CF000F*)
  - Outline = True
  - Outline Thickness = 1



- Click OK

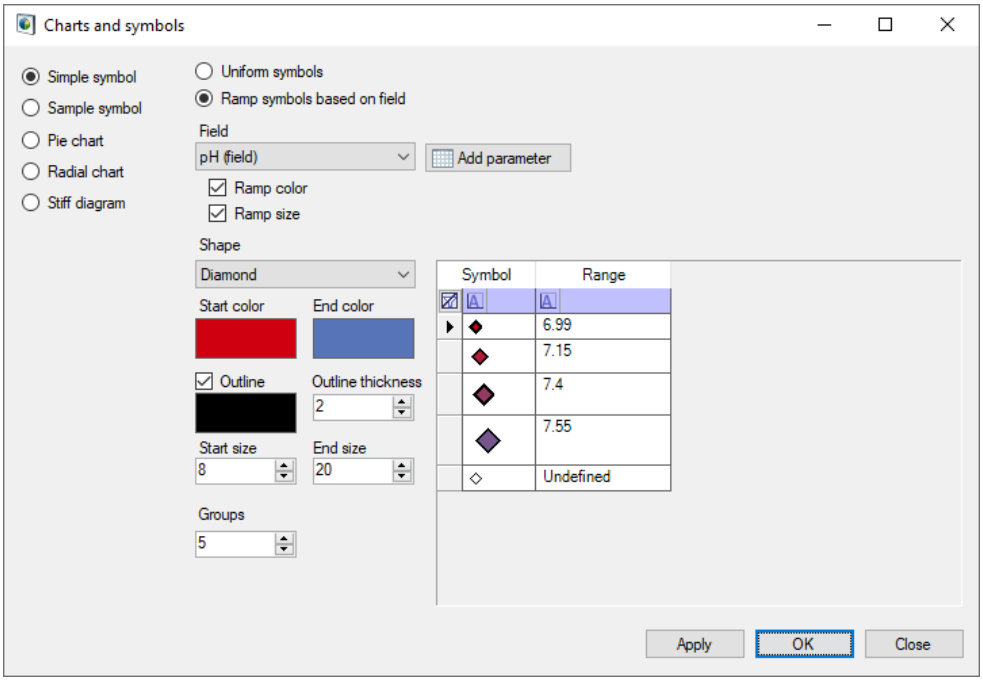


The resulting symbols are much more visible on the map, but they do not convey much information. We can add more information to the map, by using ramped symbols.

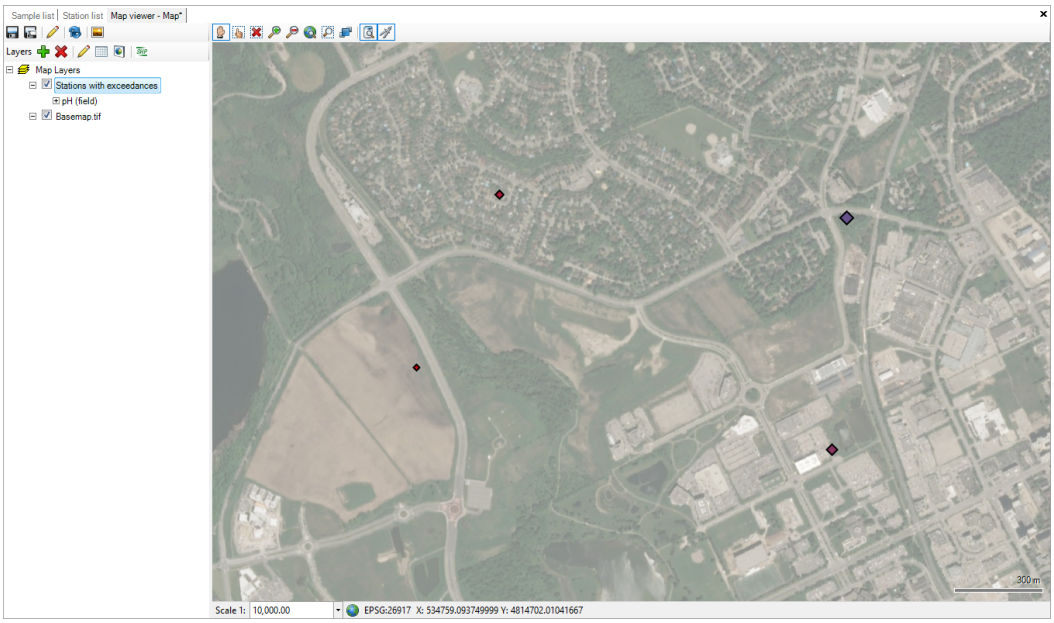
Ramped Symbols

Ramped symbols can be used to visualize the spatial distribution and magnitude of a single parameter. To create ramped symbols:

- Click the Chart Setup [ ] button to reopen the Charts and Symbols dialog:
- select the "Ramp symbols based on field" option and the following additional settings shown in the dialog:



o Click OK

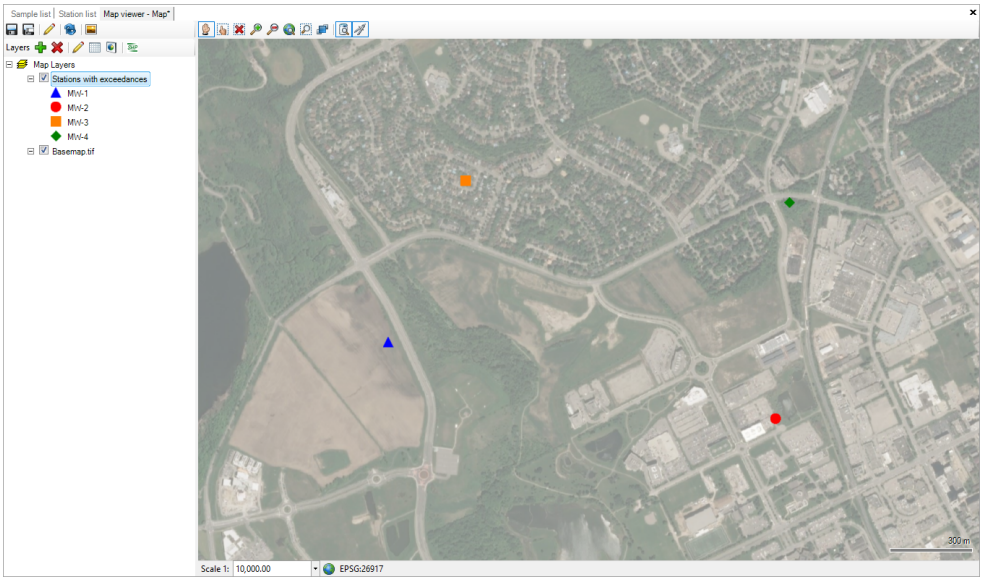


The resulting symbols are now more informative and such a map may be useful when plotting a lot of data from many stations. Another way to render the data is the use the symbols from the Station List so that the map uses the same symbols as the plot collections we explored earlier in the tutorial.

Sample Symbols

To create sample symbols:

- Click the Chart Setup [] button to reopen the Charts and Symbols dialog:
- Select the Sample Symbol option
- Click OK



Plot Symbols

The map viewer allows you to render project data-driven layers as location-based Pie Chart, Radial Chart, or Stiff Diagram plots. As mentioned above, one plot will be rendered per sample as defined in the Data Settings and based on the aggregate data option. The format of the plot will be based on the current default settings as defined using the Source data tab of the relevant plot type.

In this section we will add the Station Group again so we can keep the current Sample-based symbols on the map:

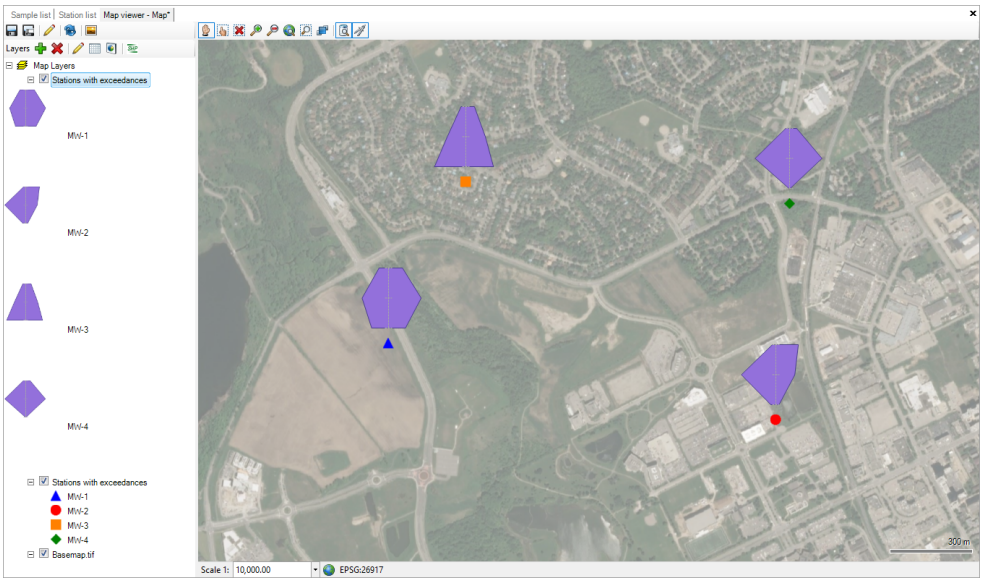
- Drag and drop the "**Stations with exceedances**" station group from the project tree onto the map
- Click the Chart Setup [] button to reopen the Charts and Symbols dialog
- Select the Stiff Diagram option
- Click Apply

Note that a Stiff diagram has been added to the map, but each covers the Sample symbols. To show both we will add an offset so that the Stiff plots are rendered above the Station locations. The offset should generally be a little larger than half of its size, since plots are anchored at their center and we generally want the plot to be rendered a small distance away from the station location.

- Change the plot size settings:
  o X offset = 0

- Y offset = 55
- Size = 100

- Click OK



The map is now quite informative and we have examined how to add multiple types of information to the map. The controls for adding radial plots and pie charts are similar to the controls for adding Stiff diagrams. Feel free to experiment with adding and styling these charts. Next we will add some labels.

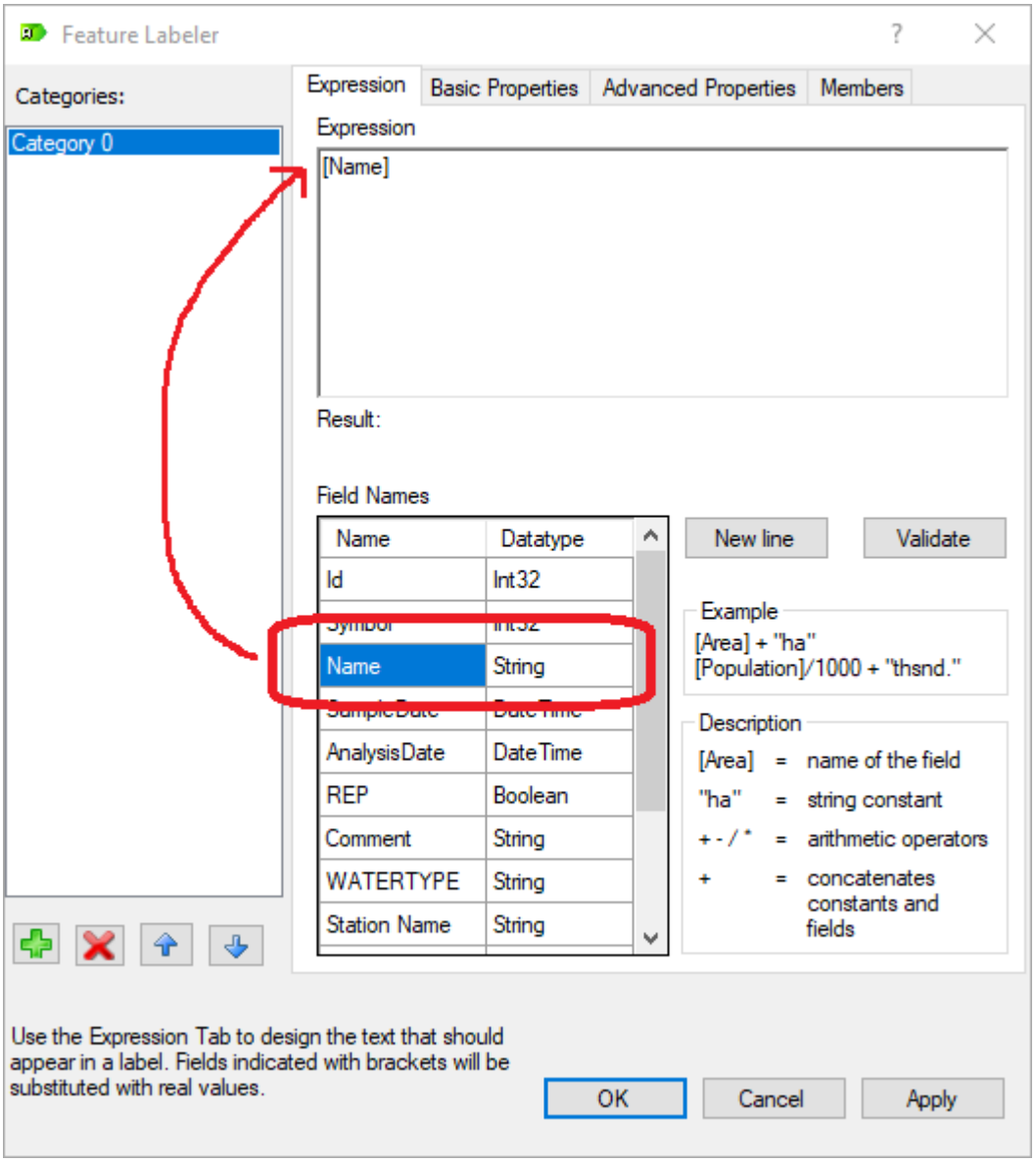
Layer Labels

The map viewer allows you to add labels to vector layers (i.e. project data-driven layers and/or shapefiles) based on one or more attributes. To access the label settings:

- Select the desired layer to which you wish to add labels, in our case, select the "Stations with exceedances" layer that is based on the Sample symbols from the Symbol Editor
- Click the Labels [ ] button in the Layer toolbar to open the Feature Labeler window

The Feature Labeler provides a fairly comprehensive set of controls to customize your labels organized by tabs, as discussed in the **XXX** section. For this exercise, we will first add some simple labels and then add supplemental information using a more complex expression.

- Double-click the "Name" field in the Field Names list presented in the Expression tab so that it appears in the Expression form:



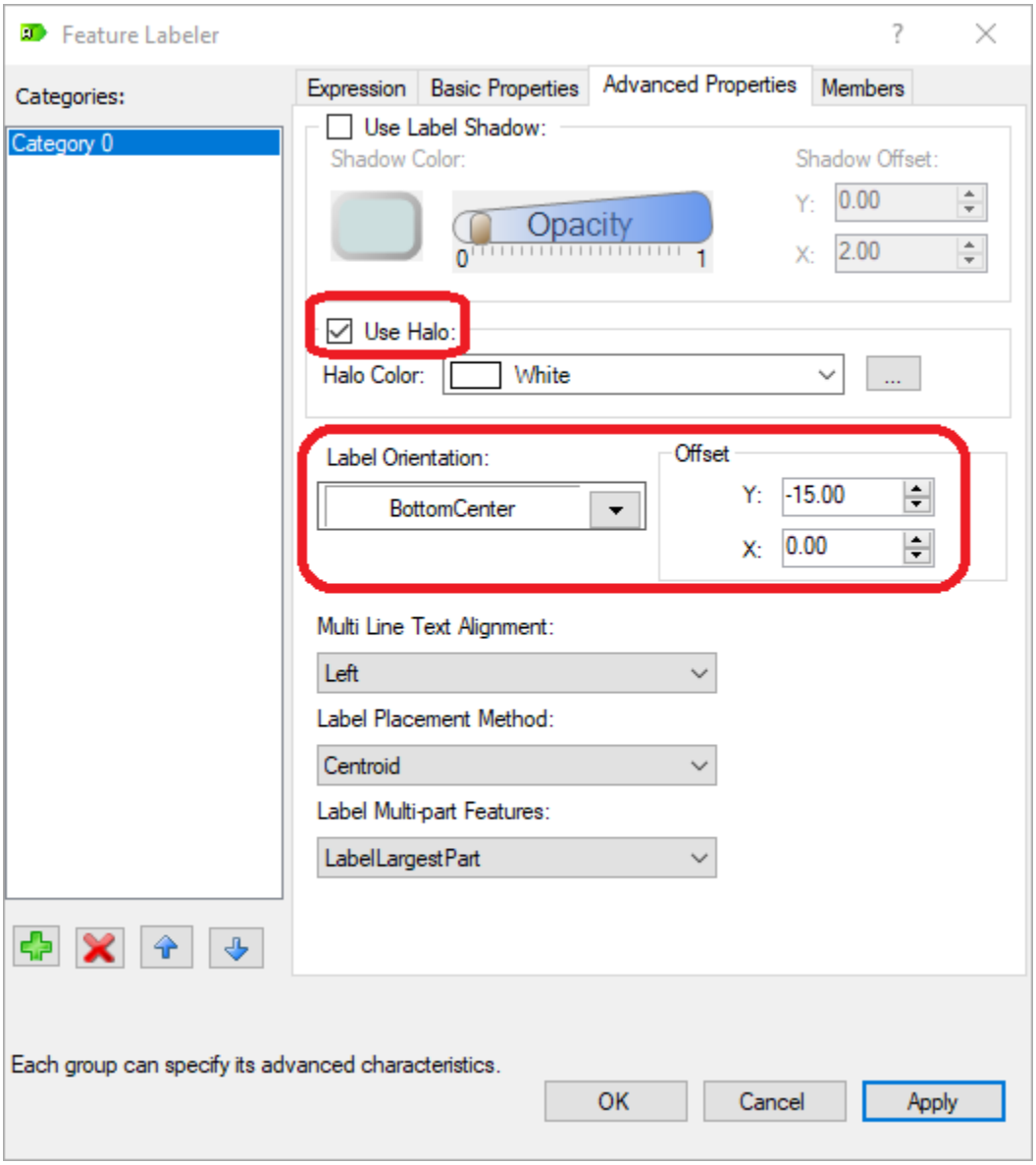
- Click Apply

Note that the labels appear on top of the symbol; similar to the default location of the Stiff diagrams, the labels are anchored to their location. To make the labels more legible and useful, let's add some formatting

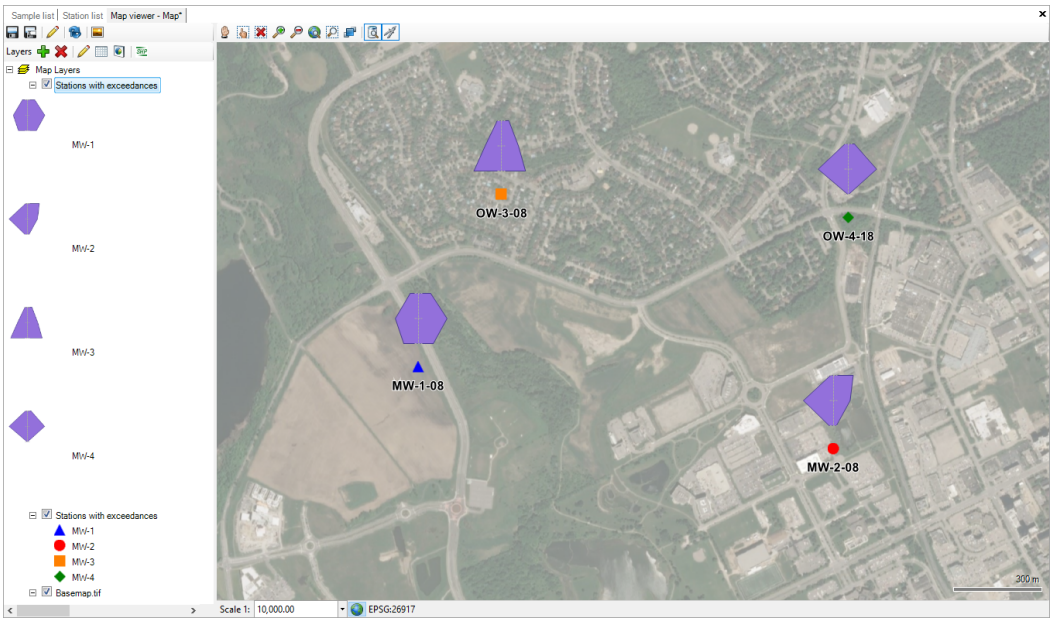
- Click on the Basic Properties tab
  - Select Size = 12
  - Style = Bold
  - Click Apply

- Click on the Advanced Properties tab
  - Select ☑ for the Use Halo option

- Select Bottom Center for the Label Orientation
- Set the Y-Offset = -10
- Click OK



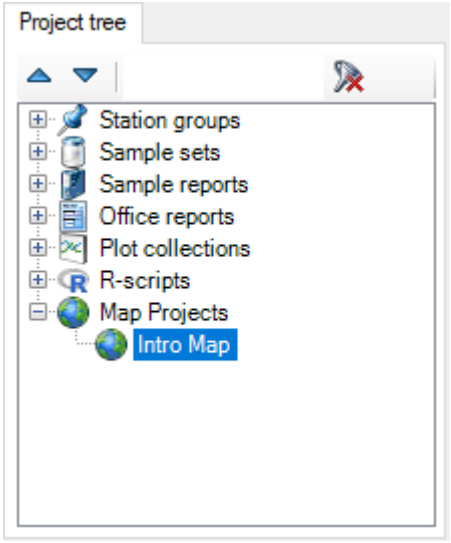
The map now has legible labels.



We can now save the map to make use of it in the future.

- Click the Rename map [ ] button in the Map Toolbar to provide a name for the map
- Enter a name for the map: "Intro Map"
- Click OK
- Click the Save [ ] button in the Map Toolbar

Note that the Map is now saved in the Project Tree as "Map" for future use.



This concludes the introduction to plot collection. In the next section of the tutorial, you will review some basic scripting with the R-Console module.

2.1.6 Basic Scripting with the R-Console

R is an open-source language for statistical computing, analysis and graphics. The **R-Console Module** allows you to run scripts in the R scripting language and leverage the thousands of available libraries that facilitate data analyses, visualization, categorization, and much more.

> **Please Note:** this tutorial is not designed to be a comprehensive introduction to the R scripting language. If you are not familiar with the R-scripting language, you may want to do a bit of supplemental research, since this tutorial is only designed to introduce you to the AquaChem interface for creating R-scripts. A great place to start learning about R is on the R Foundation website (https://www.r-project.org/).

To use the R scripting module you must first install R to your computer. If you haven't already installed R please take a moment to follow the instructions provided in the Installing R section of this user manual.

Once R has been installed, you can access the R-console from the main menu (click 'Modules > R-console'), or you can double-click one of the existing R-scripts that have been saved to the Project Tree. Three 'Basic Scripts' are saved to the AquaChem Demo Project:

1. Install Packages - this script will install the packages and libraries required for the remaining scripts.

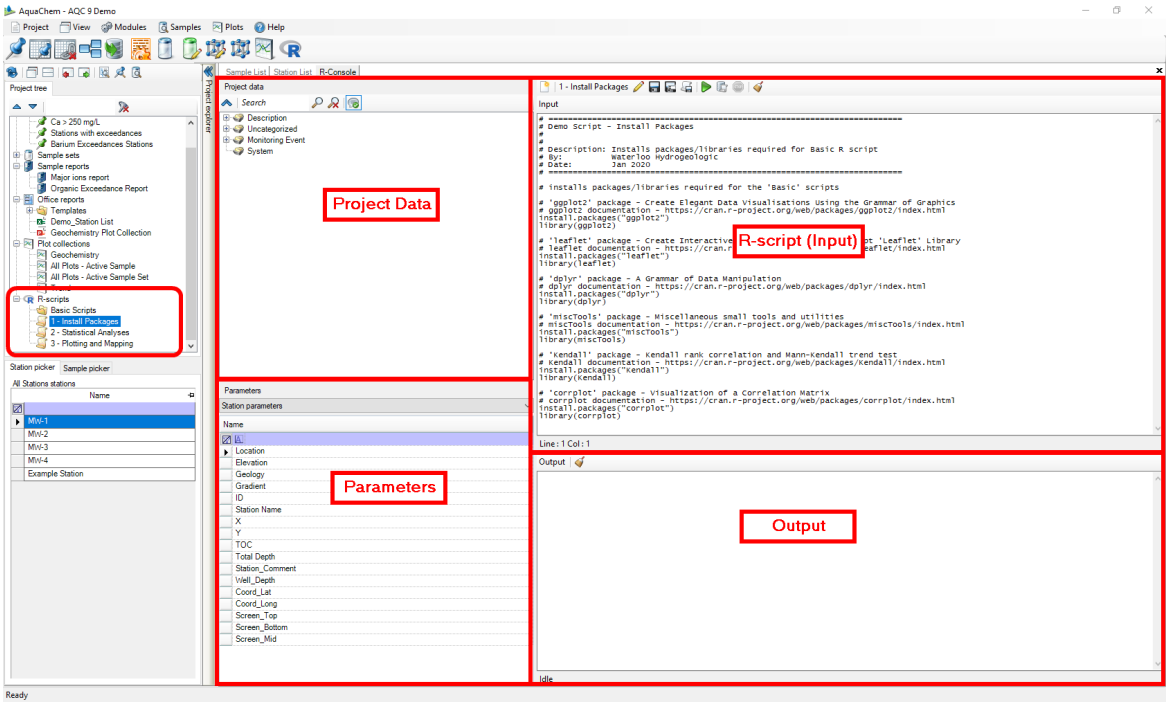
2. Statistical Analyses - this script collects some water quality data from the project (i.e. major ions including Ca, K, Na, Cl, Mg, CO3 and HCO3) and performs a series of statistical analyses such as calculating basic statistics (mean/standard deviation/min/max/quartiles), estimating trends using the Mann-Kendall test, and creating a correlation matrix.

3. Plotting and Mapping - this script retrieves some station data (i.e. station name, coordinates, elevations), plots them on an interactive map in your default browser using the Leaflet package, and creates a series of simple scatter plots.

All three of these basic scripts are annotated - script lines that begin with a '#' are comment lines which have been included to help you understand what the script is designed to do.

Install Packages

Double-click the **'1-Install Packages**' script under the R-Scripts node of the Project Tree and the R-console will open as shown below:



There are four main panes in the R-console interface:

1. The **Project data pane** facilitates the selection of data from field in the project database tables based on (or filtered by) a given station or station group. When using the project data pane, a command that defines the selected data as a (list) vector is automatically inserted into the R-script Input pane cursor location.

2. The **Parameters pane** facilitates the selection of parameter data from database tables based on (or filtered by) a given sample set. When using the Parameters pane a command that defines the selected data as a (list) vector is automatically inserted into the R-script Input pane cursor location.

3. The **Input pane** is where the R-script itself is written. The Project data and Parameters panes can be used to facilitate the creation of data variable, and the R-script associated with these data will be automatically added to the input section.

4. The **Output pane** records the results or output of the R-script as it is processed.

The '**1 - Install Packages**' script is quite basic and will not require the use of the Project Data or Parameters panes. Take a moment to review the script and you will see that it simply is designed to install the following packages/libraries:

- **'ggplot2' package** - Create Elegant Data Visualisations Using the Grammar of Graphics
- **'leaflet' package** - Create Interactive Web Maps with the JavaScript 'Leaflet' Library
- **'dplyr' package** - A Grammar of Data Manipulation
- **'miscTools' package** - Miscellaneous small tools and utilities
- **'Kendall' package** - Kendall rank correlation and Mann-Kendall trend test

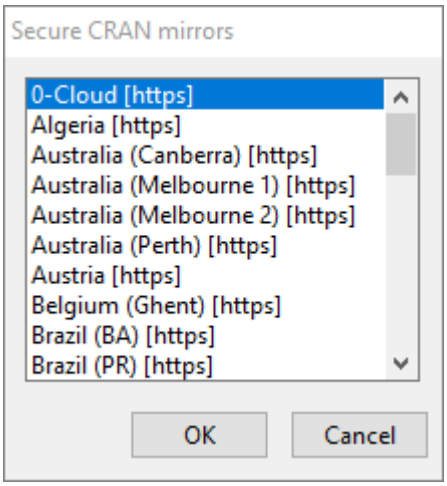
- **'corrplot' package** - Visualization of a Correlation Matrix

Note once more that all lines beginning with a '#' are comment lines and simply provide some context/explanation as to what the script is meant to accomplish. You can find more information about each of the packages by visiting the URL provided in these comment lines, which will bring you to the associated page of each package at the R Foundation website.

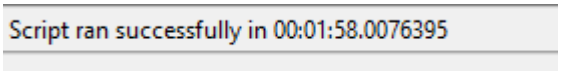
For now, simply click the **'Run'** [ ] button in the toolbar which will execute the 'Install Packages' script.

Please note: If you receive an error at this point, this likely means that you do not have write access to folder where the R package installs a targeted. If this is the case, please follow the steps in the Installing R guide; in particular, see step 3.

Since these packages have not been installed previously, you will see a 'Secure CRAN mirrors' window open, as shown below:

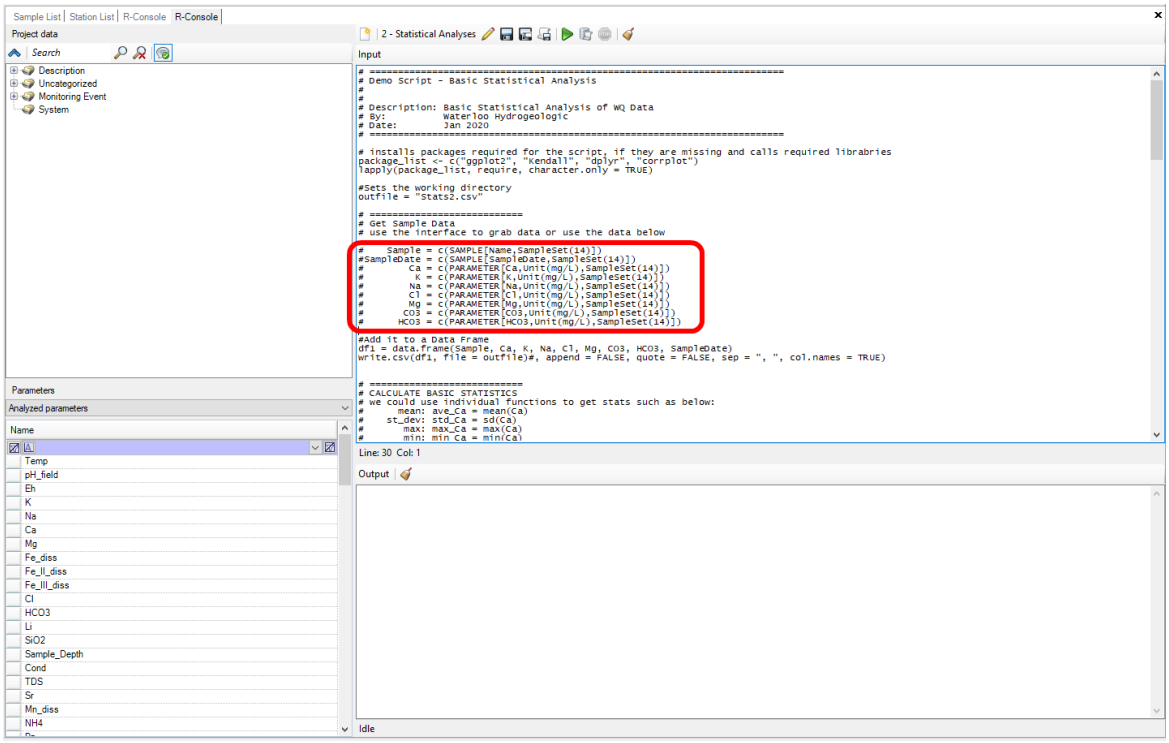


This window allows you to choose from a number of secure mirrors which host the packages that you are trying to install. Select any of them, and then click the 'OK' button at the bottom. After a few moments the script should finish running, and you will see a message in the Status Bar at the bottom of the 'Output' section indicating that the script ran successfully:



Statistical Analyses

Now that the packages/libraries required for the two remaining scripts have been installed, you can proceed to the second script. Double-click the '**2 - Statistical Analyses**' script in the Project Tree and you should see the following:



The Statistical Analyses script is designed to fetch a set of major ion data (Ca, K, Na, Cl, Mg, CO3 and HCO3) from the 'MW-4 samples' sample set, and to perform a series of statistical analyses on that data. You will notice that the highlighted portion of the script in the image above has been 'commented out' by using a '#'. This is because you will use the Parameters section of the interface to facilitate the selection of this sample data. We need to recreate the data selection commands for Sample Name, Sample Date, Ca, K, Na, Cl, Mg, CO3 and HCO3.

To start, make sure that the cursor lies just below the line that reads:

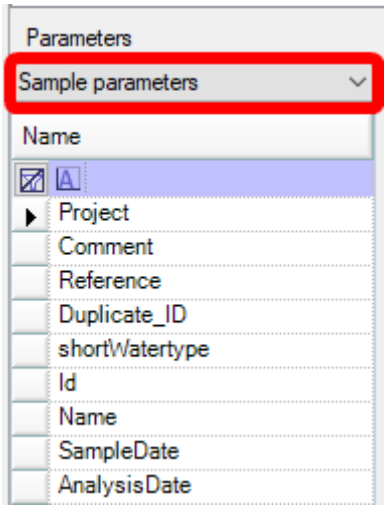
```
#       HCO3 = c(PARAMETER[HCO3,Unit(mg/L),SampleSet(14)])
```

as highlighted below:

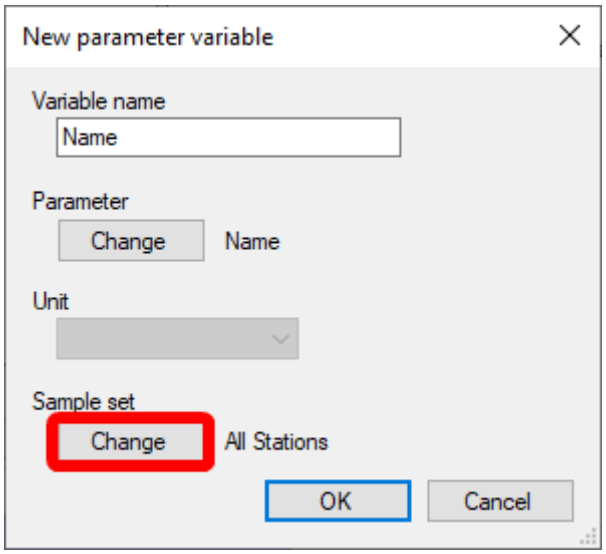
Input

```
#Sets the working directory
outfile = "Stats2.csv"

# ============================
# Get Sample Data
# use the interface to grab data or use the data below

#    Sample = c(SAMPLE[Name,SampleSet(14)])
#SampleDate = c(SAMPLE[SampleDate,SampleSet(14)])
#        Ca = c(PARAMETER[Ca,Unit(mg/L),SampleSet(14)])
#         K = c(PARAMETER[K,Unit(mg/L),SampleSet(14)])
#        Na = c(PARAMETER[Na,Unit(mg/L),SampleSet(14)])
#        Cl = c(PARAMETER[Cl,Unit(mg/L),SampleSet(14)])
#        Mg = c(PARAMETER[Mg,Unit(mg/L),SampleSet(14)])
#       CO3 = c(PARAMETER[CO3,Unit(mg/L),SampleSet(14)])
#      HCO3 = c(PARAMETER[HCO3,Unit(mg/L),SampleSet(14)])


#Add it to a Data Frame
df1 = data.frame(Sample, Ca, K, Na, Cl, Mg, CO3, HCO3, SampleDate)
write.csv(df1, file = outfile)#, append = FALSE, quote = FALSE, sep = ", ", col.names = TRUE)


# ============================
# CALCULATE BASIC STATISTICS
# we could use individual functions to get stats such as below:
#      mean: ave_Ca = mean(Ca)
#    st_dev: std_Ca = sd(Ca)
#       max: max_Ca = max(Ca)
#       min: min_Ca = min(Ca)
# quartiles: q25_Ca = quartile(Ca, 0.25)
#
# let's do this a bit more efficiently using functions
# the first function we'll need is the coefficient of variation
#
cv <- function(val) {sd(val)/mean(val)}

# next let's collect multiple stats into one vector:
get_stats = function(val) {c(mean(val), sd(val), cv(val), max(val), quantile(val,  c(.75, 0.50, 0.25)), min(val))}
```

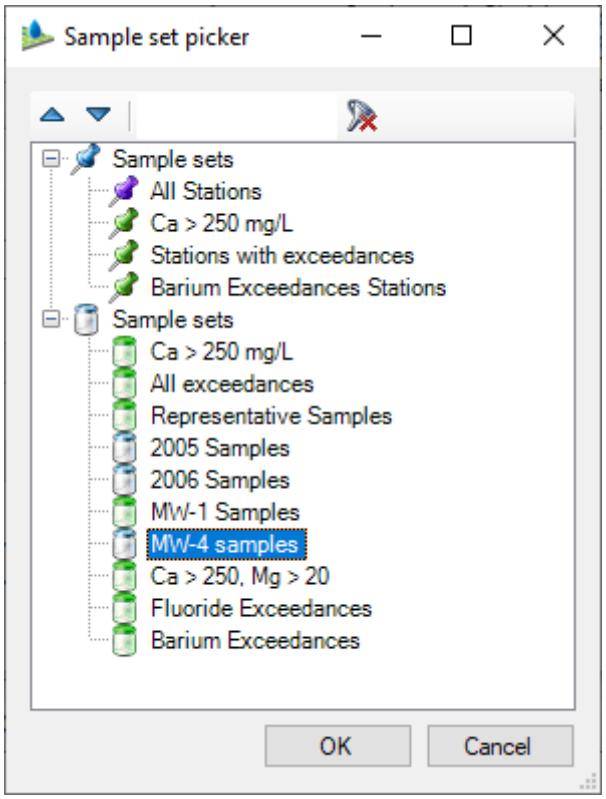
Now in the Parameters section select the 'Sample Parameters' parameter group, which allows you to select sample metadata (e.g. Sample 'Name' and 'SampleDate'):



Double-click the 'Name' parameter in the Sample parameters list, and the following 'New parameter variable' window will appear:

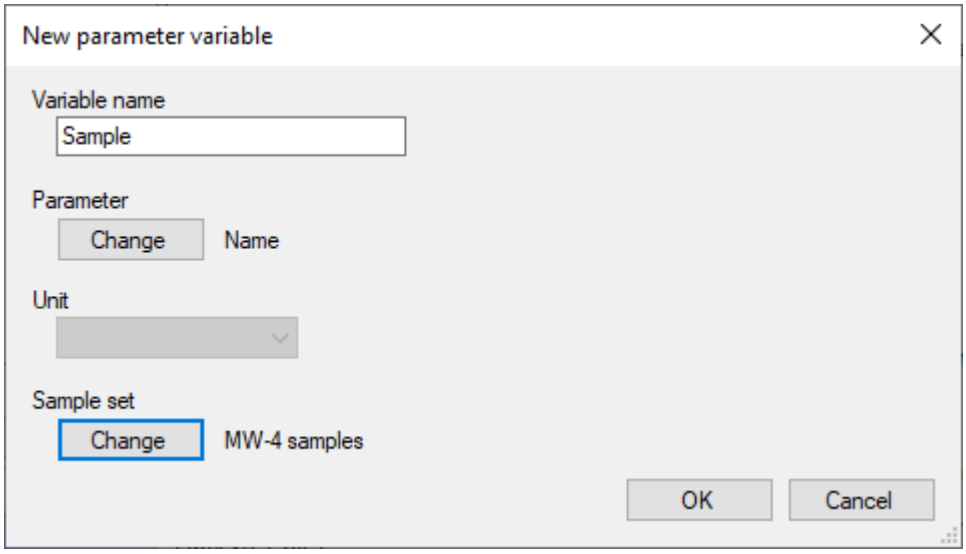


In this example we are ONLY interested in sample data from the 'MW-4 samples' sample set, so click the Change button under the 'Sample set' area (highlighted in the image above), to open the 'Sample set picker' window. Select the 'MW-4 samples' set, as indicated in the image below and click OK:



Back in the 'New parameter variable' window, change the 'Variable name' to 'Sample'.

The 'New parameter variable' window should now indicate that you are selecting a new variable called 'Sample' from the 'MW-4 samples' sample set:



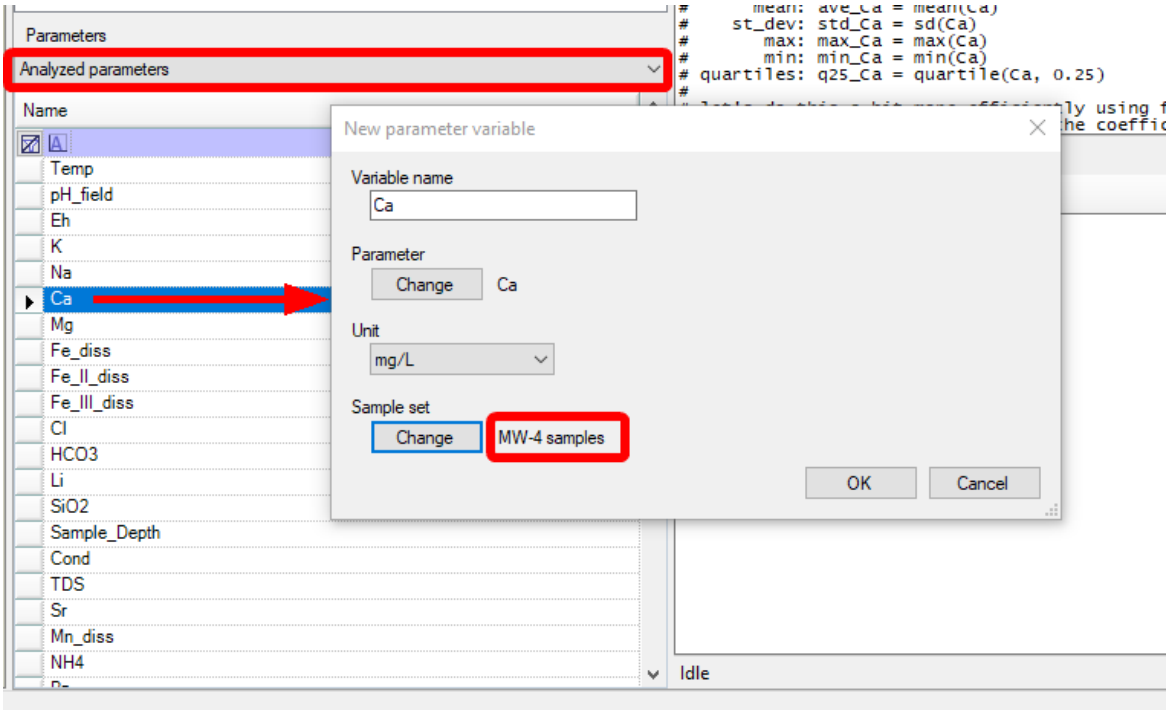
Click OK and you will see a new line of script is added to the 'Input' section. Other than the comment character '#' and blank spacing, this new line of script should be identical to the first line of 'commented' script in the 'Get Sample Data' section:

```
# ============================
# Get Sample Data
# use the interface to grab data or use the data below
#     Sample = c(SAMPLE[Name,SampleSet(14)])
#         Ca = c(PARAMETER[Ca,Unit(mg/L),SampleSet(14)])
#          K = c(PARAMETER[K,Unit(mg/L),SampleSet(14)])
#         Na = c(PARAMETER[Na,Unit(mg/L),SampleSet(14)])
#         Cl = c(PARAMETER[Cl,Unit(mg/L),SampleSet(14)])
#         Mg = c(PARAMETER[Mg,Unit(mg/L),SampleSet(14)])
#        CO3 = c(PARAMETER[CO3,Unit(mg/L),SampleSet(14)])
Sample = c(SAMPLE[Name,SampleSet(14)])
```

You must now repeat these steps for the rest of the required data. Retrieve the 'SampleDate' data field from the 'Sample parameters' group in the same manner (making sure to change the sample set to 'MW-4 samples'), and you should see the script updated with a new line for SampleDate as shown below:

```
# ============================
# Get Sample Data
# use the interface to grab data or use the data below

#     Sample = c(SAMPLE[Name,SampleSet(14)])
#SampleDate = c(SAMPLE[SampleDate,SampleSet(14)])
#         Ca = c(PARAMETER[Ca,Unit(mg/L),SampleSet(14)])
#          K = c(PARAMETER[K,Unit(mg/L),SampleSet(14)])
#         Na = c(PARAMETER[Na,Unit(mg/L),SampleSet(14)])
#         Cl = c(PARAMETER[Cl,Unit(mg/L),SampleSet(14)])
#         Mg = c(PARAMETER[Mg,Unit(mg/L),SampleSet(14)])
#        CO3 = c(PARAMETER[CO3,Unit(mg/L),SampleSet(14)])
#       HCO3 = c(PARAMETER[HCO3,Unit(mg/L),SampleSet(14)])
Sample = c(SAMPLE[Name,SampleSet(14)])
SampleDate = c(SAMPLE[SampleDate,SampleSet(14)])
```

Next you can retrieve the calcium (Ca) data. In the Parameters section change the parameter group to 'Analyzed Parameters' and repeat this selection process (once again making sure to change the sample set to 'MW-4 samples'). You can leave the default units of 'mg/L', as shown in the image below:



Repeat the parameter selection for K, Na, Cl, Mg, CO3 and HCO3, and finally your script should look like this:

```
# ============================
# Get Sample Data
# use the interface to grab data or use the data below

#    Sample = c(SAMPLE[Name,SampleSet(14)])
#SampleDate = c(SAMPLE[SampleDate,SampleSet(14)])
#        Ca = c(PARAMETER[Ca,Unit(mg/L),SampleSet(14)])
#         K = c(PARAMETER[K,Unit(mg/L),SampleSet(14)])
#        Na = c(PARAMETER[Na,Unit(mg/L),SampleSet(14)])
#        Cl = c(PARAMETER[Cl,Unit(mg/L),SampleSet(14)])
#        Mg = c(PARAMETER[Mg,Unit(mg/L),SampleSet(14)])
#       CO3 = c(PARAMETER[CO3,Unit(mg/L),SampleSet(14)])
#      HCO3 = c(PARAMETER[HCO3,Unit(mg/L),SampleSet(14)])
Sample = c(SAMPLE[Name,SampleSet(14)])
SampleDate = c(SAMPLE[SampleDate,SampleSet(14)])
Ca = c(PARAMETER[Ca,Unit(mg/L),SampleSet(14)])
K = c(PARAMETER[K,Unit(mg/L),SampleSet(14)])
Na = c(PARAMETER[Na,Unit(mg/L),SampleSet(14)])
Cl = c(PARAMETER[Cl,Unit(mg/L),SampleSet(14)])
Mg = c(PARAMETER[Mg,Unit(mg/L),SampleSet(14)])
CO3 = c(PARAMETER[CO3,Unit(mg/L),SampleSet(14)])
HCO3 = c(PARAMETER[HCO3,Unit(mg/L),SampleSet(14)])
```

This demonstrates the power of the R-console module within AquaChem, which facilitates the selection of sample data and the automatic scripting of the data into a new vector data object.

At this point you can click the **'Run'** [ ] button in the toolbar to execute the script, but it is recommended that you take some time to review the entirety of the script before you do. Each portion of the script is explained through annotation within the script itself, so this tutorial doesn't review everything in fine detail. However, a short description of each 'section' of this script is provided below:

- **Description section** - the first section (Lines 1-15) provides a basic description of the script, invokes the required libraries, and sets the the name of the output file. Please note that by default in AquaChem the location of output data will be in the 'Scripts' sub-directory in your project folder.

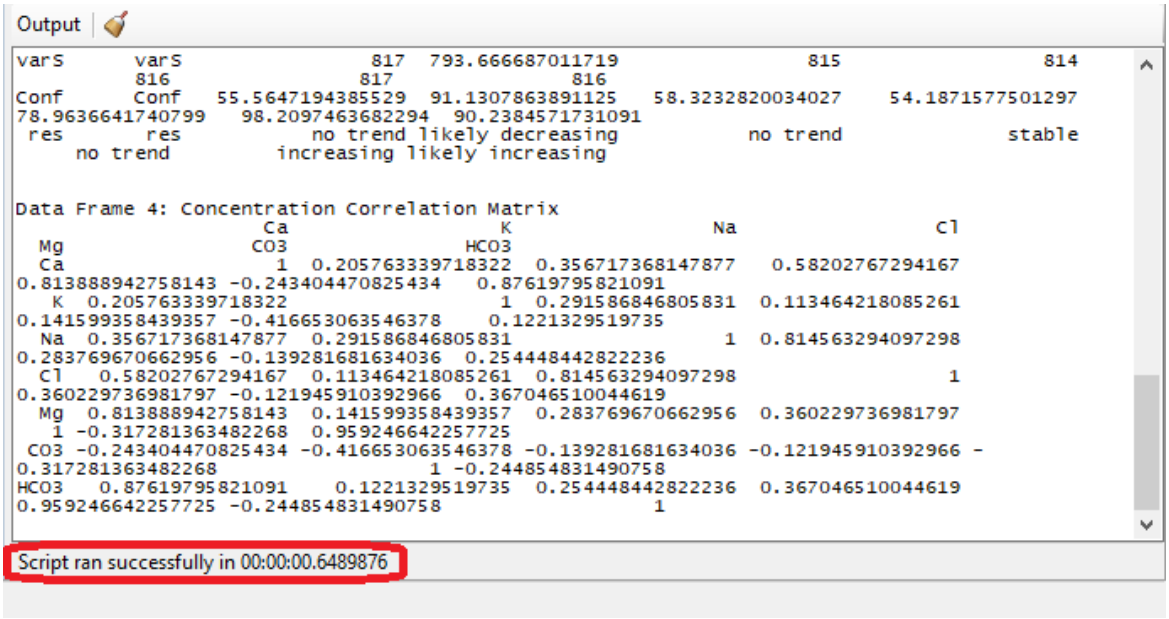
- **Get Sample Data** - the 2nd section (Lines 16- 46) is the section we have just worked on above. This section retrieves the desired data from the project database. The final portion of this section combines the new data vectors into a 'data frame' (i.e. table) and writes the data frame to an output data file (i.e. Stats2.CSV)

- **Calculate Basic Statistics** - the 3rd section (Lines 47-96) uses the new data vectors and calculates basic summary statistics (i.e. mean, standard deviation, coefficient of variation, max value, quantiles (75%, 50%, 25%) and minimum values) for the water quality parameters (Ca, K, Na, Cl, Mg, CO3 and HCO3). These summary statistics are written to vectors using the 'get_stats' function, and these vectors are then appended to the output file (i.e. Stats2.CSV)

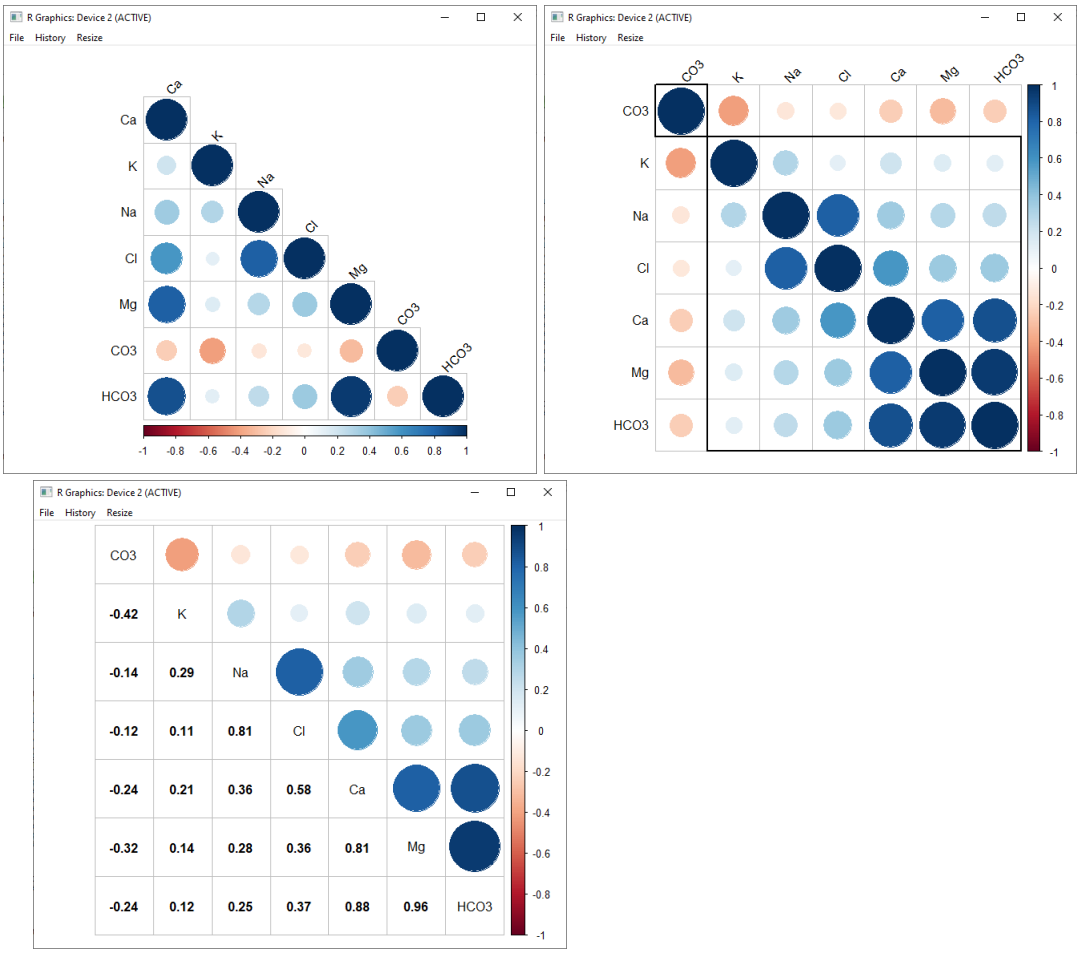
- **Estimate Mann-Kendall Trends** - the 4th section (Lines 97-180) uses the functionality of the 'Kendall' package to calculate the Mann-Kendall trend statistics for each of the water quality parameters. A function ('res') is then scripted to determine if there is an 'increasing', 'likely increasing', 'decreasing', 'likely decreasing', 'stable' or 'no trend' for each a parameter. Once again, the results of the trend test are then appended to the output file (i.e. Stats2.CSV)

- **Correlation Statistics** - the 5th and final section (Lines 181-206) calculates a correlation matrix between all available water quality parameters and then plots the results into three separate correlation matrix plots.

When you click the **'Run'** [ ] button a couple of things will happen as the script is executed. First, you should see that the script ran successfully as indicated under the 'Output' section:



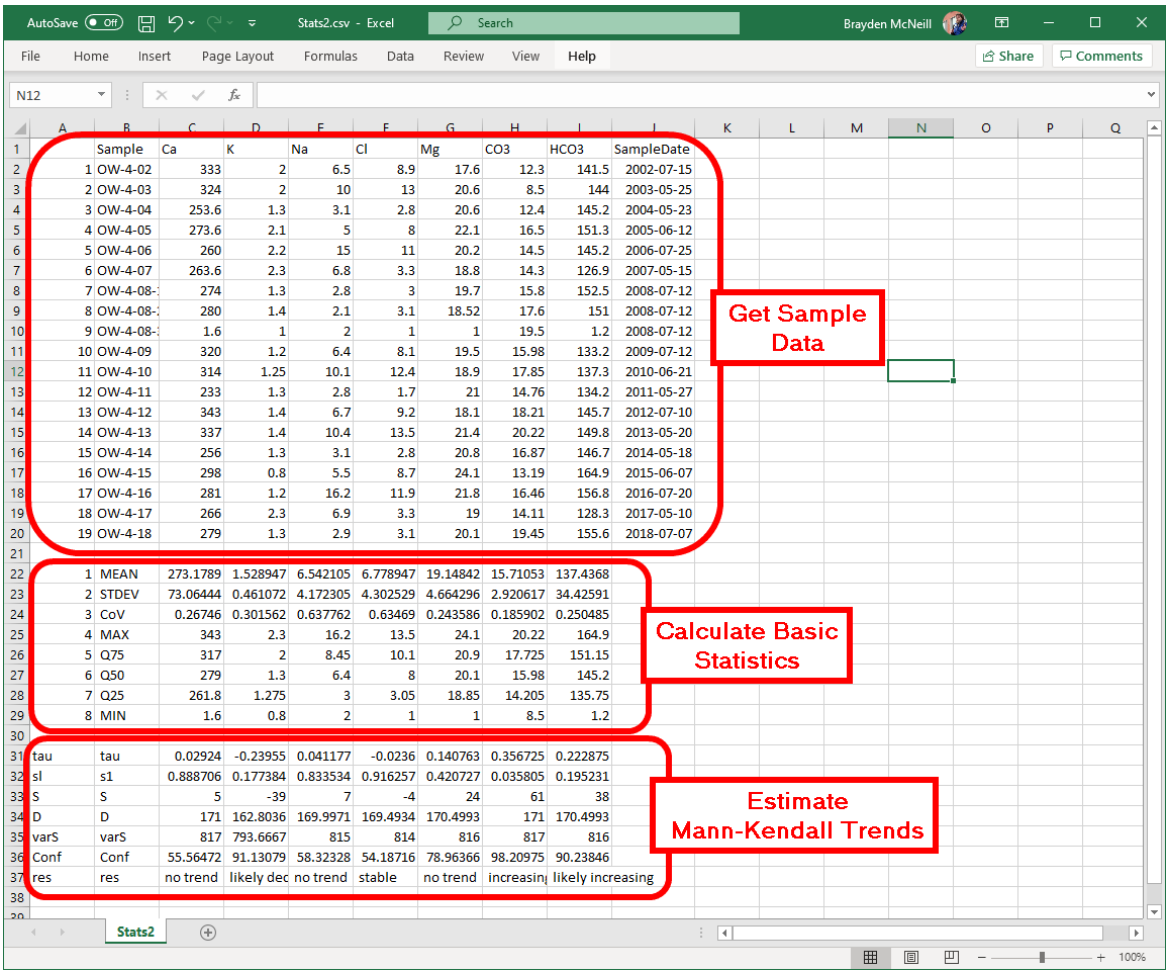
You should also see a new window entitled '**R-Graphics**' appear. You can click the 'Page Up' and 'Page Down' buttons on your keyboard to scroll between the available correlation plots, as shown below:



And finally, if you navigate to the 'Scripts' folder within the AquaChem Demo Project folder:

C:\Users\[username]\Documents\AquaChem\Projects\AQC 9 Demo\Scripts

you should find a new file called **'Stats2.CSV'** as shown below. The output file contains the results of the **'Get Sample Data**', '**Calculate Basic Statistics**' and '**Estimate Mann-Kendall Trends**' sections of the script described above:

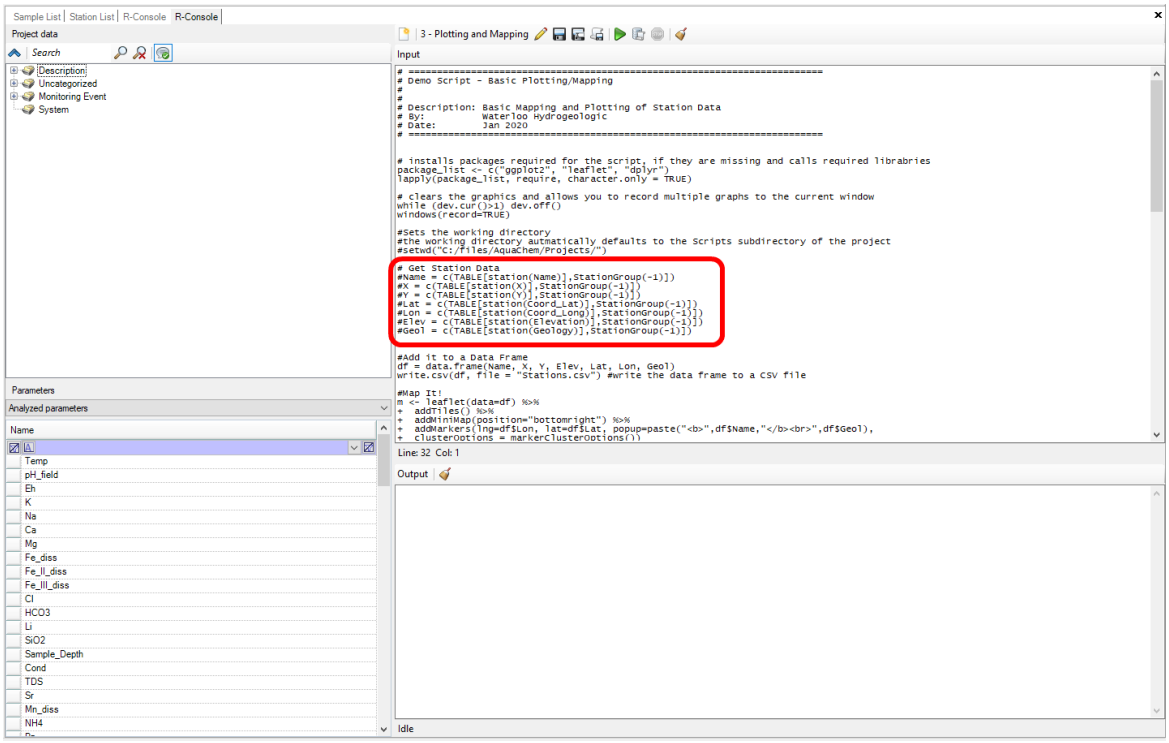


		Sample	Ca	K	Na	Cl	Mg	CO3	HCO3	SampleDate
2	1	OW-4-02	333	2	6.5	8.9	17.6	12.3	141.5	2002-07-15
3	2	OW-4-03	324	2	10	13	20.6	8.5	144	2003-05-25
4	3	OW-4-04	253.6	1.3	3.1	2.8	20.6	12.4	145.2	2004-05-23
5	4	OW-4-05	273.6	2.1	5	8	22.1	16.5	151.3	2005-06-12
6	5	OW-4-06	260	2.2	15	11	20.2	14.5	145.2	2006-07-25
7	6	OW-4-07	263.6	2.3	6.8	3.3	18.8	14.3	126.9	2007-05-15
8	7	OW-4-08-	274	1.3	2.8	3	19.7	15.8	152.5	2008-07-12
9	8	OW-4-08-	280	1.4	2.1	3.1	18.52	17.6	151	2008-07-12
10	9	OW-4-08-	1.6	1	2	1	1	19.5	1.2	2008-07-12
11	10	OW-4-09	320	1.2	6.4	8.1	19.5	15.98	133.2	2009-07-12
12	11	OW-4-10	314	1.25	10.1	12.4	18.9	17.85	137.3	2010-06-21
13	12	OW-4-11	233	1.3	2.8	1.7	21	14.76	134.2	2011-05-27
14	13	OW-4-12	343	1.4	6.7	9.2	18.1	18.21	145.7	2012-07-10
15	14	OW-4-13	337	1.4	10.4	13.5	21.4	20.22	149.8	2013-05-20
16	15	OW-4-14	256	1.3	3.1	2.8	20.8	16.87	146.7	2014-05-18
17	16	OW-4-15	298	0.8	5.5	8.7	24.1	13.19	164.9	2015-06-07
18	17	OW-4-16	281	1.2	16.2	11.9	21.8	16.46	156.8	2016-07-20
19	18	OW-4-17	266	2.3	6.9	3.3	19	14.11	128.3	2017-05-10
20	19	OW-4-18	279	1.3	2.9	3.1	20.1	19.45	155.6	2018-07-07
22	1	MEAN	273.1789	1.528947	6.542105	6.778947	19.14842	15.71053	137.4368	
23	2	STDEV	73.06444	0.461072	4.172305	4.302529	4.664296	2.920617	34.42591	
24	3	CoV	0.26746	0.301562	0.637762	0.63469	0.243586	0.185902	0.250485	
25	4	MAX	343	2.3	16.2	13.5	24.1	20.22	164.9	
26	5	Q75	317	2	8.45	10.1	20.9	17.725	151.15	
27	6	Q50	279	1.3	6.4	8	20.1	15.98	145.2	
28	7	Q25	261.8	1.275	3	3.05	18.85	14.205	135.75	
29	8	MIN	1.6	0.8	2	1	1	8.5	1.2	
31	tau	tau	0.02924	-0.23955	0.041177	-0.0236	0.140763	0.356725	0.222875	
32	sl	s1	0.888706	0.177384	0.833534	0.916257	0.420727	0.035805	0.195231	
33	S	S	5	-39	7	-4	24	61	38	
34	D	D	171	162.8036	169.9971	169.4934	170.4993	171	170.4993	
35	varS	varS	817	793.6667	815	814	816	817	816	
36	Conf	Conf	55.56472	91.13079	58.32328	54.18716	78.96366	98.20975	90.23846	
37	res	res	no trend	likely dec	no trend	stable	no trend	increasin	likely increasing	

You can close the resulting output file and plot windows and proceed to the third and final script.

Plotting and Mapping

Double-click the script '**3 - Plotting and Mapping**' from the Project Tree and you should see the following:

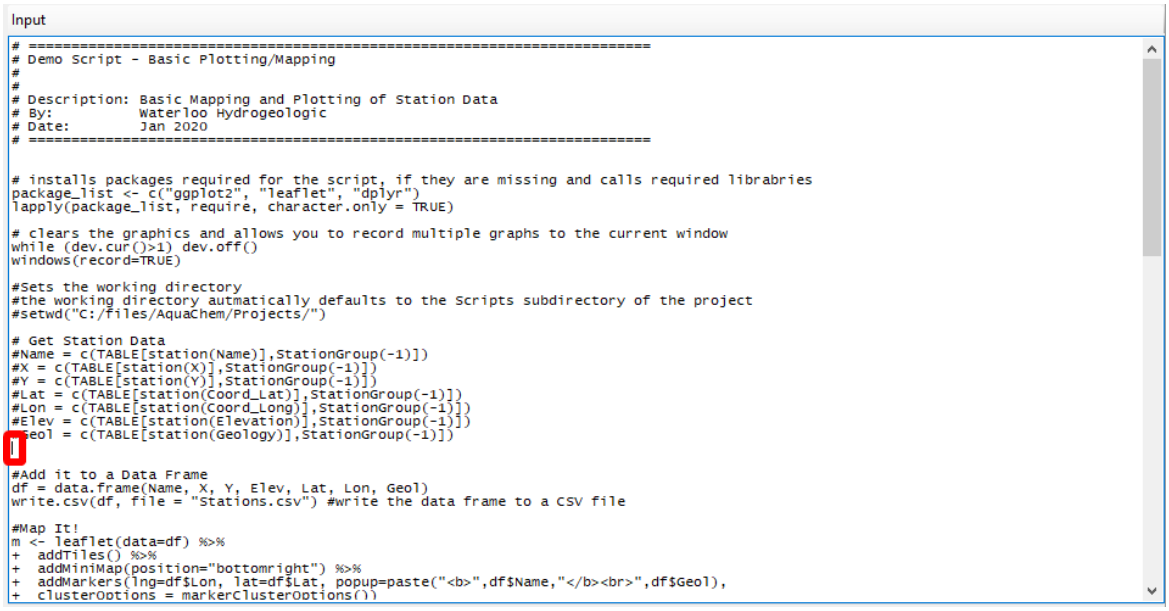


The Plotting and Mapping script is designed to fetch a set of station data from the Station Data table and perform some mapping and plotting based on that data. You will notice that the highlighted portion of the script in the image above has been 'commented out' by using a '#'. This is because you will use the 'Project data' section of the interface to facilitate the selection of this station data. We need to recreate the data variable definition commands for the Station Name, X, Y, Latitude, Longitude, Elevation and Geology list variables.

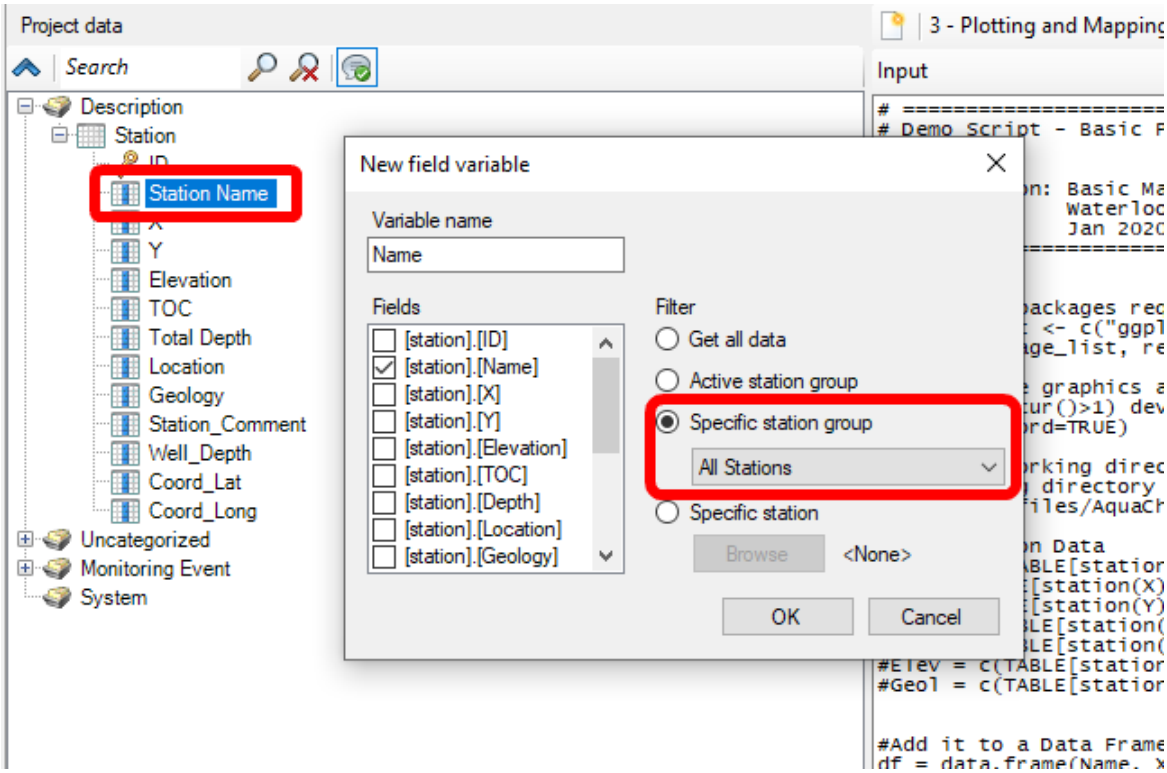
To start, make sure that the cursor lies just below the line that reads:

```
#Geol = c(TABLE[station(Geology)])
```

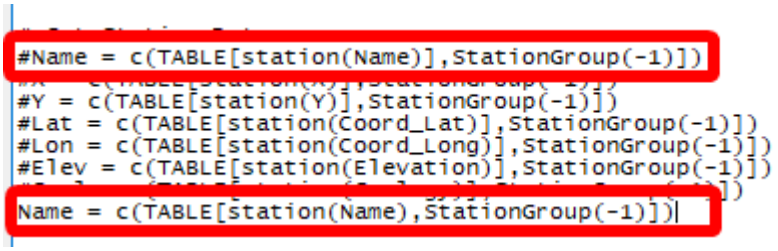
as highlighted in the script below:



Next, in the Project data section expand the 'Description' data category and further expand the 'Station' table. Double-click the 'Station Name' data field and the '**New field variable**' window will open as shown below. The default variable name (i.e. 'Name') will suffice, and if the 'All Stations' station group is not already active, please ensure that you specify it by selecting the 'Specific station group' option:



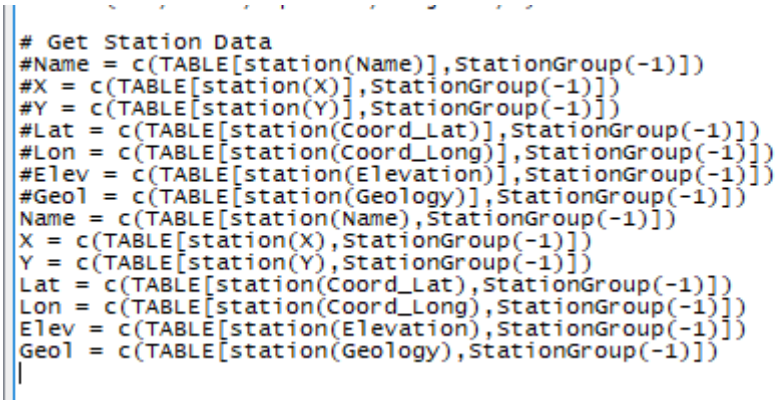
Click OK and you should see the new vector of station data added into the script as shown below, effectively recreating the first line in the 'Get Station Data' portion of this script:



Repeat these steps to create a new data object for the X, Y, Coord_Lat [Lat], Coord_Long [Lon], Elevation [Elev] and Geology [Geol] fields.

> **Please Note**: make sure to rename the variable to the name in [square brackets] above (i.e. the same variable as indicated in the original script)

Once you have selected all the necessary data fields the script should look like the image below:



This demonstrates the power of the R-console module within AquaChem, which facilitates the selection of Station Data table fields and the automatic scripting of the data into a new vector data object.

At this point you can click the **'Run'** [▶] button in the toolbar to execute the script, but it is recommended to take some time to review the entirety of the script before you do. Each portion of the script is explained through annotation within the script itself, so this tutorial doesn't review everything in fine detail. However, a short explanation of each 'section' of this script is provided below:

- **Description section** - the first section (Lines 1-21) provides some basic description of the script, invokes the required libraries and sets the 'working directory' (i.e. the name of the output file). Please note that by default in AquaChem, the location of output data will be in the 'Scripts' folder within the AquaChem project folder.

- **Get Station Data section** - the second section (Lines 22-43) is the section we have just altered in order to retrieve the necessary station data fields. The final portion of this section combines the new data vectors into a 'data frame' (i.e. table) and writes the data frame to an output data file (i.e. Stations.CSV)

- **Map It! section** - the third section (Lines 44-51) relies on the functionality of the 'leaflet' library to map the station data to a webpage. When this section of the script is run a new tab will open in your web-browser and will display the location of the project stations.

- **Plot It! section** - the fourth and final section (Lines 52-114) relies on the functionality of the 'ggplot2' librabry to create five different charts. chart1 and chart2 plot the X vs. Y data and X vs. Elev data, respectively. On and following Line 66, some additional sample data (i.e. Na and Cl data from station MW-1) is retrieved and plotted in 3 additional charts: chart3 displays the Cl concentrations at MW-1 over time, chart4 provides a scatter plot of Cl vs Na data at MW-1, and chart5 displays both Na and Cl concentrations over time (and includes 'regression' lines)

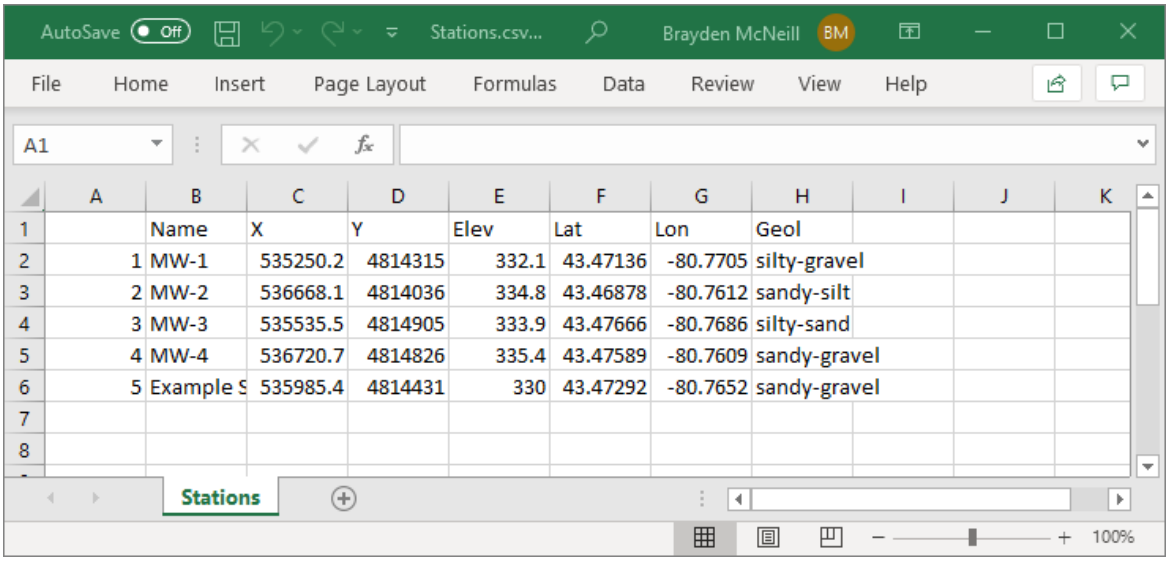
So when you click the **'Run'** [▶] button a couple of things will happen as the script is executed.

First, you should see that the script ran successfully as indicated under the 'Output' section.

Secondly, if you navigate to the 'Scripts' folder within the AquaChem Demo Project folder:

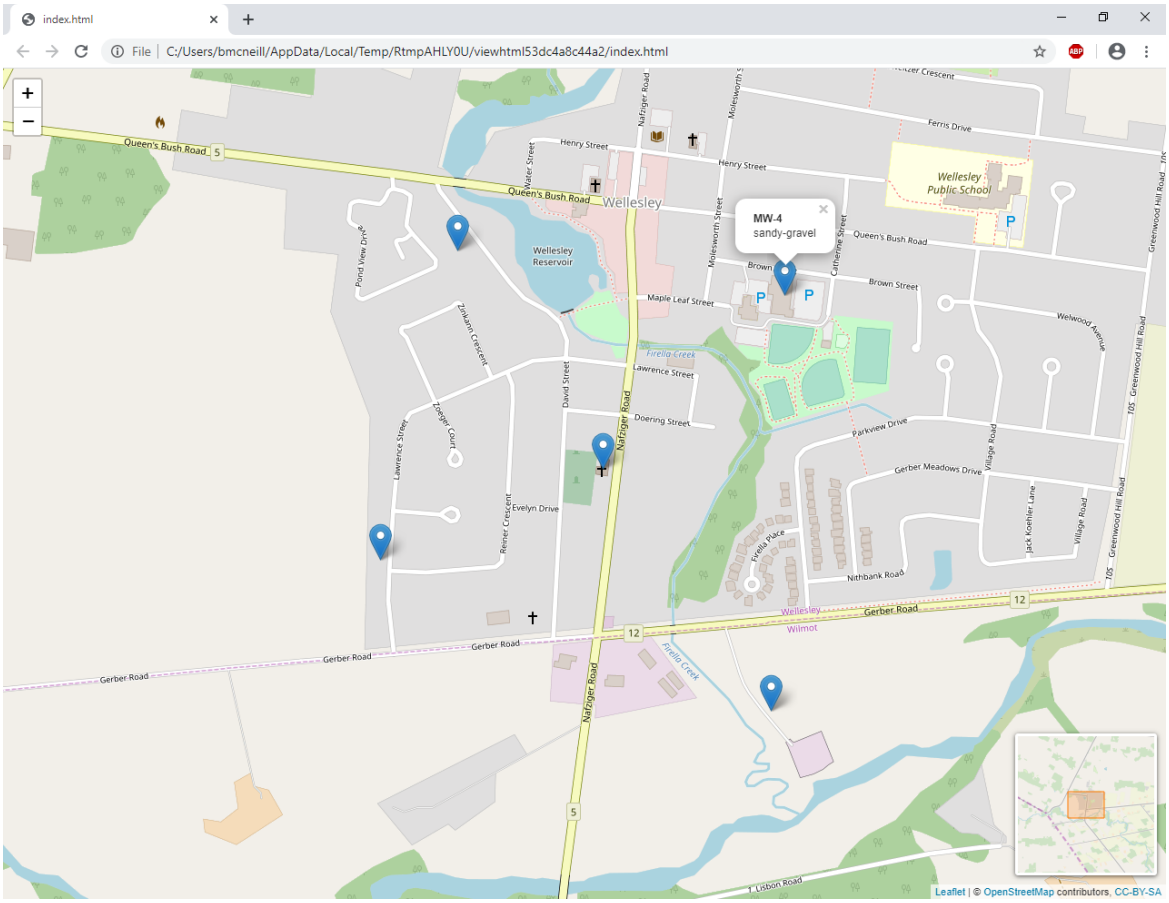
C:\Users\[username]\Documents\AquaChem\Projects\AQC 9 Demo\Scripts

you should find a new file called **'Stations.CSV'** as shown below. The output file contains the results of the 'Get Station Data' section (i.e. Station Name, X, Y, Elevation, Latitude, Longitude and Geology data):



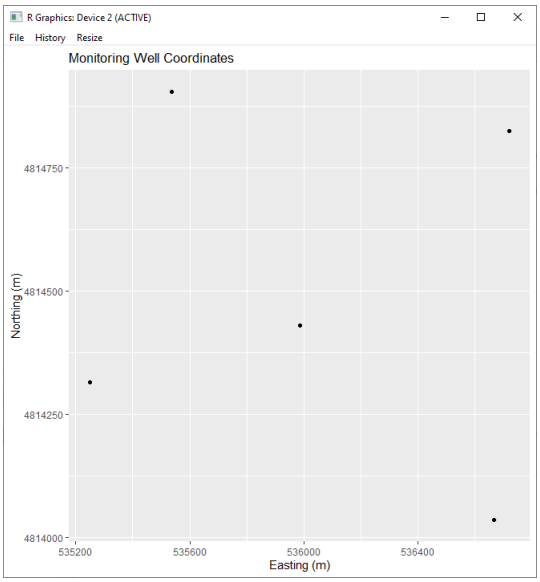
	A	B	C	D	E	F	G	H
1		Name	X	Y	Elev	Lat	Lon	Geol
2	1	MW-1	535250.2	4814315	332.1	43.47136	-80.7705	silty-gravel
3	2	MW-2	536668.1	4814036	334.8	43.46878	-80.7612	sandy-silt
4	3	MW-3	535535.5	4814905	333.9	43.47666	-80.7686	silty-sand
5	4	MW-4	536720.7	4814826	335.4	43.47589	-80.7609	sandy-gravel
6	5	Example S	535985.4	4814431	330	43.47292	-80.7652	sandy-gravel
7								
8								

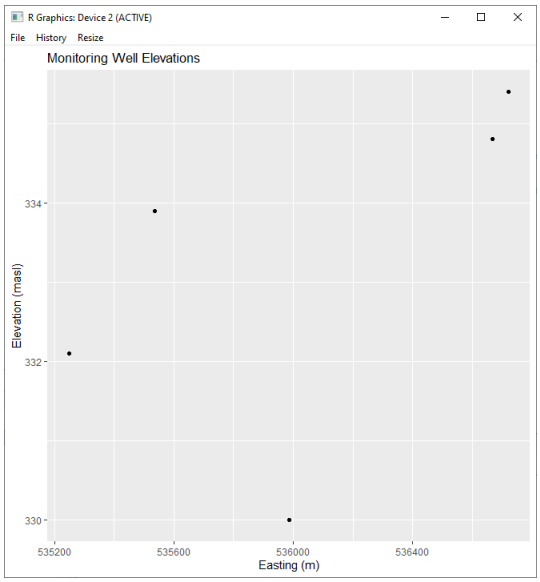
Third, a new tab should open in your default internet browser with the results of the Map It! section. You should see all five of the stations from this project displayed within the associated map (all stations are located in 'Wellesley', a small town near Waterloo, Ontario, Canada). If you click on any of the stations, a small info bubble will appear to display the station name and geology designation, as shown below:

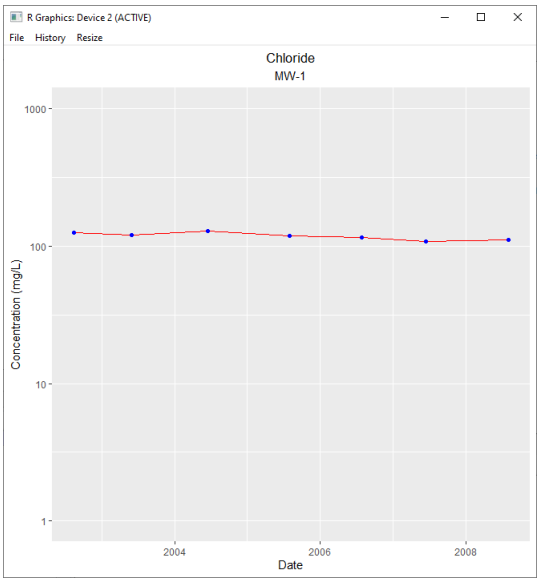


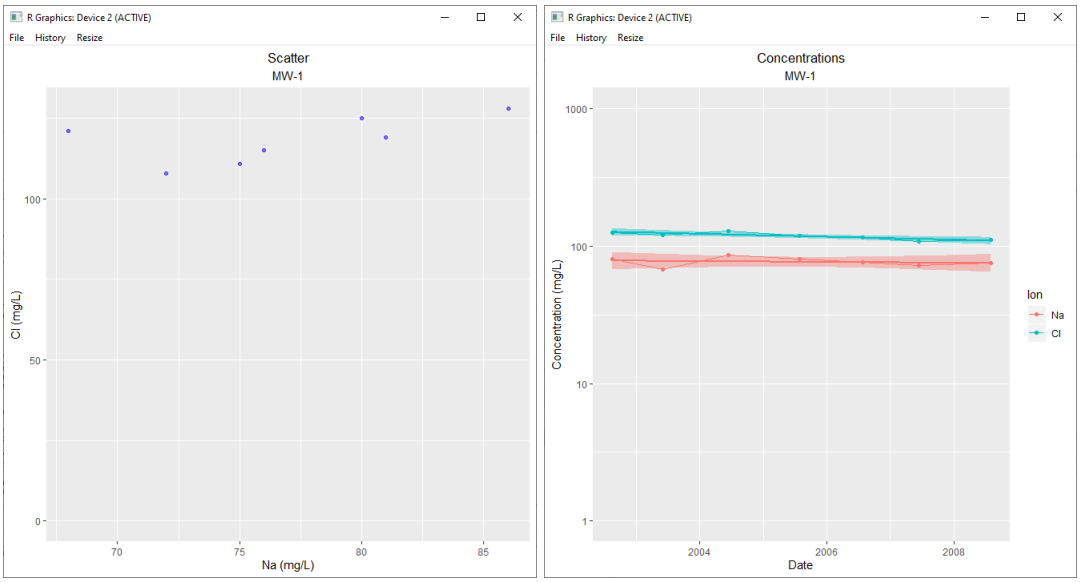
Please Note: this is a fully interactive map of the world. Feel free to zoom in and out, scroll around, etc. In fact, if you zoom out far enough, you will notice that the location markers will cluster; which is useful if you have a lot of data concentrated in a given area of the map. You may also notice the map inset in the lower right corner of the map which may be useful when you need to view the map at different scales of interest.

And finally, you should also see a new window 'R-Graphics' appear. You can click the 'Page Up' and 'Page Down' buttons on your keyboard to scroll between the available correlation plots, as shown below:


R Graphics: Device 2 (ACTIVE)
File History Resize
Monitoring Well Coordinates
Northing (m)
4814750
4814500
4814250
4814000
535200
535600
536000
536400
Easting (m)


R Graphics: Device 2 (ACTIVE)
File History Resize
Monitoring Well Elevations
Elevation (masl)
334
332
330
535200
535600
536000
536400
Easting (m)


R Graphics: Device 2 (ACTIVE)
File History Resize
Chloride
MW-1
Concentration (mg/L)
1000
100
10
1
2004
2006
2008
Date



Once again, it bears repeating that this tutorial is not a comprehensive introduction to the R scripting language. By reviewing the basic scripts included in the AquaChem Demo Project, you may be able to learn how to apply some of these scripts to your own projects. However, it is highly recommended that you study the available resources at the R Foundation website in order to better familiarize yourself with R.

- This concludes the AquaChem Demo Project tutorial -

2.2 Creating a New Project and Importing Data

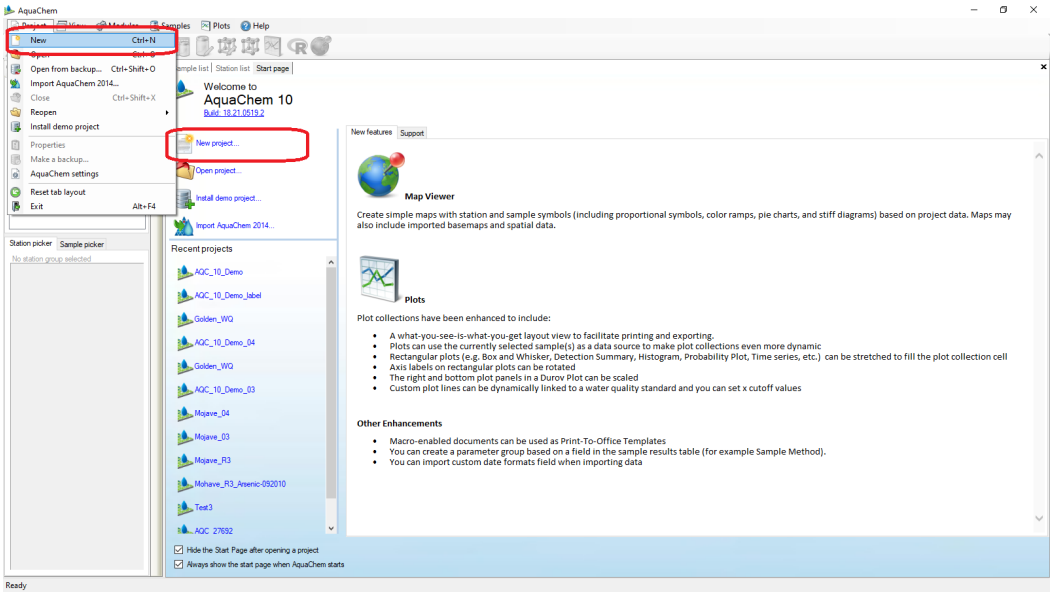
Creating new projects in AquaChem 10.0 is fairly simple process: to create a new project, you first specify the project name and location and select an existing database template to define the initial structure of the database. When the project has been created, you may want to customize the database structure to suit the needs of your specific project. Once the database structure has been updated to match your data requirements, you will populate the project with data using any of the available import methods (General, Samples, or Images).

This entire process is explained in this short tutorial, which has three sections:

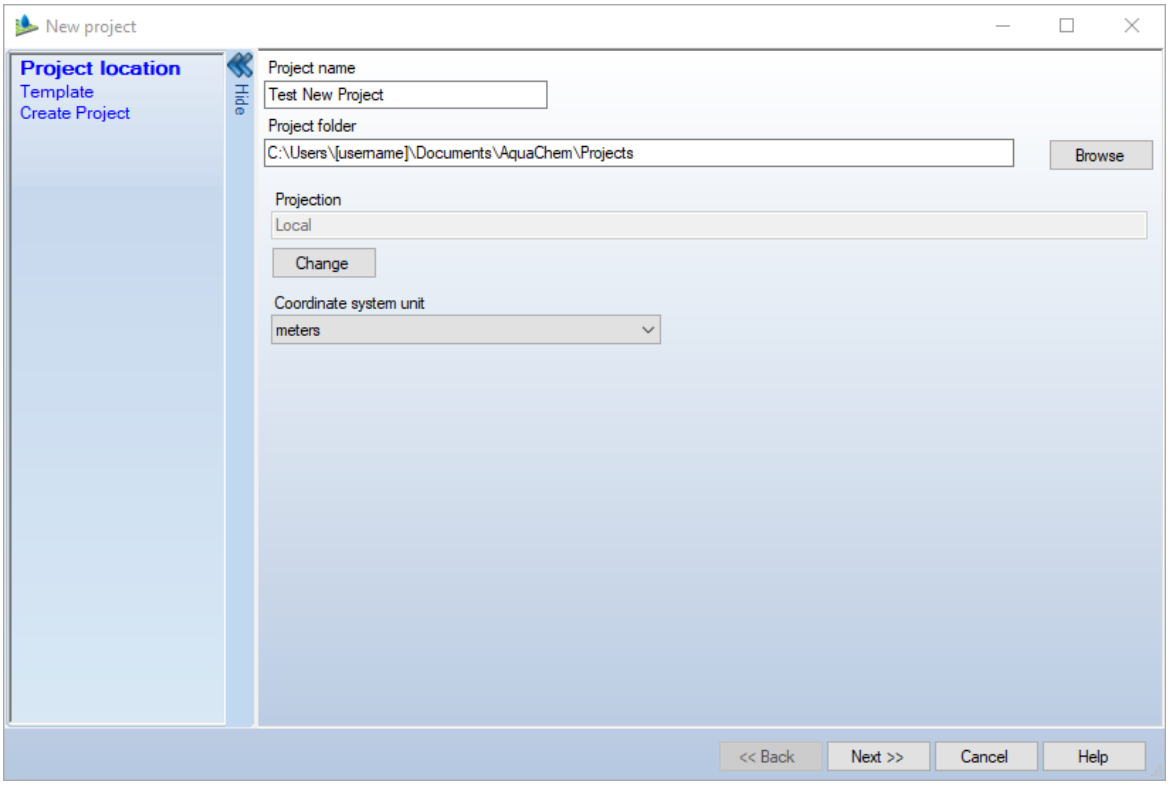
- **Creating a Database**
- **Configuring the Database**
- **Importing Data**

2.2.1 Creating a Database

To create a new AquaChem 10.0 project, first launch the application and access the Start Page. You should see a '**New project...**' button. Alternatively, you can click '**Project > New**' from the main menu:



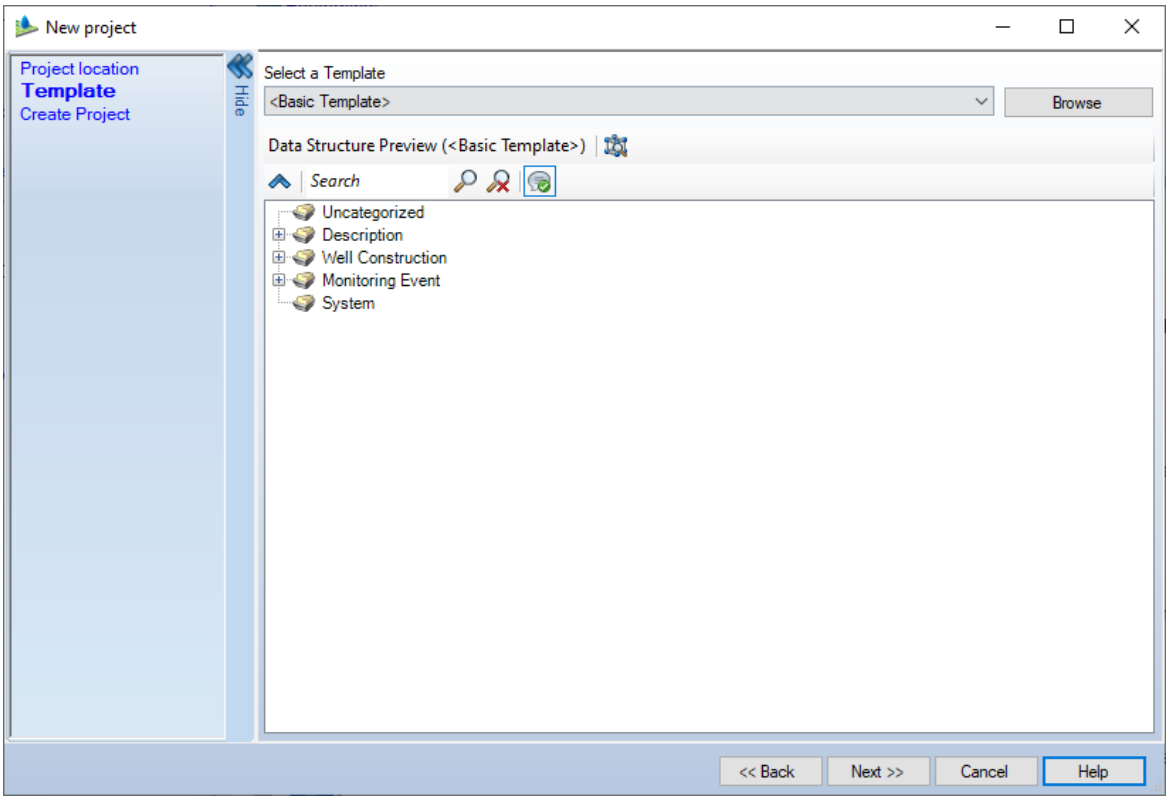
Clicking either of these buttons will open the 'New Project' window, as shown below:



Enter a name of your choice (e.g. 'Test New Project'), and specify the location of the Project Folder. By default the new project will be saved to the AquaChem Projects folder:

- *C:\Users\[username]\Documents\AquaChem\Projects*

When you have entered a name selected the project folder, click the Next >> button to proceed to the template selection step, as shown below:

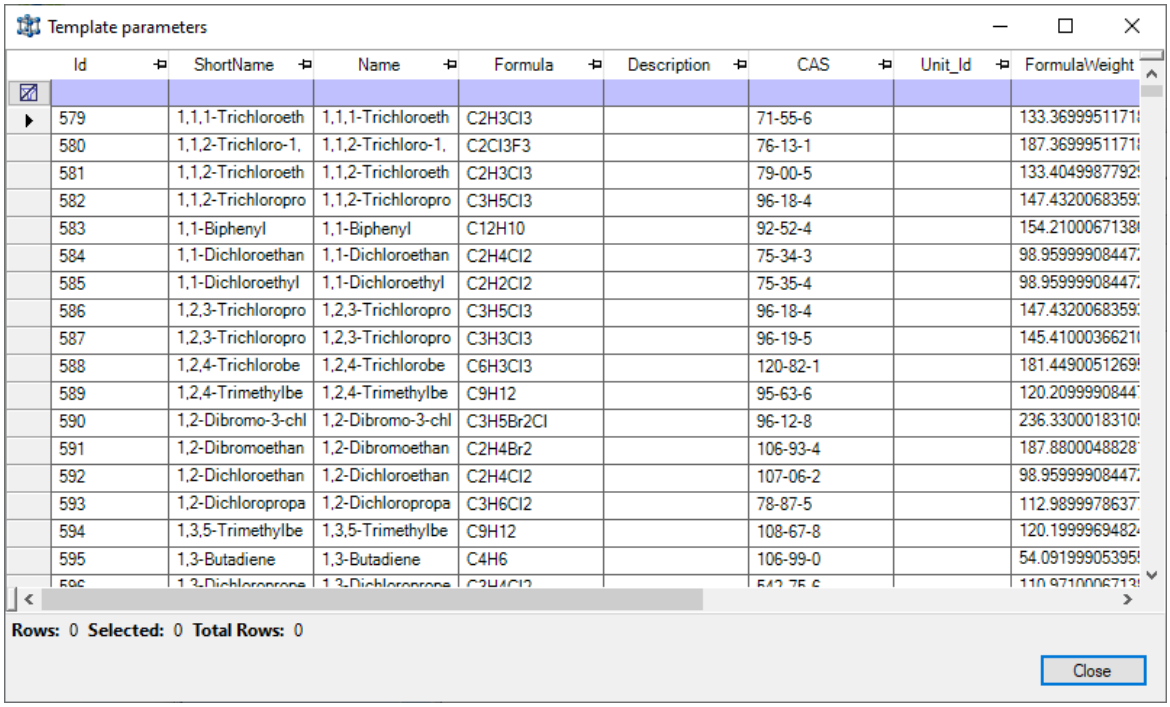


The template is an empty database that contains all necessary data tables, parameters, settings, etc., but does not contain sample or station data. When you create a new database, the database template is copied to the specified filename and location. Choosing a template simply means that your project will use the same data structure (e.g. same Sample, Station, and Analytical Parameters) as the selected template.

Two default database templates are available upon installation of AquaChem; a **Basic** template, and an **Advanced** template. The database structure (including database tables and fields) can be reviewed for both of these templates by expanding the data categories listed in the 'Data Structure Preview' table.

The primary differences between the Basic and Advanced templates are in the Station and Sample tables, each of which contain several additional fields. For example, the Station table in the Advanced template includes fields for Location, Geology, Lat, Long and many others, in addition to the fields available within the Basic template (i.e. ID, Station Name, X, Y, Elevation, TOC and Total Depth). In both templates the Sample table contains fields for the SampleID, Name, SampleDate, AnalysisDate, Symbol and Station, whereas the Advanced template includes additional descriptive fields such as REP (indicating whether the sample is representative), Comment, WaterType, LabCode, DuplicateID, Odor, Color, etc.

You can also review the water quality parameters available in the templates by clicking the 'View Parameters' [ ] button, which opens the 'Templates parameters' window, as shown below (table below is for the Basic template):

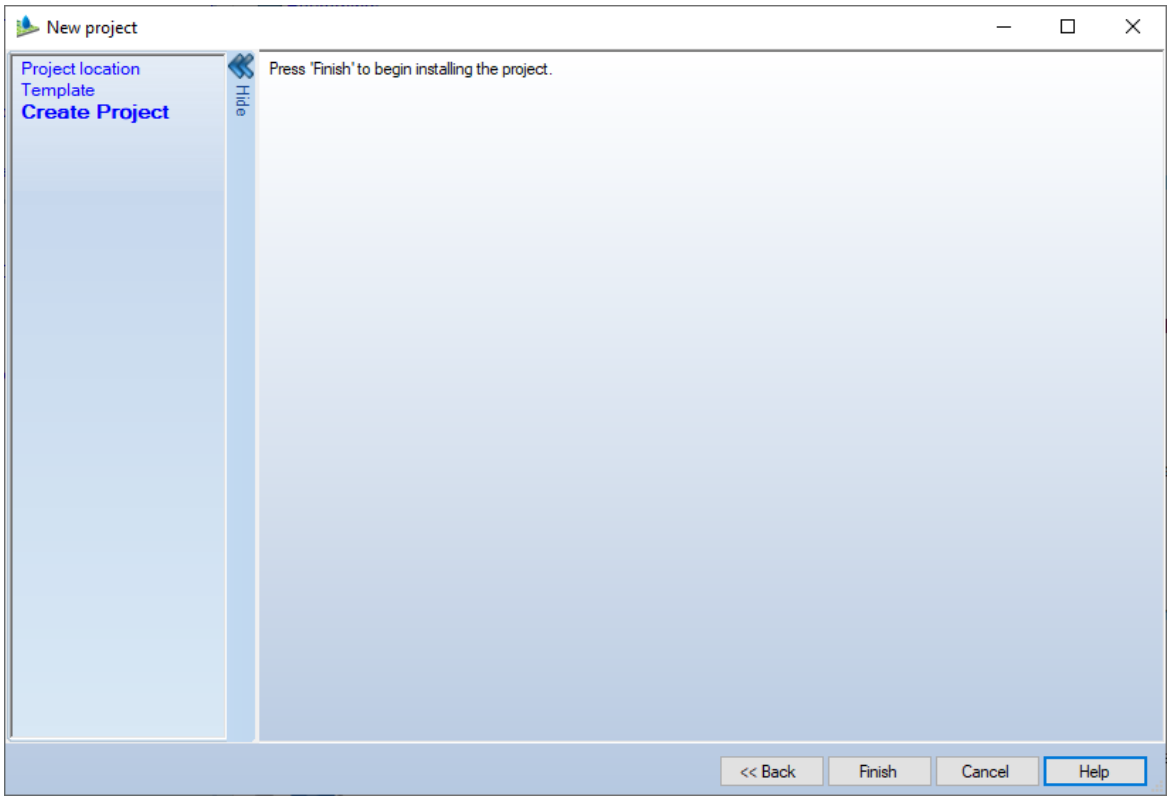


Id	ShortName	Name	Formula	Description	CAS	Unit_Id	FormulaWeight
579	1,1,1-Trichloroeth	1,1,1-Trichloroeth	C2H3Cl3		71-55-6		133.3699951171
580	1,1,2-Trichloro-1,	1,1,2-Trichloro-1,	C2Cl3F3		76-13-1		187.3699951171
581	1,1,2-Trichloroeth	1,1,2-Trichloroeth	C2H3Cl3		79-00-5		133.4049987792
582	1,1,2-Trichloropro	1,1,2-Trichloropro	C3H5Cl3		96-18-4		147.4320068359
583	1,1-Biphenyl	1,1-Biphenyl	C12H10		92-52-4		154.2100067138
584	1,1-Dichloroethan	1,1-Dichloroethan	C2H4Cl2		75-34-3		98.95999908447
585	1,1-Dichloroethyl	1,1-Dichloroethyl	C2H2Cl2		75-35-4		98.95999908447
586	1,2,3-Trichloropro	1,2,3-Trichloropro	C3H5Cl3		96-18-4		147.4320068359
587	1,2,3-Trichloropro	1,2,3-Trichloropro	C3H3Cl3		96-19-5		145.4100036621
588	1,2,4-Trichlorobe	1,2,4-Trichlorobe	C6H3Cl3		120-82-1		181.4490051269
589	1,2,4-Trimethylbe	1,2,4-Trimethylbe	C9H12		95-63-6		120.2099990844
590	1,2-Dibromo-3-chl	1,2-Dibromo-3-chl	C3H5Br2Cl		96-12-8		236.3300018310
591	1,2-Dibromoethan	1,2-Dibromoethan	C2H4Br2		106-93-4		187.8800048828
592	1,2-Dichloroethan	1,2-Dichloroethan	C2H4Cl2		107-06-2		98.95999908447
593	1,2-Dichloropropa	1,2-Dichloropropa	C3H6Cl2		78-87-5		112.9899978637
594	1,3,5-Trimethylbe	1,3,5-Trimethylbe	C9H12		108-67-8		120.1999969482
595	1,3-Butadiene	1,3-Butadiene	C4H6		106-99-0		54.09199905395

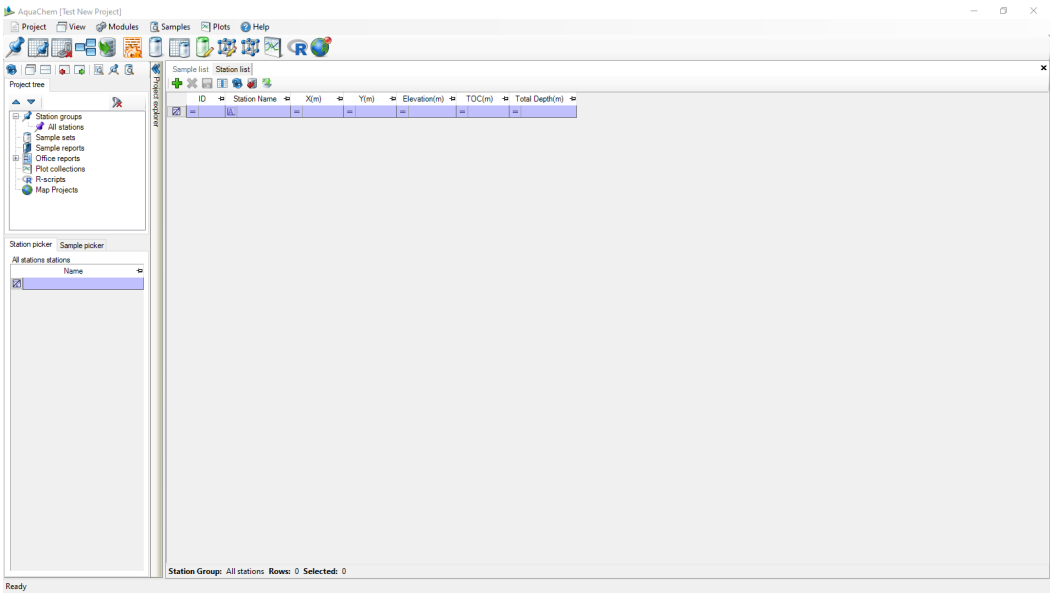
Once again, the Advanced template provides a larger selection of database parameters compared to the Basic template.

Spend some time reviewing the database templates. Keep in mind that these templates may not contain ALL the database fields or parameters that are required for your project. However, once the project has been created you will be able to update the database structure and parameters to meet your needs. The customized database structure can then be saved as a new database template, which can be reused for future projects. If/when a custom database template is required simply click the 'Browse' button. Any custom database templates (*.hgat) which you have created can be used by selecting them with the Windows file explorer that opens.

For now, simply select the <Basic Template> from the 'Select a Template' menu, and click the Next >> button. This brings you to the 'Create Project' step, as shown below:



At this stage simply click Finish button to create the new (empty) database. Once the database has been created the 'Station List' tab will be shown:



At this point it's a good idea to use the Template Manager module to configure the database structure, before eventually importing your data.

2.2.2 Configuring the Database

Database configuration is the process of updating the structure of your database so that it meets all of your project needs. You will be importing a small data set from two Microsoft Excel spreadsheets, one for station data and a second for water quality measurements. Let's review those spreadsheets and determine if any database configuration is required. The data sources for this tutorial (**'Stations.xlsx'** and **'Water Quality Data.xlsx'**) can be found in the following location:

C:\Users\[username]\Documents\AquaChem\Tutorial Files\New Project Tutorial

Recall that stations are records that represent a single location with an X- and Y-coordinate, often including associated metadata. A review of the **'Stations.xlsx'** data file reveals that there are four stations to be imported (MW-1, MW-3, OW-2 and OW-4) and that the following metadata are available for each station:

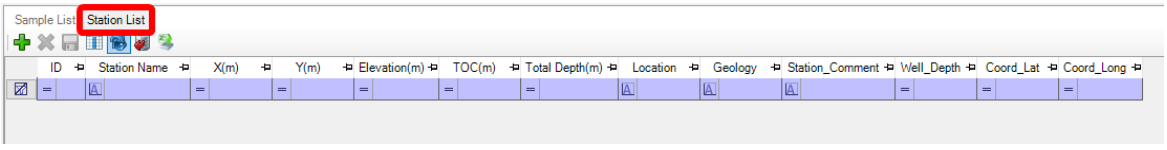
- **Station Name** - project specific name associated with each location (not to be confused with Station IDs, which are unique identifying codes used internally by AquaChem)
- **Geology** - describes the soil type/geology of the sample location
- **X/Y** - coordinate data
- **Elevation** - ground elevation at the sample location
- **TOC** - elevation of the well casing at the sample location
- **Well_Depth** - total depth of the sample well
- **Depth_to_Sample_Point** - depth from the TOC elevation to the sample point
- **Station_Comment** - information regarding installation date/contractor
- **Aquifer_Code** - simple project based code identifying the aquifer in which the sample point resides

A review of the **'Water Quality Data.xlsx'** file indicates that there are 28 samples to import with up to 33 parameters each. Sample metadata include the following:

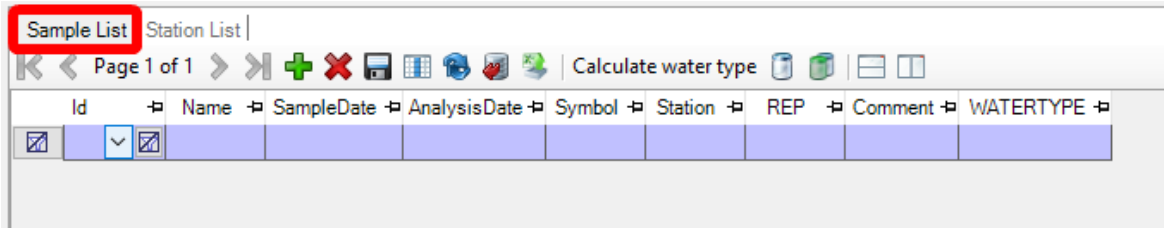
- **Sample_Name** - unique name for each sample (not to be confused with Sample IDs which are unique identifying codes used internally by AquaChem)
- **Station_Name** - same as above
- **Sample_Date** - specific date/time that the sample was collected
- **Analysis_Date** - specific date/time that the sample was analyzed by the laboratory

The available station and sample metadata can be compared against the current database structure by simply reviewing the columns listed in the 'Station List' and 'Sample List' tabs:

Station List:



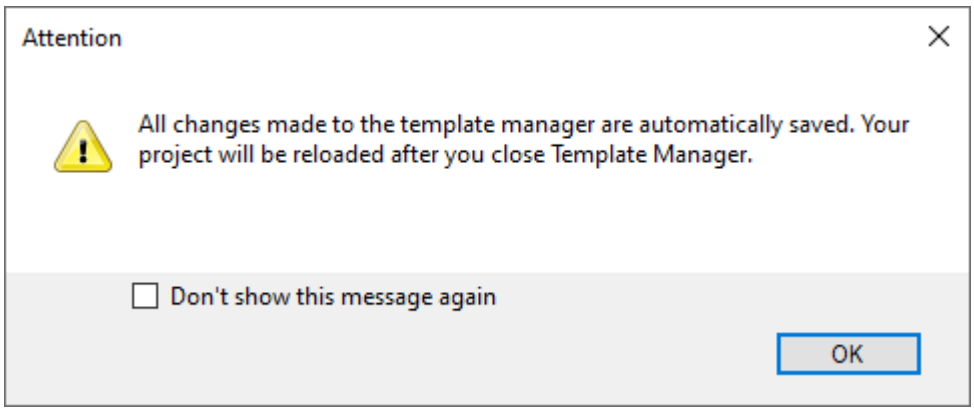
Sample List:



As you can see from the image above, the Station List does not include a column for all the metadata associated with our samples. You can review specific information about individual database tables/fields using the Template Manager module, which also allows you to add, remove or otherwise customize any database table.

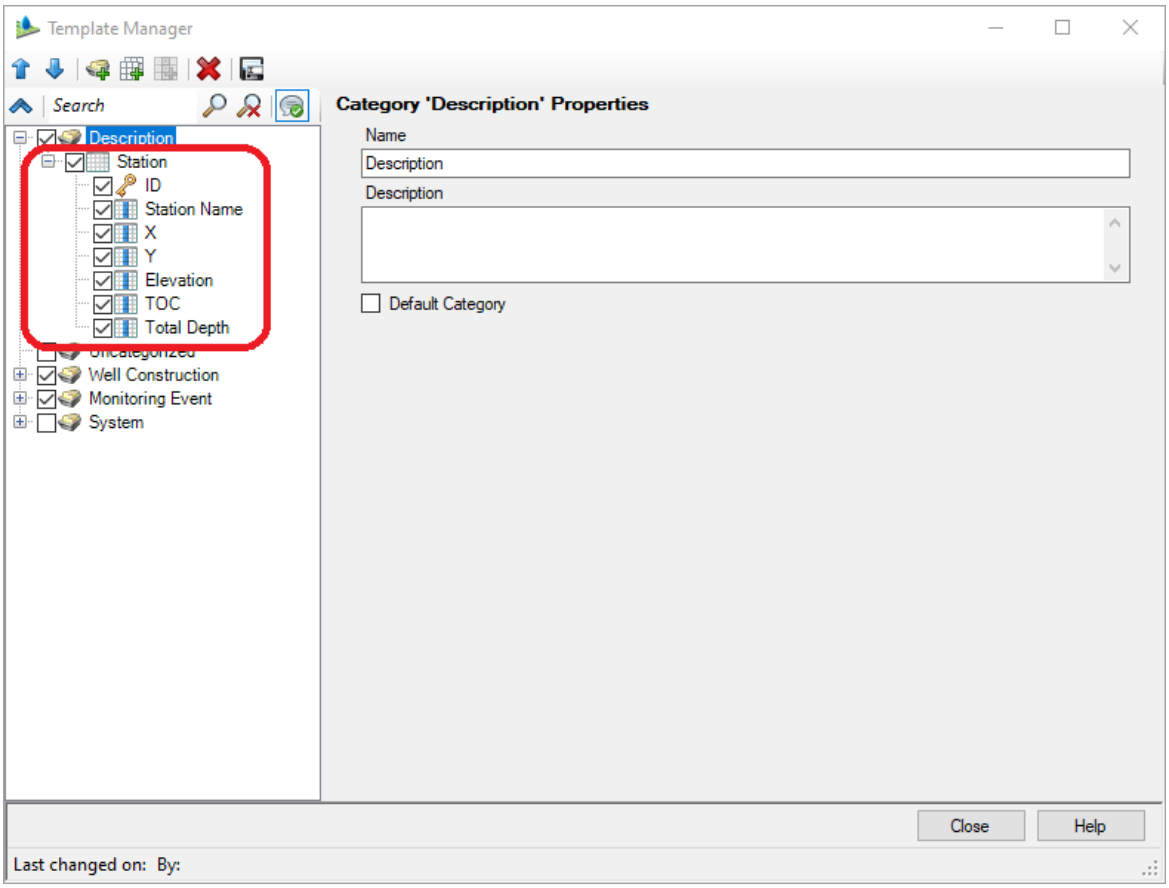
Access the Template Manager module by clicking **'Modules > Template Manager**' from the main menu or by clicking the button in the main toolbar.

A notification will appear indicating that all changes to the template manager are automatically saved and permanent.

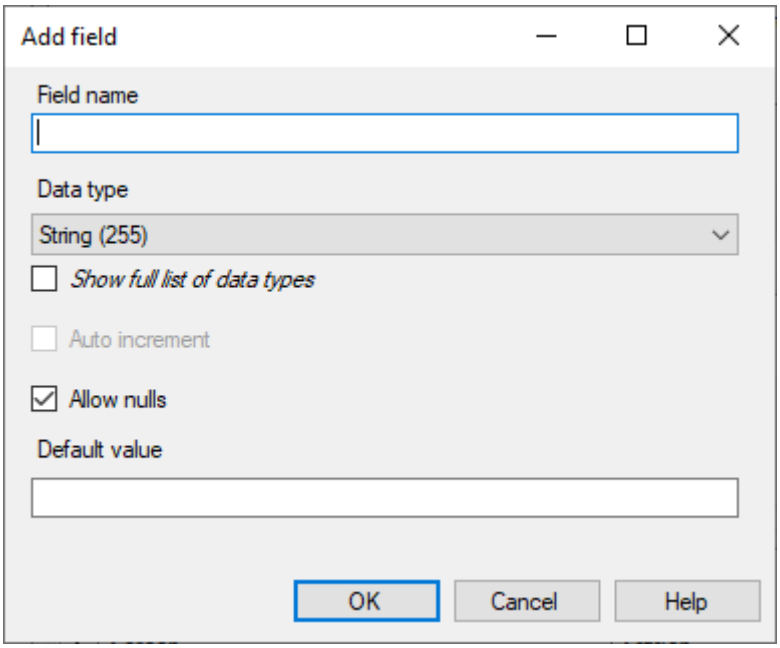


WARNING: Please take special note of the message above!
AquaChem provides you with near absolute control over the structure of the database, but this control does present some dangers! If any database tables/fields are deleted the data records associated with those fields will be permanently lost. With that in mind, **it's always preferable to customize the database structure *BEFORE* you begin importing your data!**

Click OK to dismiss the message and the **Template Manager** module will appear. Expand the **'Station'** node in the database tree on the left in order to review the contents of the Station table (i.e. click the ⊞ button next to 'Station'):



Let's add the missing station metadata fields (e.g. Depth_to_Sample_Point and Aquifer_Code) to the Station table by selecting the table in the database tree on the left and clicking the 'Add a new field' button [] in the toolbar. This will open the **'Add field'** window, as shown below:



At this stage you can add a name for the new field, select from available data types, and specify whether null values will be allowed in this field.

Type the name of the field (e.g. 'Aquifer_Code') into the **'Field name'** and click OK to add the field to the Station table. The 'Aquifer_Code' field is based on the 'String (255)' data type and does not require any additional changes. Repeat for the remaining station metadata, creating a new field for each, using the data types listed below (make sure to also specify the unit category and unit of the 'Depth_to_Sample_Point' and 'Well_Depth' fields):

- **Aquifer_Code** - String (255)
- **Geology** - String (255)
- **Station_Comment** - String (255)
- **Depth_to_Sample_Point** - Double
  - **Unit category** = length, Unit = meters
- **Well_Depth** - Double
  - **Unit category** = length, Unit = meters

You can also hide unneeded database fields by clicking the checkbox next to the database field, or alternatively you can delete them using the 'Delete Selected Item' [ ] button in the toolbar. Hiding unnecessary database fields is generally favorable since they can be easily reactivated and used at a later time. You can see here that there are several fields in both the Station table and the Sample table which are not required, based on the contents of the source data files.

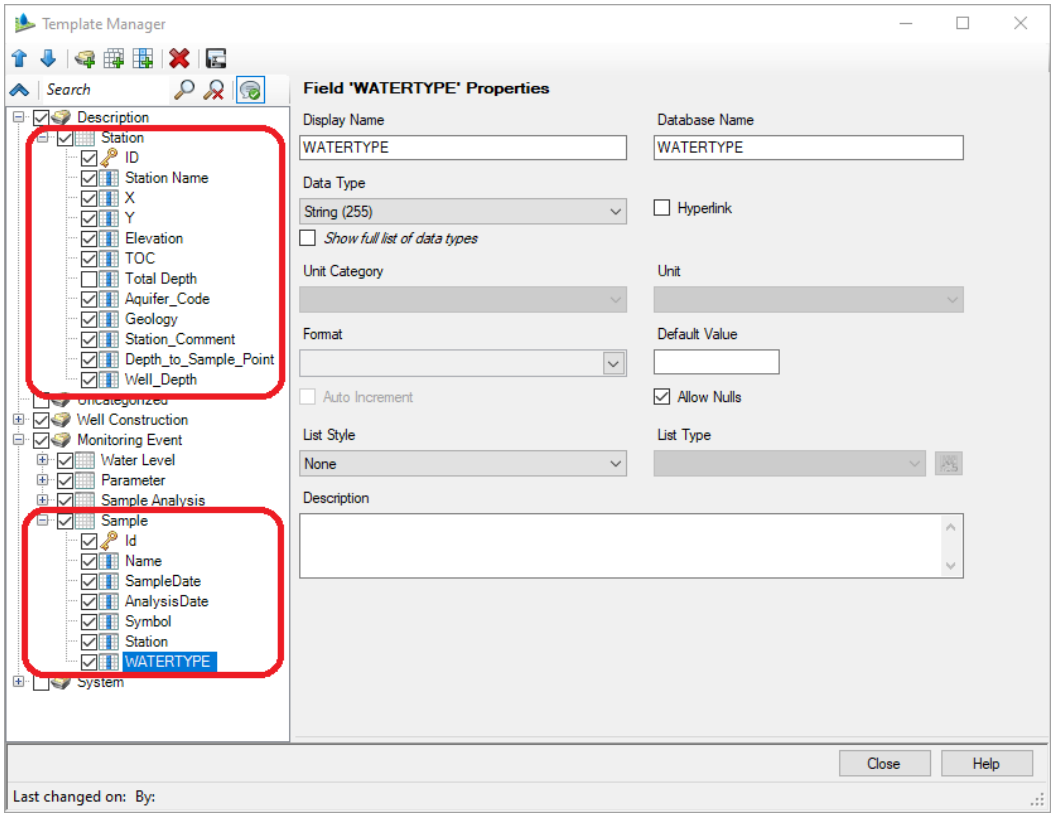
'Hide' the following field by deselecting the checkbox [☑] next to its label in the database tree on the left:

- **Total Depth**

To accommodate the sample data, you will also have to make some changes to the Sample table (under the Monitoring Event data category).

- Select and expand the Sample table under the Monitoring Event category in the database tree on the left
- Click the 'Add a new field' [ ] button
- Add the following a field called **WATERTYPE** with a type of **String (255)**
- Select the **Station** field so that it is shown

When you are finished the Template Manager should look similar to the image below:

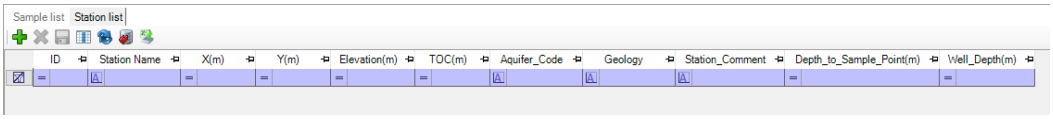


Please Note: it is also possible to rearrange the order of these data fields by dragging and dropping them or by selecting a field and using the move up/ down buttons.

If future projects are based on a similar database structure you can click the **'Export project settings as template'** button [] to save the current database structure as a template file (**.hgat* file; saved to the templates folder) which can be reused for subsequent projects.

For now, click Close to finalize the database configuration. Since changes have been made the project will be reloaded, as indicated by the information message:

Click OK reload the project. The Station List should be displayed once again, and all new data fields will be included:



This concludes a very simple tutorial on updating the AquaChem database structure by adding new data fields. However, please note that more advanced customizations can also be accomplished using the Template Manager including:

- Add or Delete tables and/or fields
- Alter the properties of tables and fields
- Define relationships between tables
- Group tables under logical data categories
- Save database templates for future projects
- Set visibility of tables and/or fields
- Set display formats for numeric and date fields
- Define required or optional lists of values

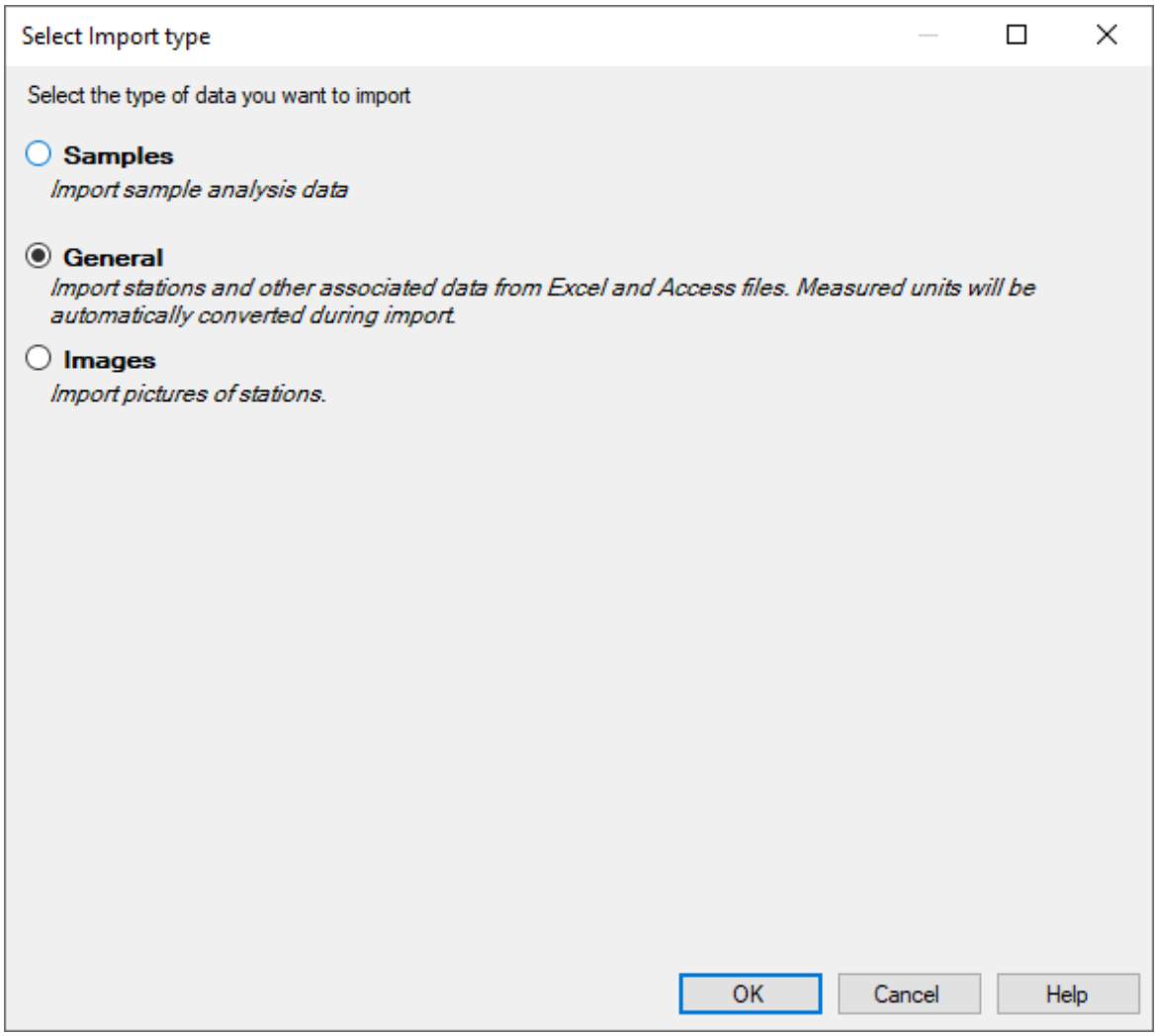
Now that the database structure has been updated to reflect our station data requirements, you can proceed to the next section of the tutorial which covers Importing Data.

2.2.3 Importing Data

Data can be brought into an AquaChem 10.0 project database in a number of ways, including manual data entry and importing a variety of file types (.txt, .csv, .xls, .xlsx, .mdb, and .accdb) with various structures (samples as rows, samples as columns, one analyzed value for each row).

In this section of the tutorial, you will review the process for importing station and sample data from Microsoft Excel spreadsheets, which is one of the more common import methods.

To initiate the data import process, open the Import Data Wizard using the main menu ('**Modules > Import Data**') or by clicking the button in the main toolbar. The first step when importing data is to select from the available data types:

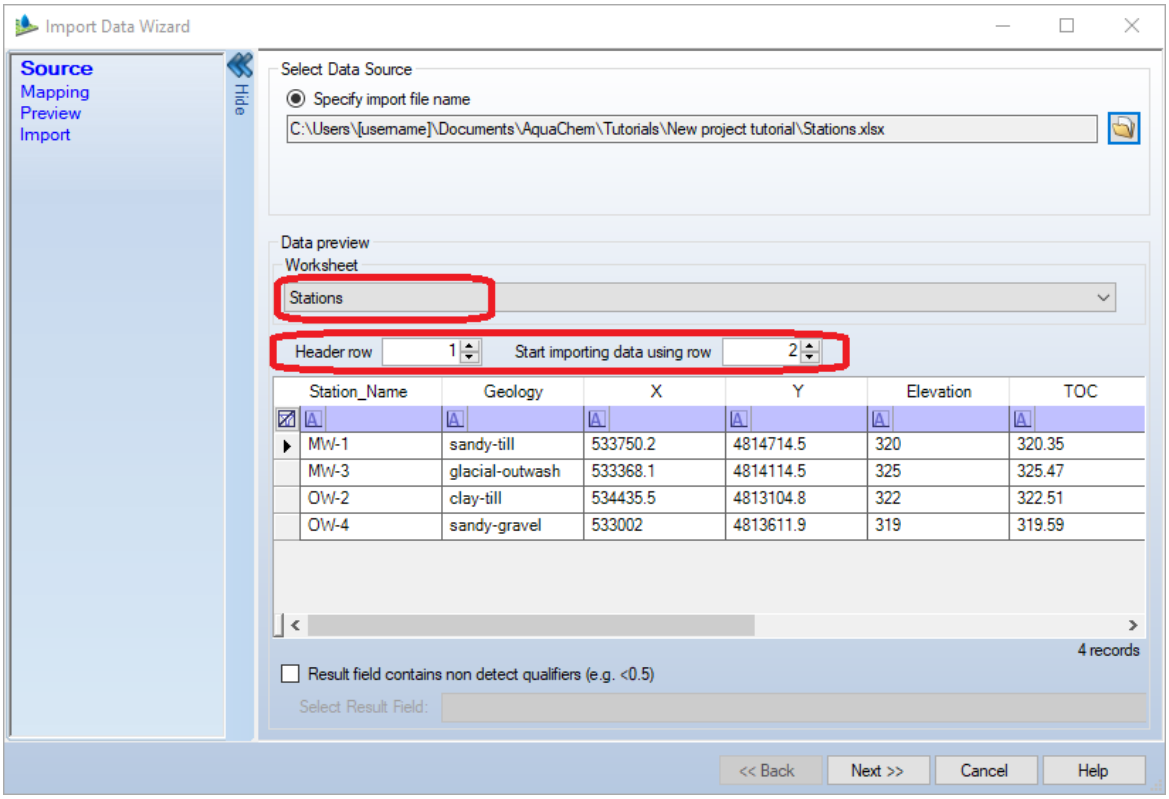


Based on the AquaChem data structure, all water quality data must be related back to a unique station ID. As such, the first step when importing project data is usually to import a list of stations. You will import the **'Stations.xlsx**' data file using the '**General**' format.

Select 'General', and click **'OK'** to proceed. You will then see the first step of the Import Data Wizard. The **'Source'** step allows you to select the data file to import. Click the **'Select Files'** button [] next to the **'Specify import file name'** field to open a Windows file explorer. Browse to 'Stations.xlsx' file, located in the following folder:

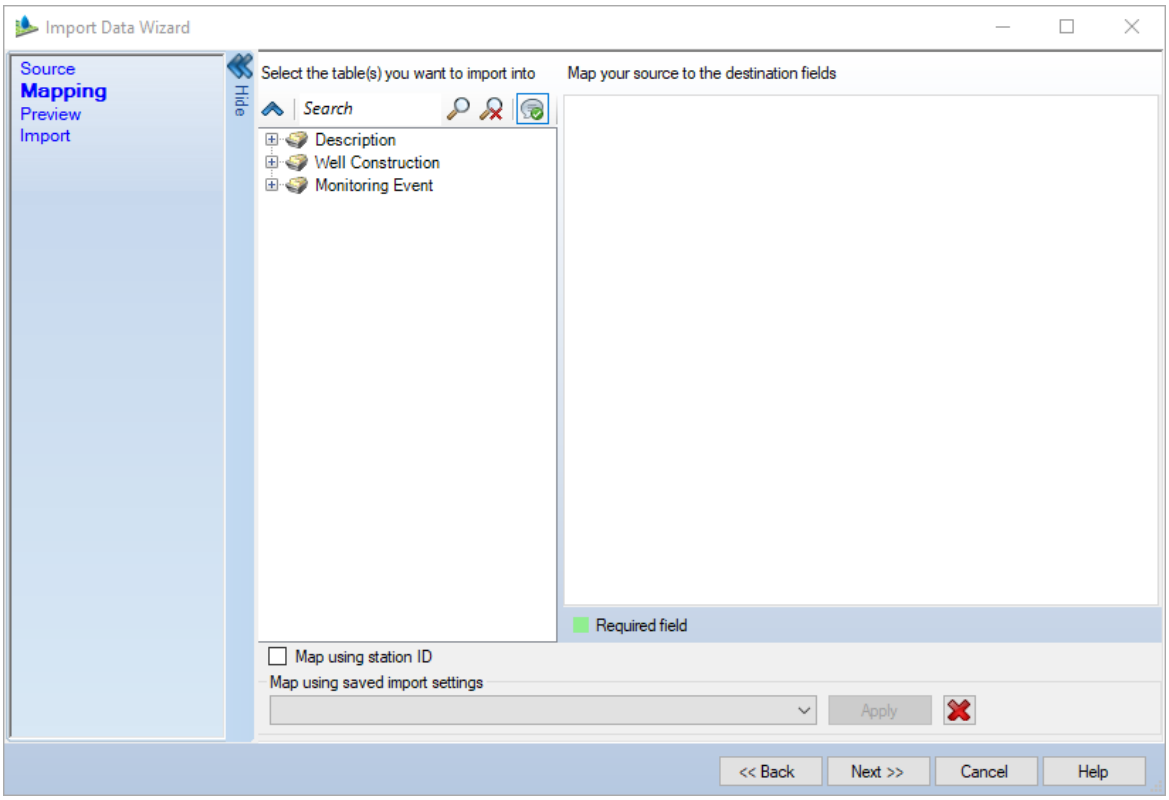
- *C:\Users\[username]\Documents\AquaChem\Tutorial Files\New Project Tutorial*

The Import Data Wizard window will be updated with a preview of the selected file, as shown below:



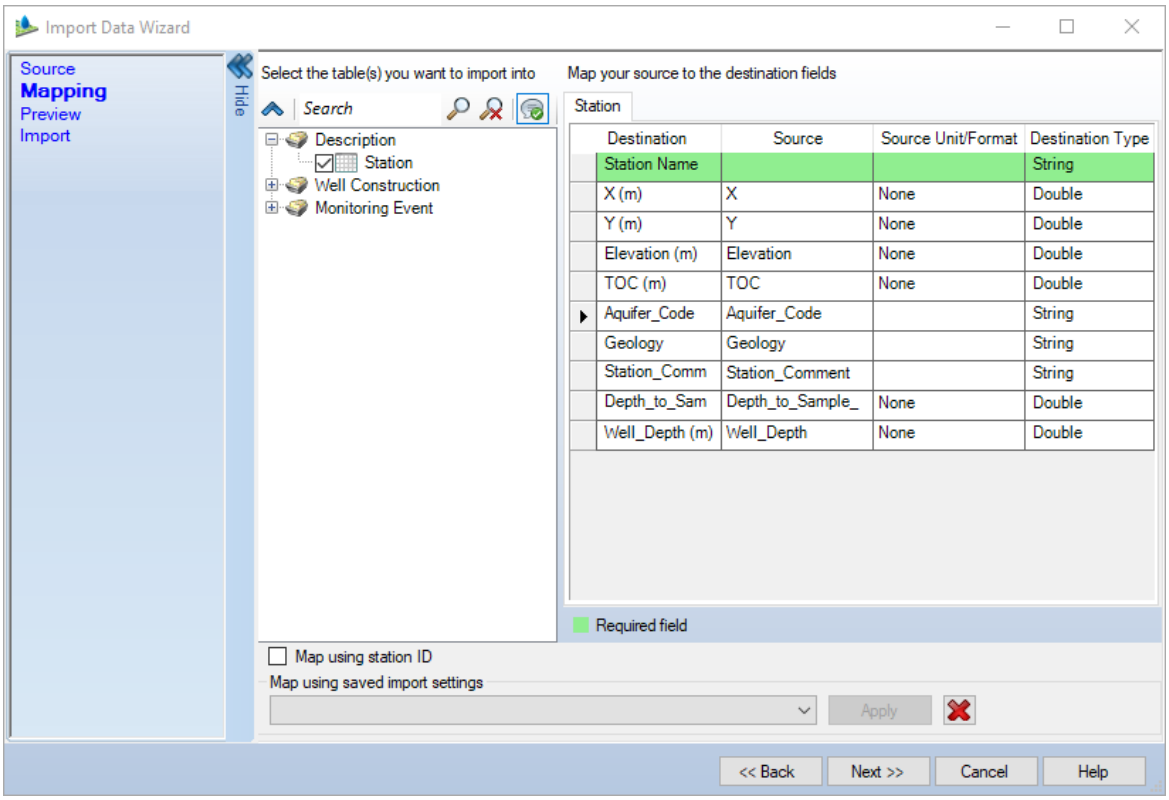
In this case the source data file only contains a single worksheet, and a single header row. However, if future data sources contain multiple worksheets you can select the desired worksheet using the menu highlighted in the image above. It is also possible to specify the exact row containing header information and the first row which contains data to be imported using the fields highlighted above.

You can proceed to the next step in the import workflow by clicking the Next >> button. You will then see the '**Mapping**' step, as shown below:



The purpose of the Mapping step is to identify which portions of your source data (i.e. which columns) are associated with individual data base fields.

Expand the 'Description' data category, and activate the 'Station' data table by using the checkbox [☑]. This adds the Station table and all associated fields to the table on the right-hand side, as shown below:



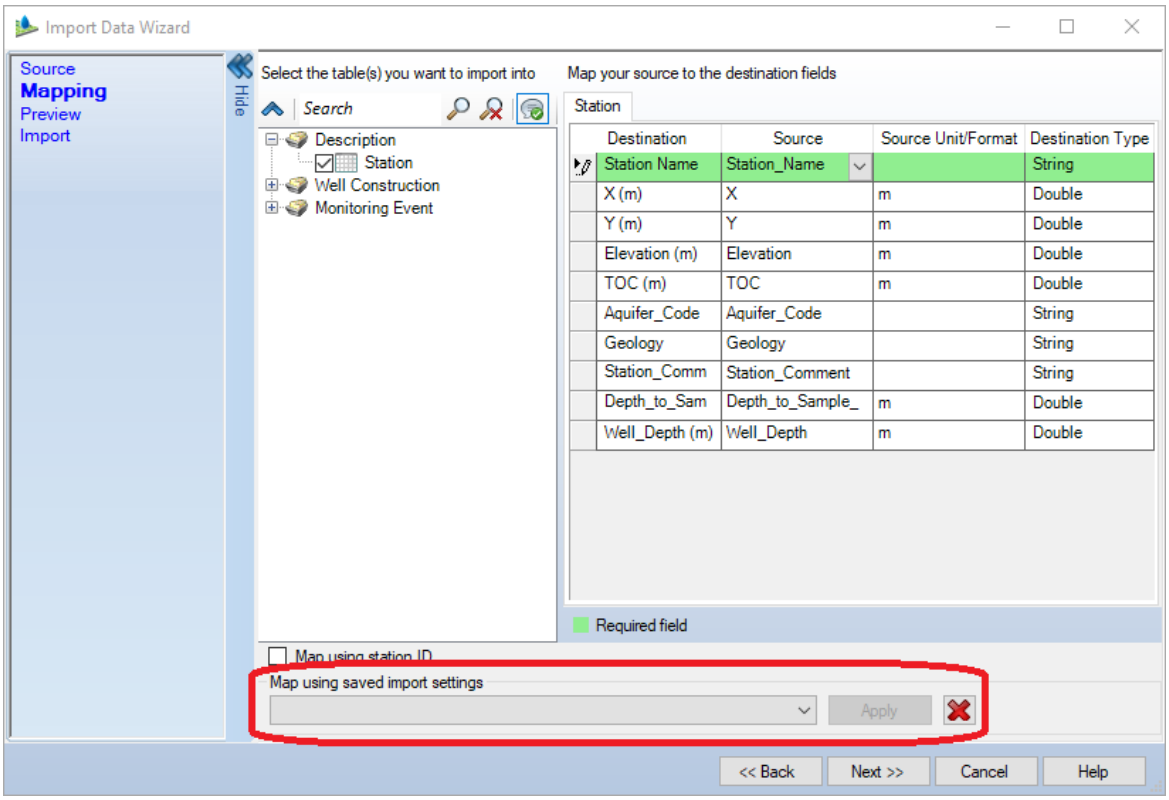
As you can see, many of the columns from the data source have been mapped automatically to the desired database fields. This is because the columns and fields have exactly matching names. However, two important fields have not been mapped automatically, namely the 'Station Name' and 'Total Depth (m)' fields.

Click the cell in the 'Source' column next to 'Station Name' and select 'Station_Name'.

You must also map the units associated with any fields which are based on a designated unit (i.e. the 'Double' type fields). Specify the source unit for all required fields as **'m'** (meters).

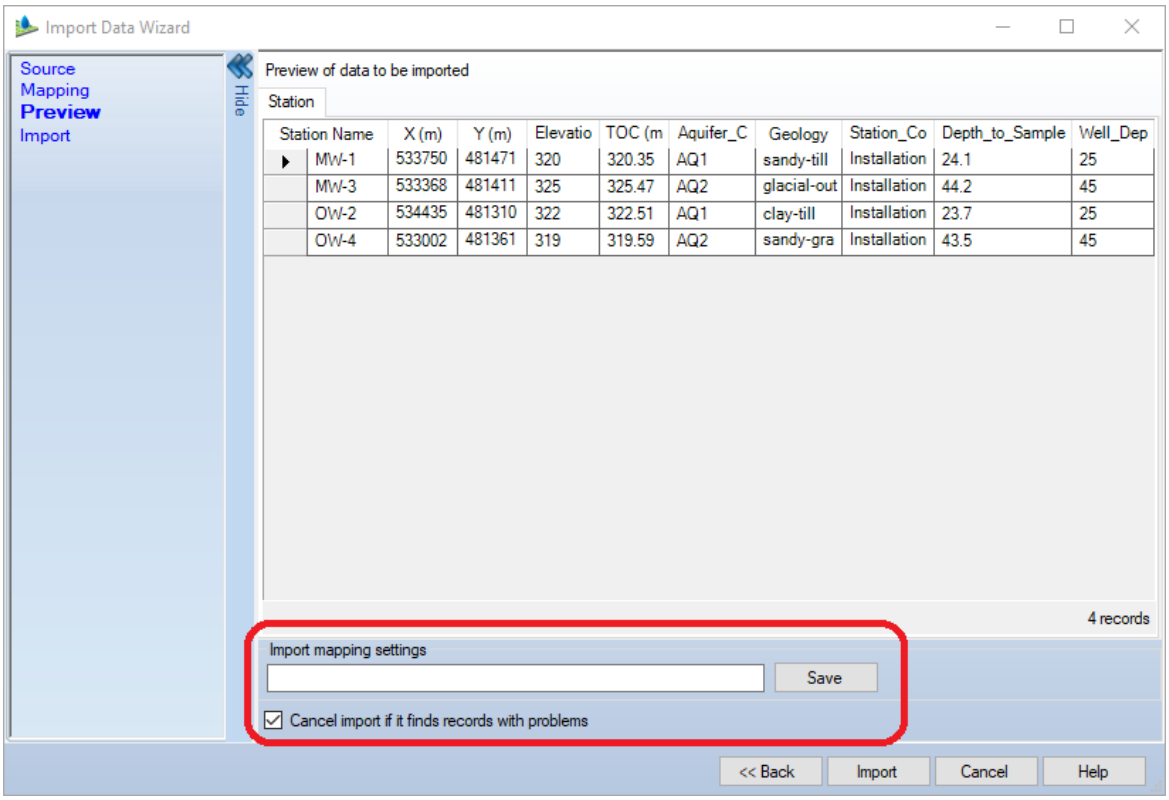
Please Note: AquaChem will automatically convert source units which do not match the units required by the database template. However, in this case the database and source file have the same units.

Once the required data mapping is complete the Import Data Wizard window should look like the image below:



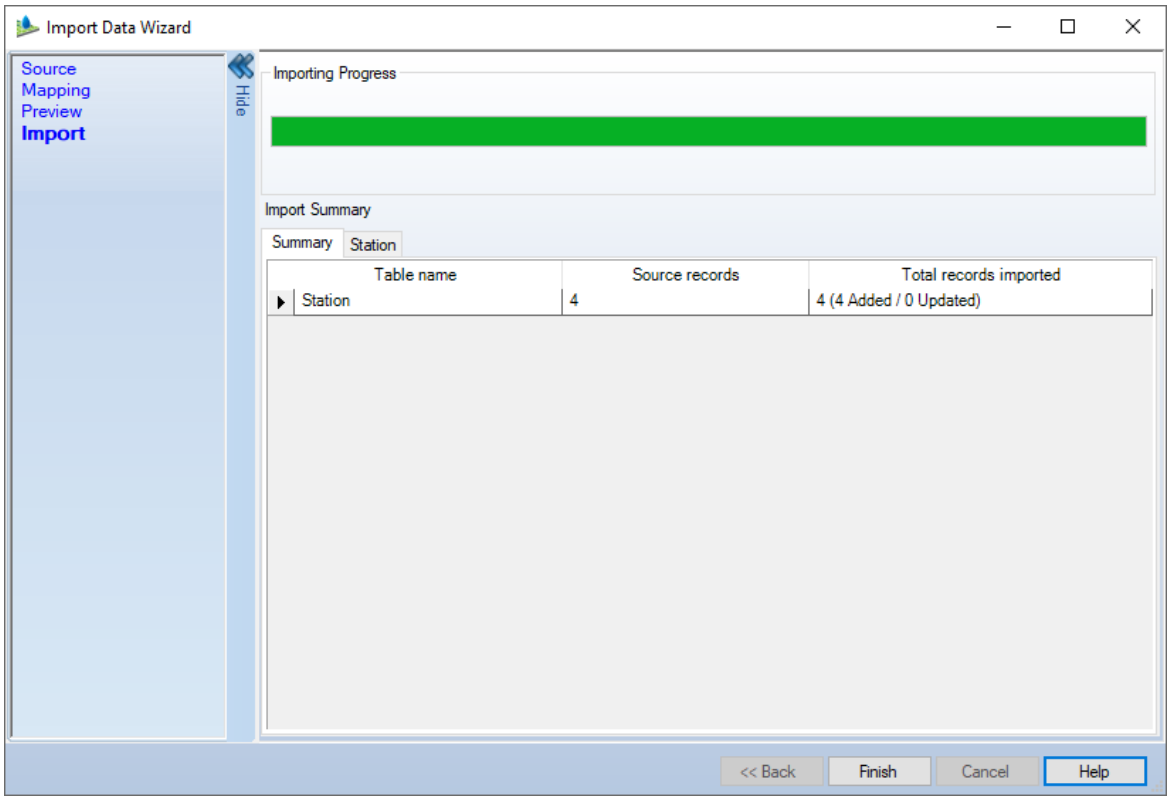
If future data sources with the exact same data mapping settings will be imported you may consider saving the import settings (on the 'Preview' step). The saved import settings can then be saved and applied using the menu/button highlighted in the image above.

Click the Next >> button to proceed to the 'Preview' step, as shown below:

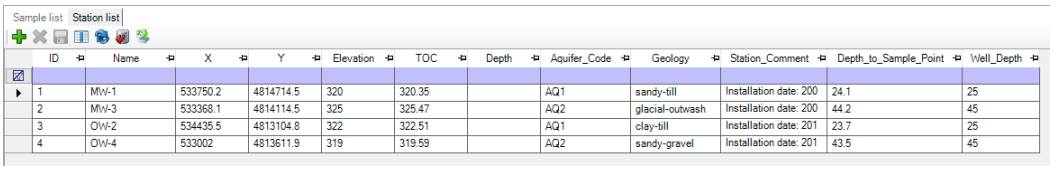


The Preview step simply provides a chance to review the data which is ready to be imported. It's also possible to save the current import/mapping settings using the field/button highlighted in the image above. The saved import/mapping settings can be reused to simplify future data imports (using the highlighted field/buttons in the 'Mapping' step).

To finish the import of station data simply click the Import button. You will then proceed to the 'Import' step, which provides a summary of the imported data as shown below:

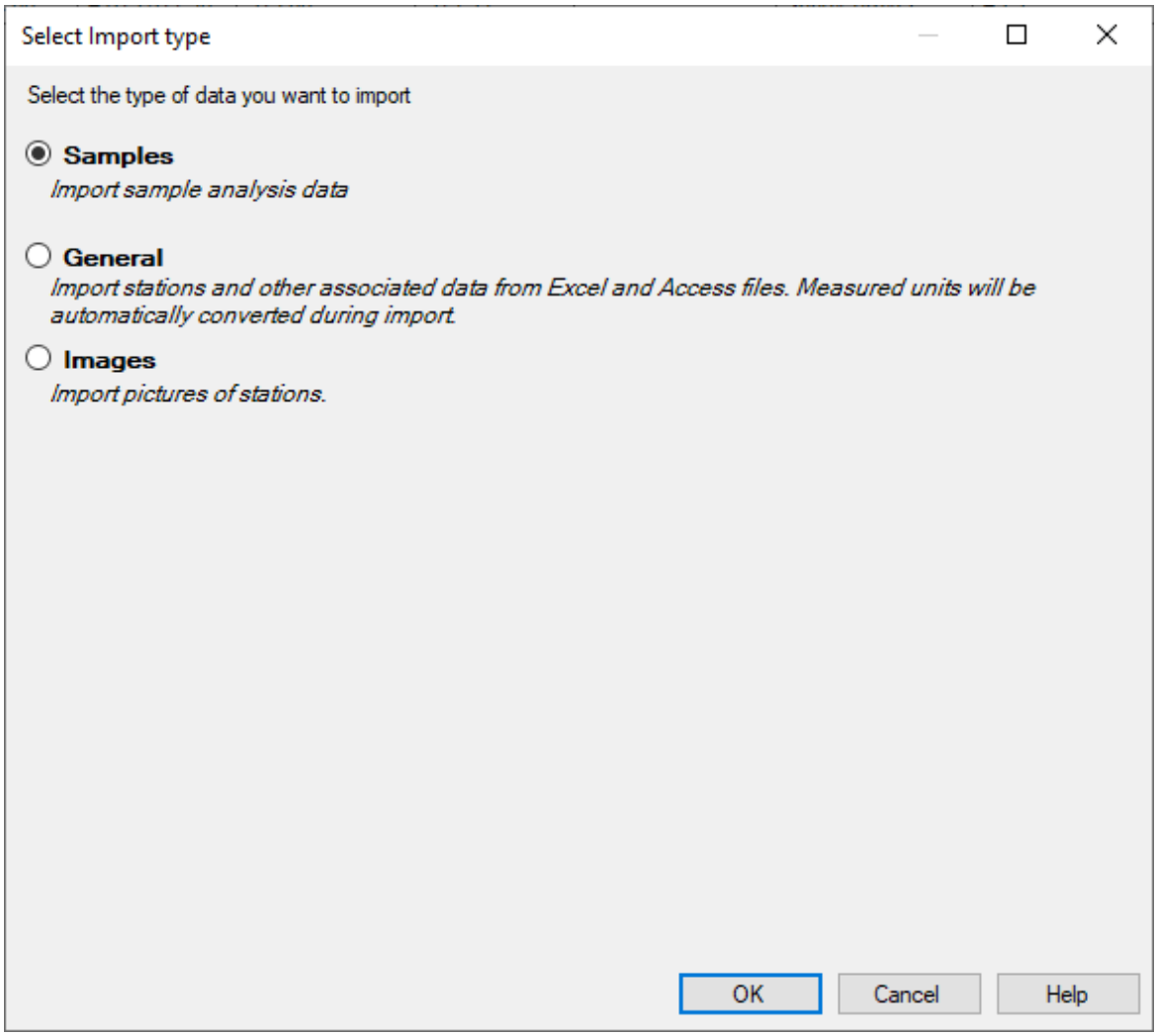


Click the Finish button to close the Import Data Wizard window and review the imported data, which should now be displayed in the 'Station List' tab:



ID	Name	X	Y	Elevation	TOC	Depth	Aquifer_Code	Geology	Station_Comment	Depth_to_Sample_Point	Well_Depth
1	MW-1	533750.2	4814714.5	320	320.35		AQ1	sandy-till	Installation date: 200	24.1	25
2	MW-3	533368.1	4814114.5	325	325.47		AQ2	glacial-outwash	Installation date: 200	44.2	45
3	OW-2	534435.5	4813104.8	322	322.51		AQ1	clay-till	Installation date: 201	23.7	25
4	OW-4	533002	4813611.9	319	319.59		AQ2	sandy-gravel	Installation date: 201	43.5	45

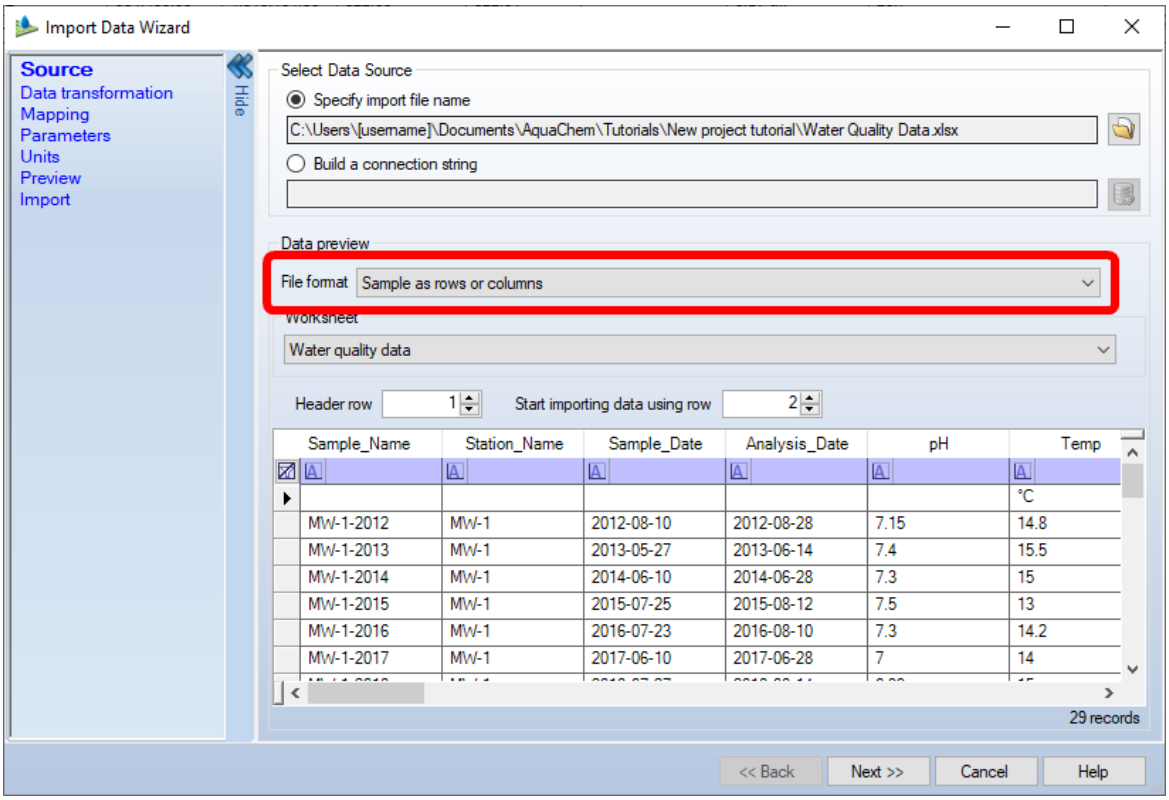
Now that the station data has been imported, you can proceed to import the sample analysis data contained in the '*Water Quality Data.xlsx*' spreadsheet. To initiate the import process you will again access the **Import Data Wizard** from the main menu ('**Modules > Import Data**'). This time the selected data type should be '**Samples**', as shown in the image below:



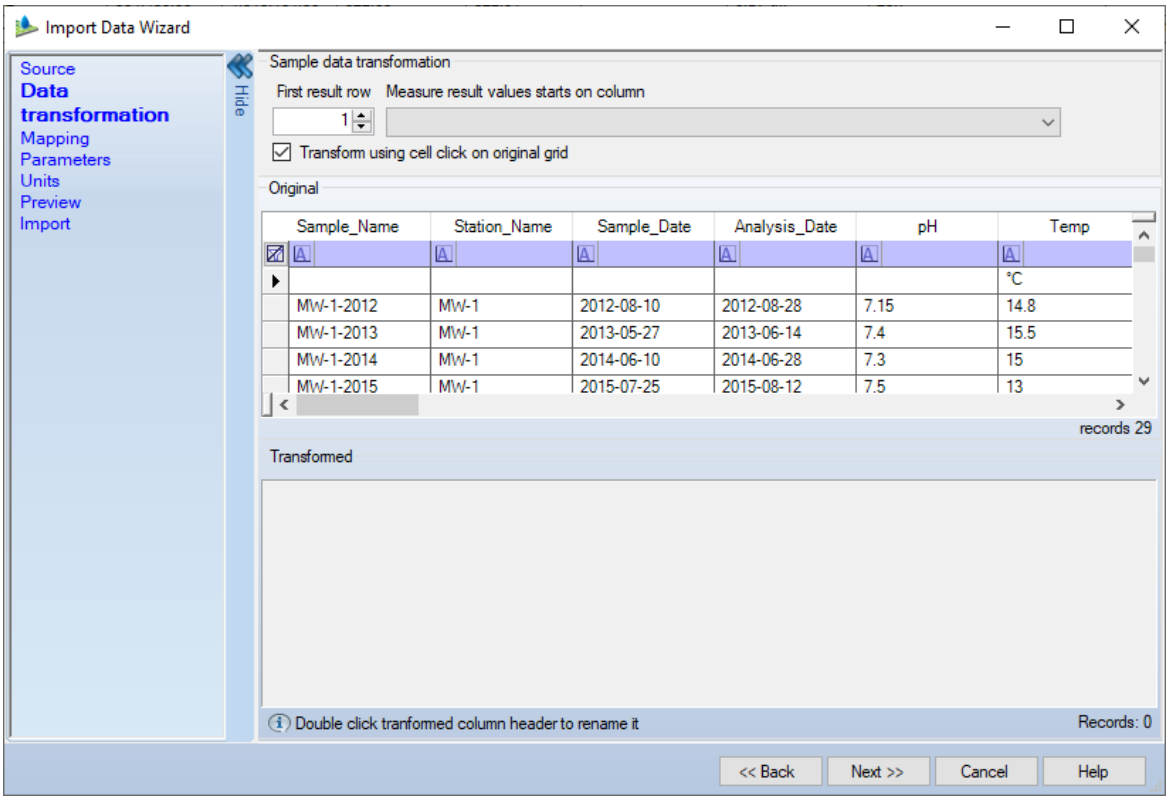
Click OK to proceed and you will again arrive at the 'Data Mapping' step. Click the **'Select Files'** button [ ] next to the 'Specify import file name' field to open a Windows file explorer. Browse to **'Water Quality Data.xlsx'** file, located in the following folder:

C:\Users\[username]\Documents\AquaChem\Tutorial Files\New Project Tutorial

Once again, at the 'Data Mapping' step, we can select from available worksheets, specify the header row, and which row to begin importing data. However, when importing sample data, there is an additional setting which must be specified, specifically the **'File format'** setting (highlighted in the image below). Select **'Samples as rows or columns'** as the desired file format, and the Import Data Wizard window should look like the image below:



Proceed by clicking Next >> and you will arrive at the **'Data Transformation'** step, as shown below:



The purpose of the Data Transformation step is to change the data into a format which can be imported into the AquaChem project (i.e. to transform the data from a 'Samples as rows/columns' format into a 'Single analyzed value per row' format).

This transformation can be accomplished two ways:

1. By specifying the first row containing results and then selecting the first column which includes measured values (using the 'Measure result values starts on column' menu), or
2. By clicking on a cell in the 'Original' grid (Note: the 'Transform using cell click on original grid' checkbox must be active)

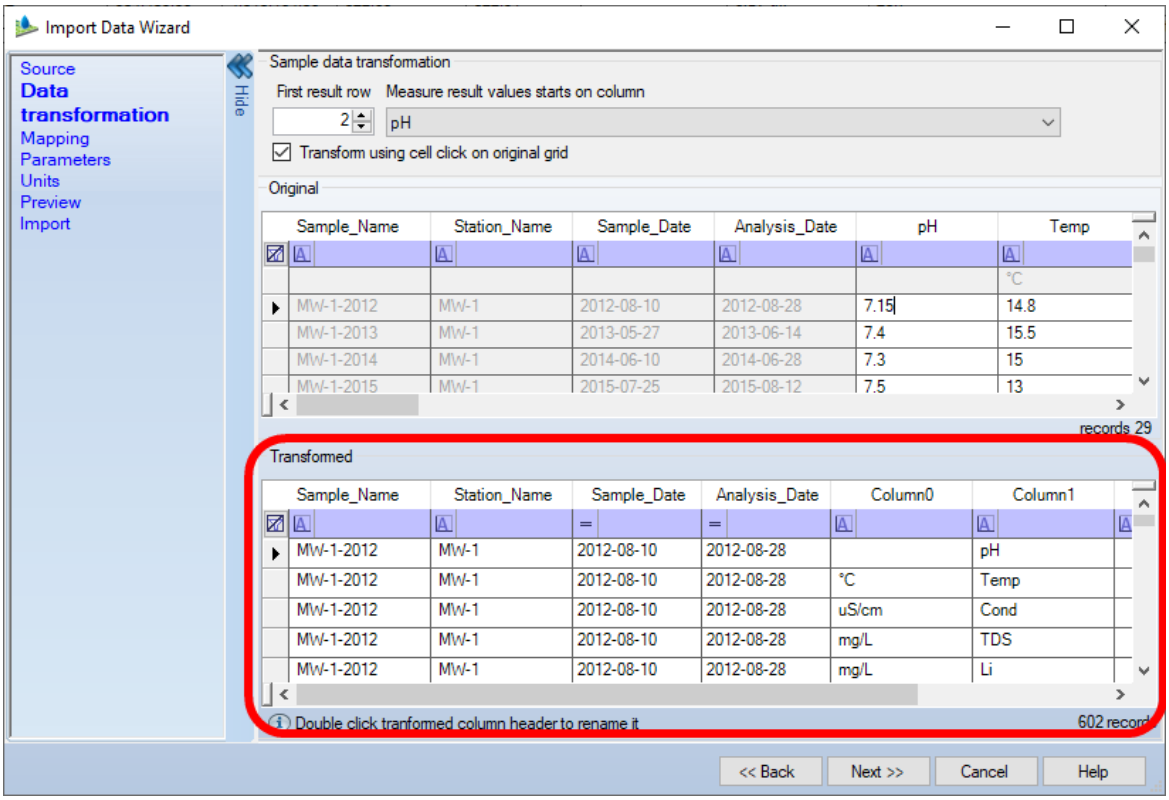
You must choose one of these options and transform the data to continue. Select **ONE** of the methods below to transform the data:

1. Specify row 2 as the 'First result row' and then select 'pH' from the 'Measure result values starts on column' menu,

   OR

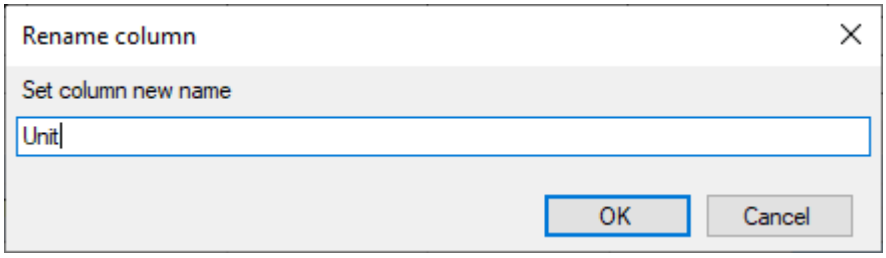
2. Click on the first result (i.e. 7.15) under the pH column

After performing one of these data transformations, the data appears in the **'Transformed'** section of the interface, as shown below:



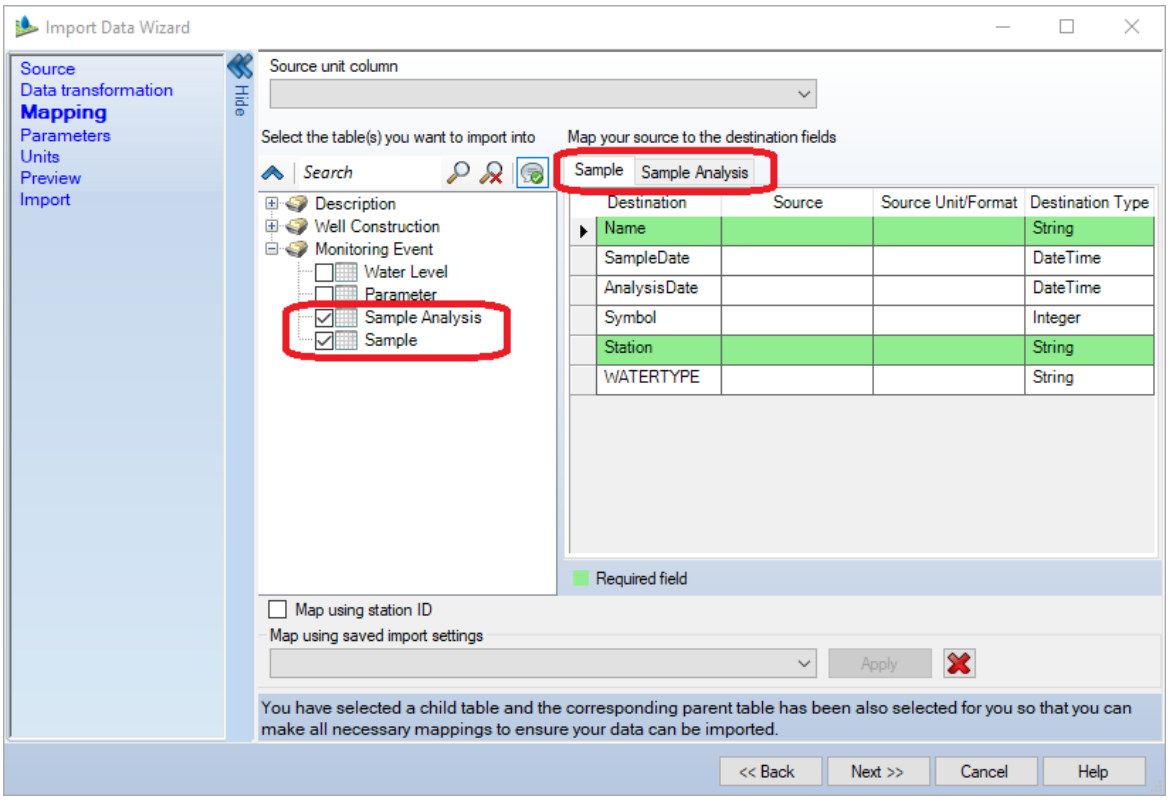
The next step in the workflow ('Mapping') requires you to map the 'transformed' columns listed here to available database fields/tables. You will notice that the columns here are not all labeled in a helpful manner (e.g. 'Column0'). As such, it is helpful to relabel these columns to make them easier to identify later.

Double-click the header for **'Column0'**, and rename the column to '**Unit**' in the window that appears:



Also, double-click the header for **'Column1'**, and rename the column to **'Parameter'** in the window that appears.

Click OK in the 'Rename column' dialogue to close it, then click Next >> to proceed to the **'Data Mapping'** step, as shown below:



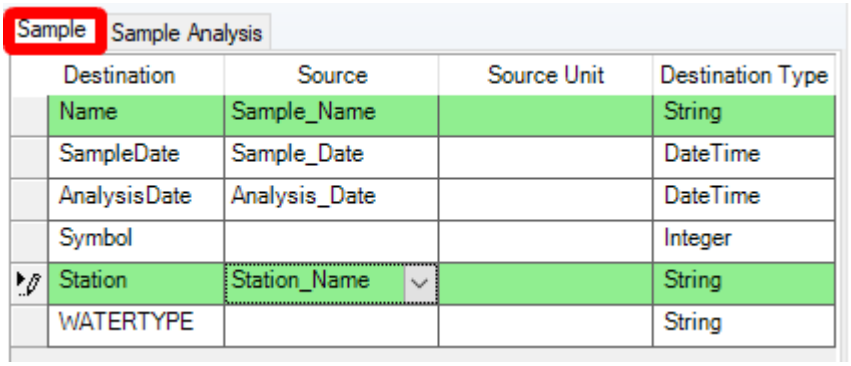
Once again we perform this data mapping step in order to identify which portions of your source data (i.e. which columns) are associated with individual data base fields.

Expand the **'Monitoring Event'** data category and as you can see from the image above the **'Sample Analysis'** and **'Sample'** data tables have been selected automatically (since you already selected the **'Samples'** data type in the first step of the data import).

Map the following source data columns to the destination fields indicated below (**[Destination field] = [Source Column]**):

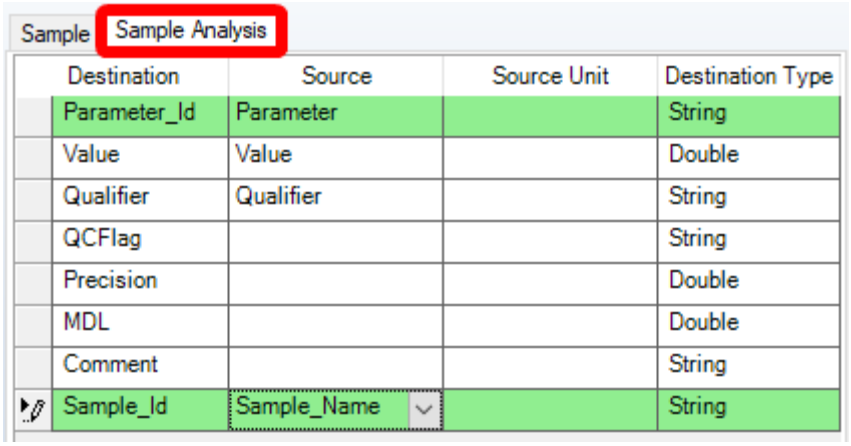
Sample Table

- [Name] = [Sample_Name]
- [SampleDate] = [Sample_Date]
- [AnalysisDate] = [Analysis_Date]
- [Station] = [Station_Name]

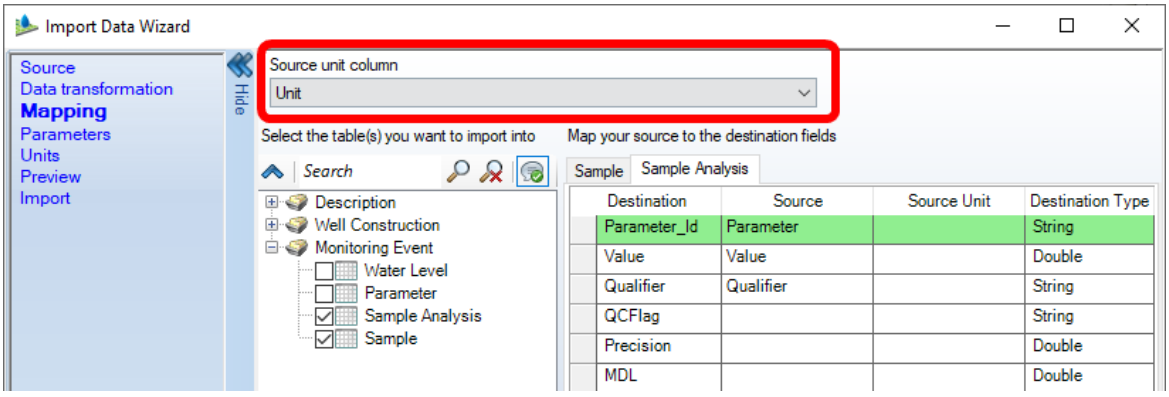


Sample Analysis Table

- [Parameter_Id] = [Parameter]
- [Sample_Id] = [Sample_Name]



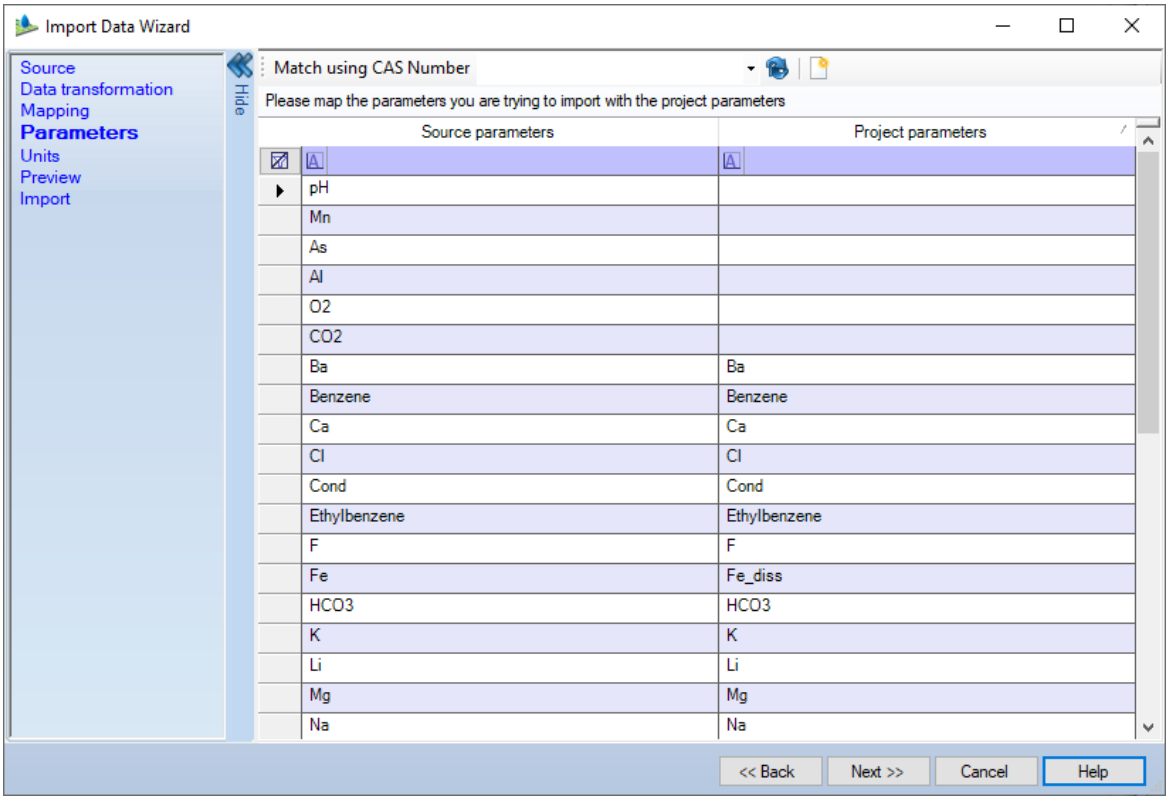
Finally, you must also map the source units column using the **'Source unit column'** menu at the top of the window:



Please Note: once again you may select a saved import setting at this step, which can be very helpful if you find yourself frequently importing

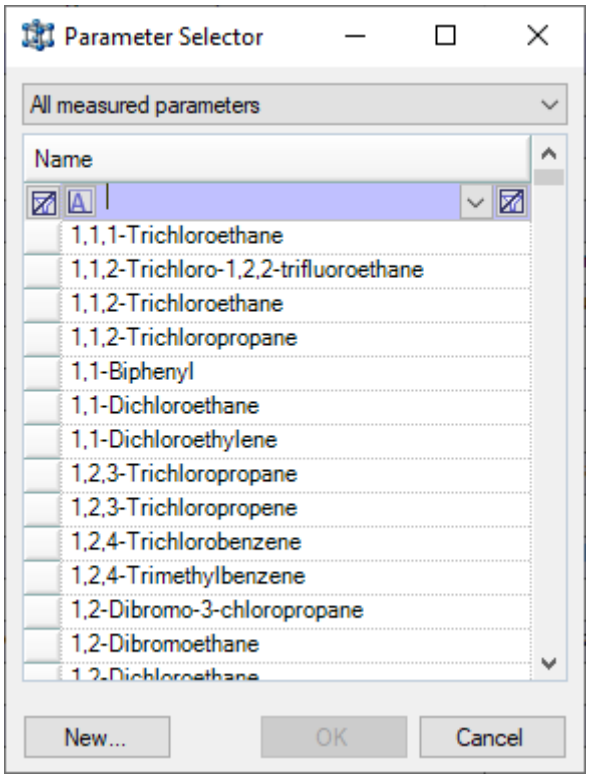
data files with the same format. The import settings can be saved at the **'Preview'** step.

Click Next >> to proceed to the **'Parameters'** step as shown below:



The **'Parameters'** step provides you with an opportunity to map any parameter names which have not been identified automatically by AquaChem. In this example you will need to map the following parameters by clicking the *empty* cells under the **'Project parameters'** column and selecting from available project parameters.

Click the empty cell in the **'Project parameters'** column for pH, and the **'Parameter Selector'** window will open:



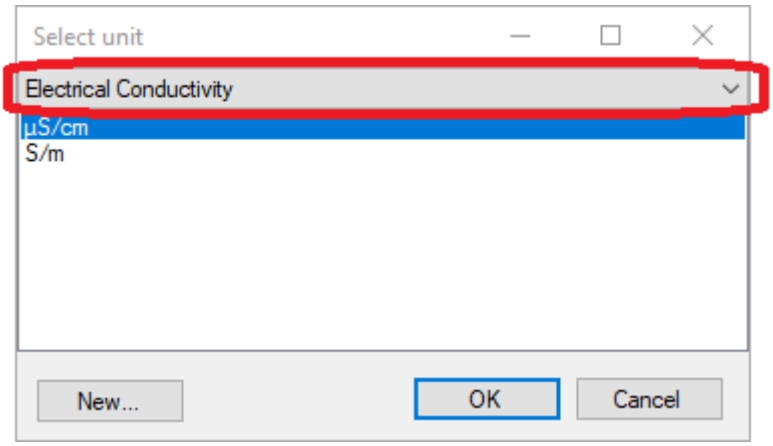
Scroll through the list until you find **'pH field'** and select it (alternatively you can type 'pH field' into the filter at the top of the list). Repeat this procedure to map the following parameters (**[Source parameters] = [Project parameters]**):

- [pH] = [pH field]
- [Mn] = [Mn_diss]
- [As] = [As_diss]
- [Al] = [Al_tot]
- [O2] = [DO]
- [CO2] - does not have an existing parameter, therefore you can click the 'Create stubs for missing parameters in your project' [ ] button

Please Note: if your source data file contains CAS numbers you may indicate which source column contains these numbers using the menu at the top of this window. AquaChem will then auto-map any parameters with matching CAS numbers.

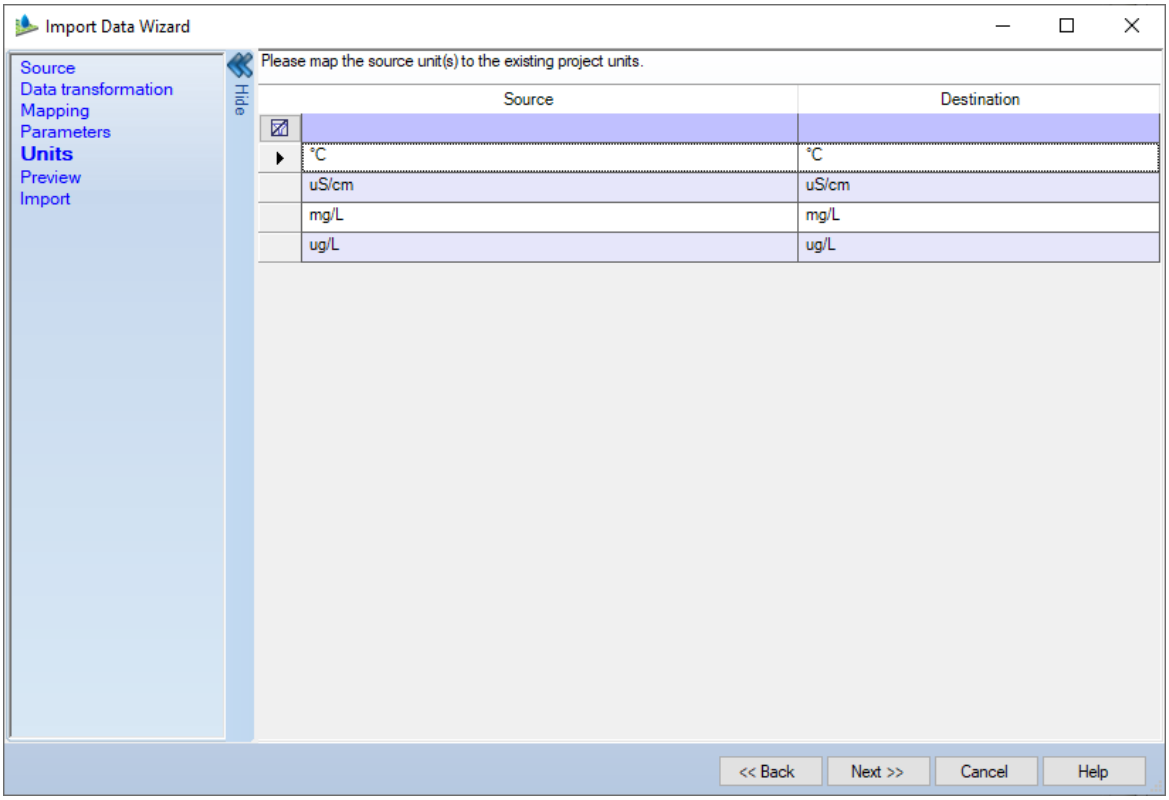
When these parameters have been mapped, click the Next >> button to proceed to the **'Units'** step, which fulfills the same role as the **'Parameters'** step but in the context of unmapped units. You can map the units using a similar set of controls as we used in for parameters:

- For uS/cm, change the unit category to **Electrical Conductivity** and select **µS/cm**

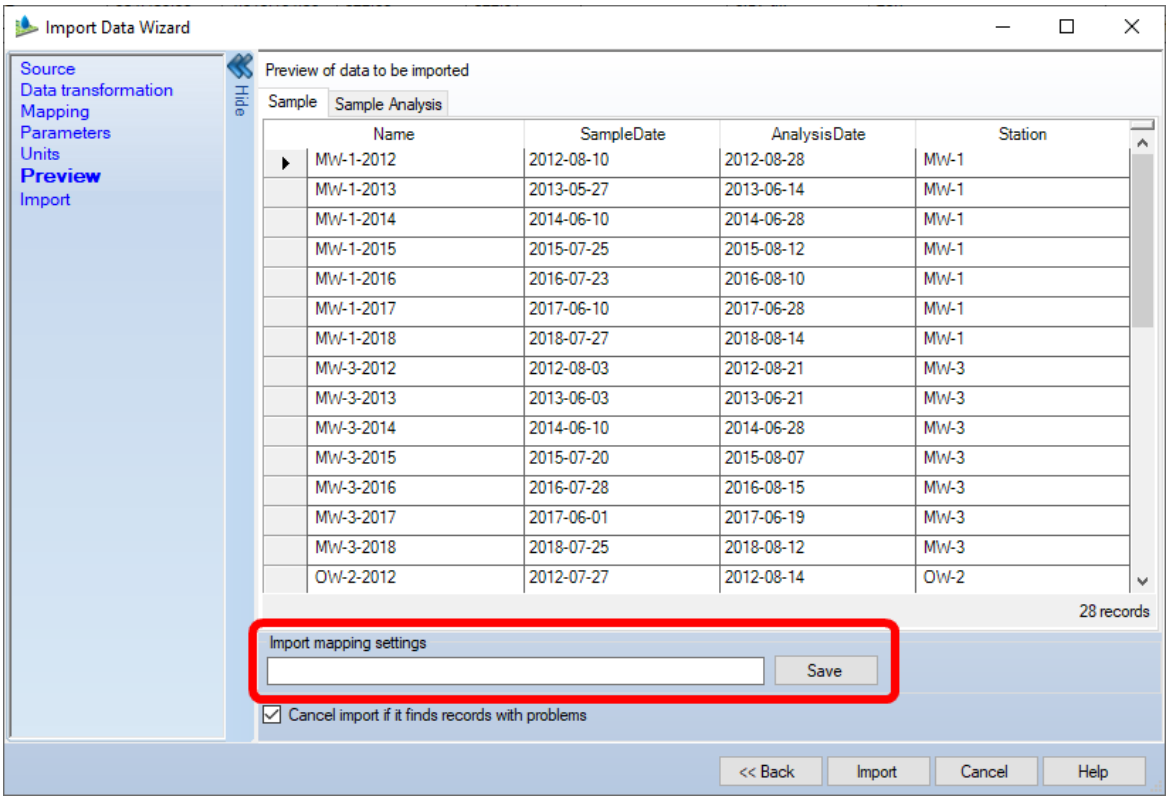


- For ug/L, change the unit category to concentration and select **µg/L**

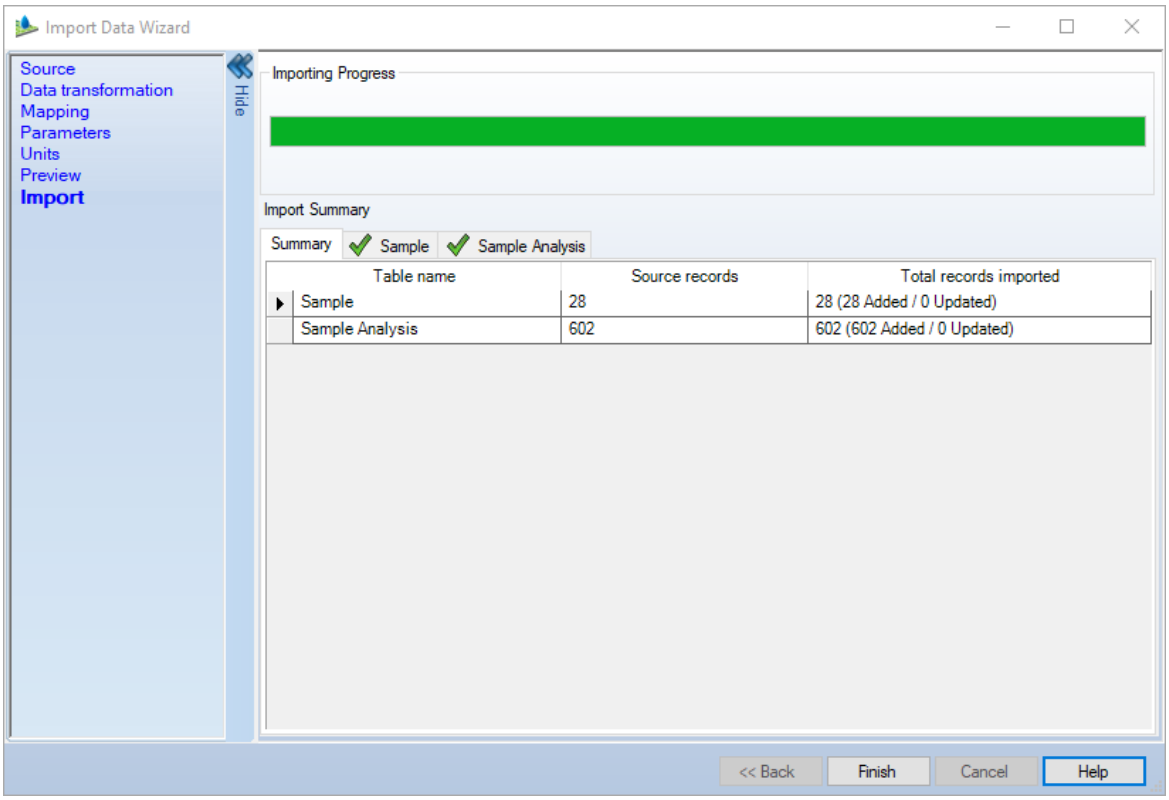
Your mappings should resemble the following:



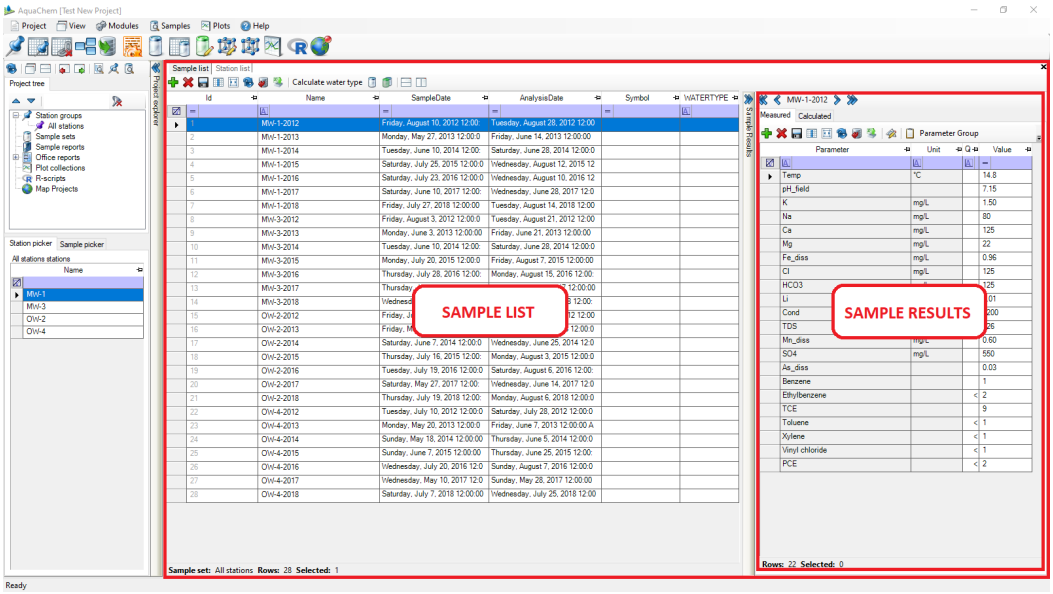
Click Next >> again to proceed to the 'Preview' step, which provides a preview of the data to be imported. At this stage you may also save the import mapping settings (which can be reused for future imports), as shown below:



Click the **'Import'** button to import the data, and you will be taken to the **'Import'** step. This step once again provides a summary of the imported records, as shown below:



Finally, click Finish to complete the import of water quality data. When you access the 'Sample List' tab and click the refresh [ ] button you will then see the imported records (28 rows), and the water quality parameters associated with each parameter will be displayed in the 'Sample Details' window to the right, as shown below:



Now that your project data has been imported you can begin analyzing the data by creating sample groups, plot collections, importing project specific water quality standards, generating sample reports, etc. For more information on these features/functions please review the AquaChem Demo Project Tutorial.

- This concludes the 'Creating a New Project and Importing Data' tutorial -

2.3 Importing Projects from AquaChem 2014

Importing existing AquaChem projects from earlier versions (i.e. 2014.2 and earlier) is a streamlined process that only requires five simple steps:

- Select the AquaChem v2014 project file (.aqc)
- Specify the name of the new AquaChem 10.0 project, and the location of the new project folder
- Map any unmapped units
- Import the project
- Map parameters required by AquaChem 10.0 (if missing)

To demonstrate this functionality, you will import the Basic Demo project from AquaChem 2014.2. It is also important to familiarize yourself with the differences in the database structure between AquaChem 2014 (and earlier versions) and the newer AquaChem 10.0 database structure. As such, this tutorial has two sections:

- **Comparing Database Structures**
- **Importing an AquaChem 2014 Project**

2.3.1 Comparing Database Structures

The general structure of AquaChem projects remains largely the same as that used in AquaChem 2014 (and earlier) projects, which is very fortunate because it means that importing projects from AquaChem 2014 is extremely simple. In both versions of the program, the database structure is based on the following key data tables:

- **Station Data Table:** contains information regarding individual 'Stations', which represent a single location with an X- and Y-coordinate, often including associated metadata.

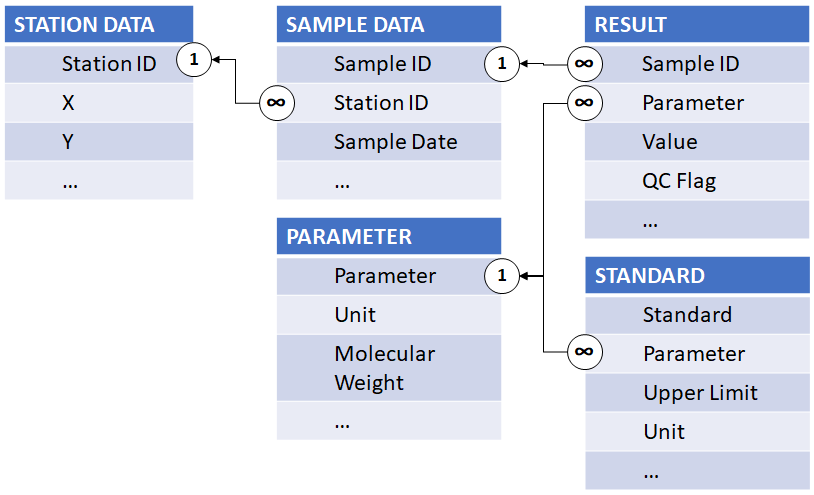
- **Sample Data Table:** contains information regarding individual 'Samples', which represent unique events where one or more physical measurements and/or analytical samples have been collected at a given location/station.

- **Analysis Results Table:** contains information regarding individual records that represent the value and associated data for a single parameter.

Analysis results data are further tied to the Parameter table, which contains information on the types of measurements and observations that are included included in the project, and

the Standards table, which contains threshold values that indicate parameter results may be be present at levels above prescribed concentrations/values (i.e. water quality standards).

These data tables are contained in a relational database, the basic structure of which is illustrated in the image below:

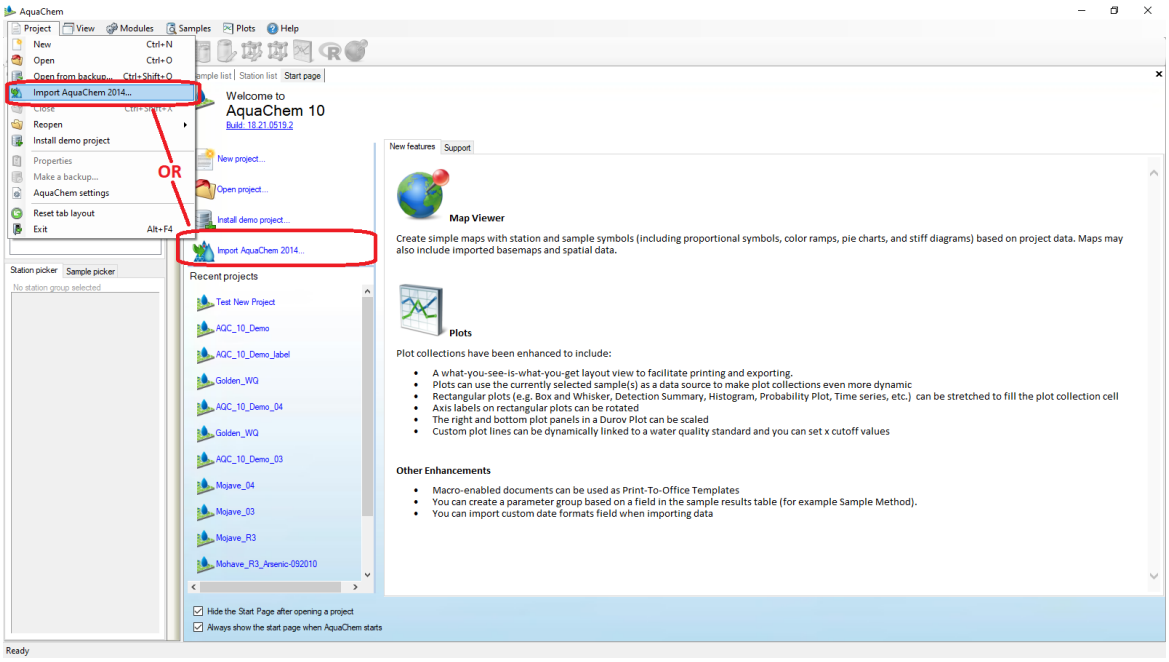


The main difference between the relational database structure used in older and newer AquaChem projects is that the database structure in newer versions include a variety of additional relationships to tables which are not listed here. These extra relationships enable a variety of additional functionality in AquaChem 10.0 compared to earlier versions, such as the ability to create Station Groups, static and dynamic Sample Sets, persistent/savable Sample Reports, Plot Collections, Maps, and more. For more information about the database structure, please review the 'Database Structure' section.

In the next section, we will import the v2014.2 Demo Project.

2.3.2 Importing the v2014 Project

To import an AquaChem 2014 project, first launch AquaChem 10.0 and launch the Start Page. You should see a button to '**Import AquaChem 2014...**'. Alternatively, you can click '**Project > Import AquaChem 2014...**' from the main menu:

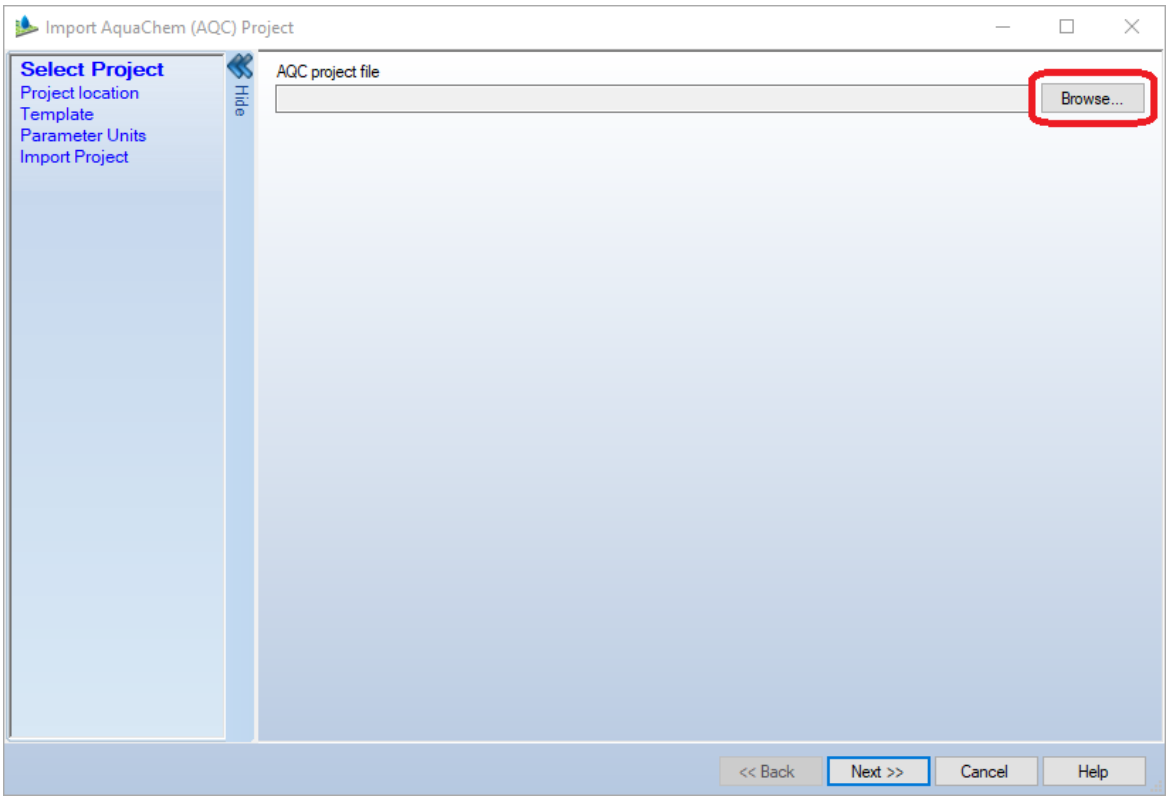


Click either of these buttons (highlighted above) and the 'Import AquaChem (AQC) Project' window will open, at the Select Project step.

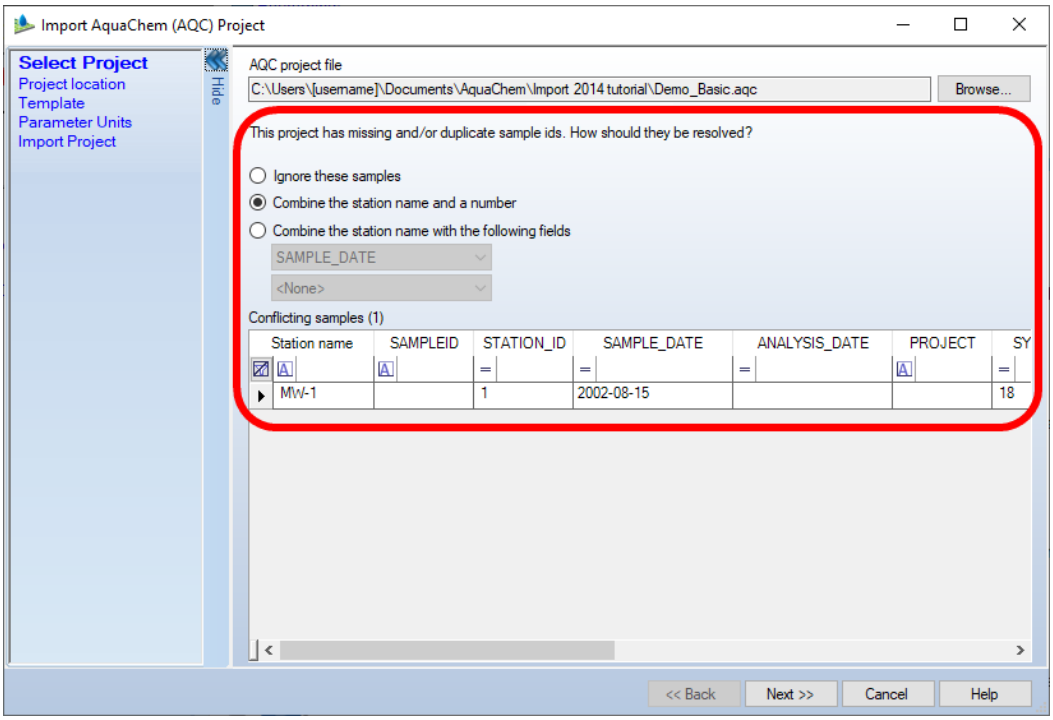
Select Project Step

The first step in the Import AquaChem 2014 process is to select the AquaChem 2014 project which we would like to import into AquaChem 10.0. Click the 'Browse' button next to the 'AQC project file' field (highlighted below) to open a Windows Explorer window and browse to the location of the project file. A copy of the basic demo project ('Demo_Basic.aqc') has been saved to the AquaChem 10.0 installation folder. Browse to the location below and select the **'Demo_Basic.aqc'** project file:

- *C:\Users\[username]\Documents\AquaChem\Tutorial Files\Import AquaChem v2014*



Please Note: if any samples in the original project file do not contain unique SampleID, you will be prompted to ignore the samples (in which case they will not be imported), or to append a number or other unique value to the Station Name. This ensures that each sample in the AquaChem 10.0 project contains unique SampleIDs. An example is shown below:



In this case, the Demo_Basic.aqc project file *does* contain unique SampleIDs for all samples, and *so you shouldn't see the highlighted message about missing/duplicated SampleIDs, as highlighted above*. The image is shown to provide an example, and in most cases existing projects will contain unique SampleIDs for all samples.

Once the file '*Demo_Basic.aqc*' has been selected you can proceed to the next step (Project Location) by clicking the Next >> button.

Project Location Step

The second step in the Import process is to specify a new name and project folder for the AquaChem 10.0 project. By default the AquaChem 10.0 project name will be the same as the original project file, and the project folder will be located in the following folder:

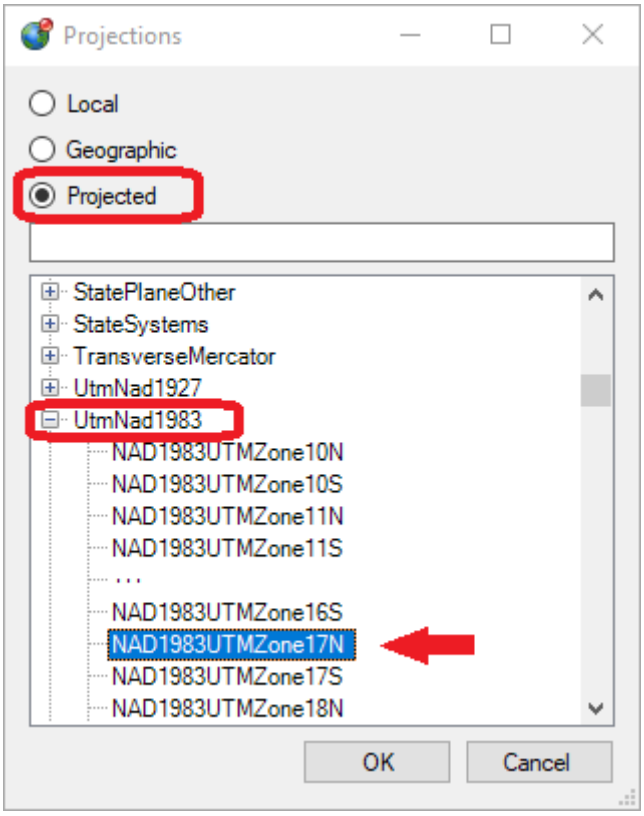
- *C:\Users\[username]\Documents\AquaChem\Projects*

If you wish to change the location, select the Browse button and navigate to the folder of your choosing.

The project location step also allows you to define the coordinate reference system for the project including the Projection and coordinate system units. In this case, the Demo_Basic project is located in Zone 17N of the UTM projection with the NAD1983 horizontal datum and measurement units of meters.

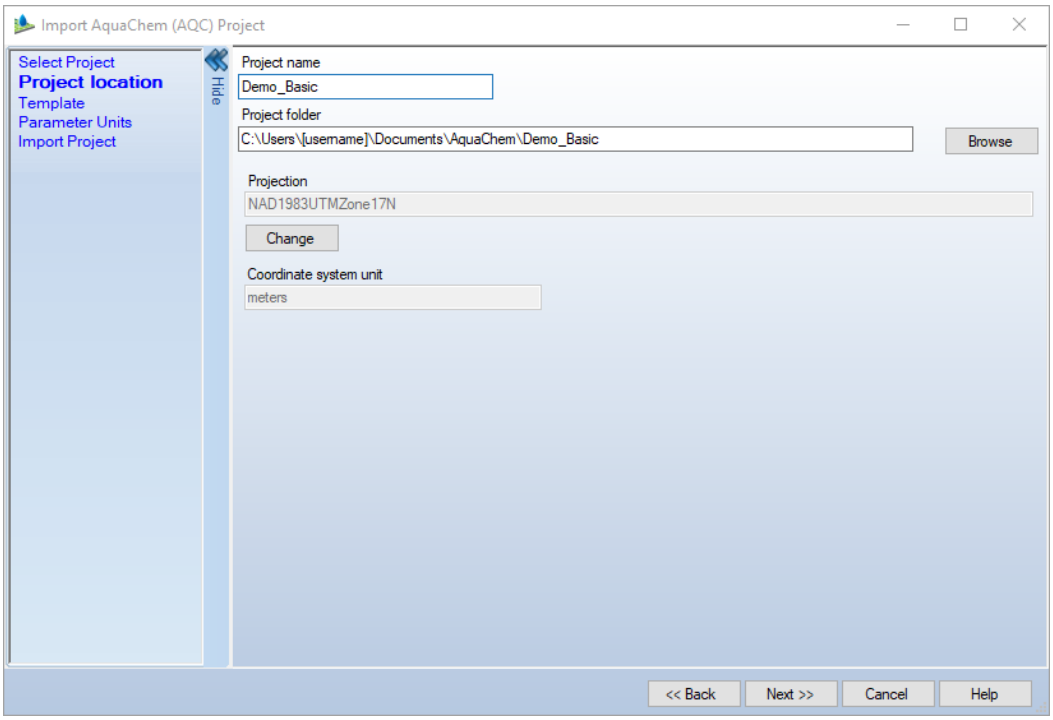
- Click the Change button to set the projection for the project:
- Select Projected
- Find and expand the UtmNad1983 branch on the tree

- Select the option "NAD1983UTMZone17N"



- Click OK

The Import wizard should look similar to the image below:

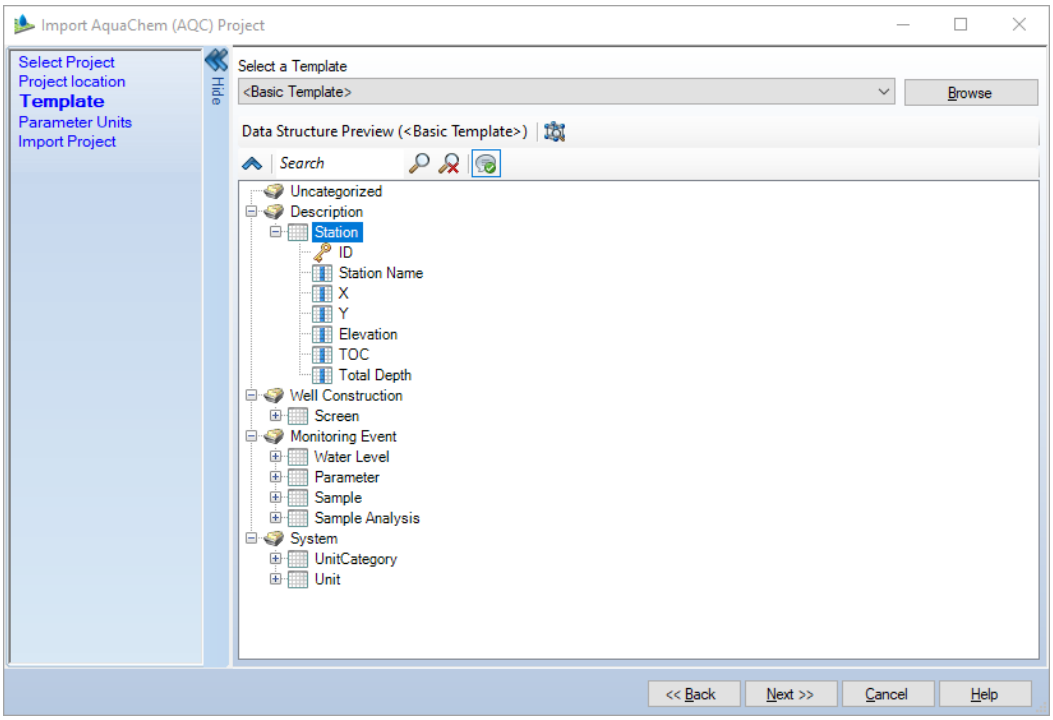


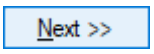
You can now proceed to the Template mapping step by clicking the Next >> button.

Template Step

On this step, you can select a project template to migrate the data into. The project template defines the structure, layout, and requirements of your database, including tables, fields, and lists. The template also includes all of the parameters to be included in your project.

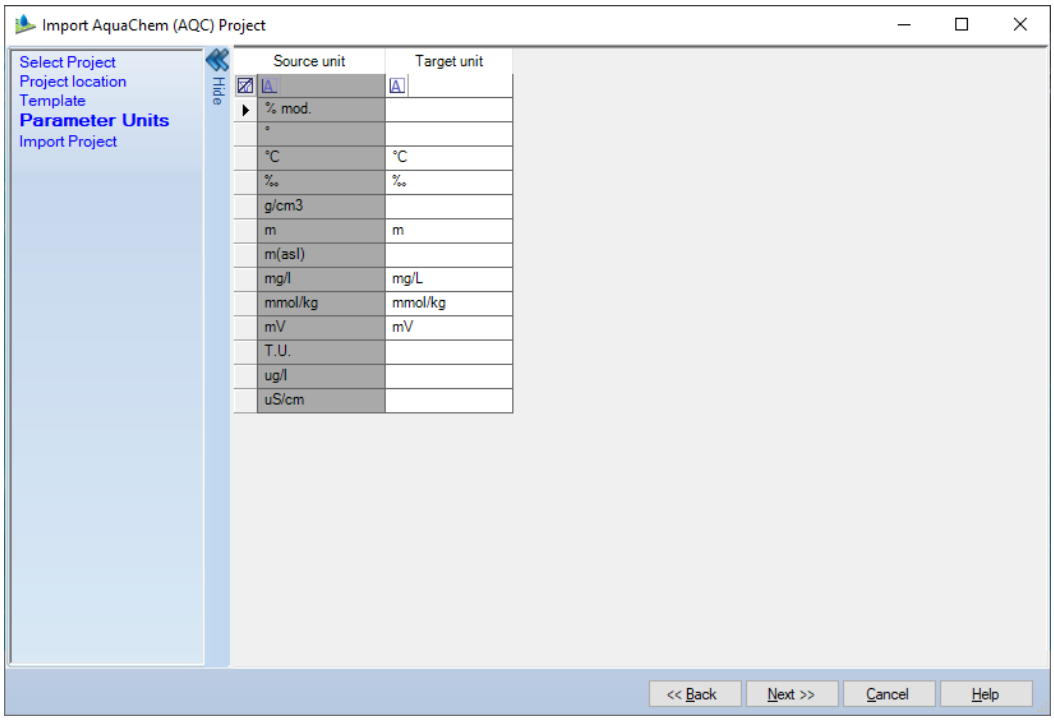
For this project, we will leave the default <Basic Template>; however feel free to explore the template by perusing through the Data Structure preview items and the template parameter list (accessed by the button). You can also browse through the Advanced template.



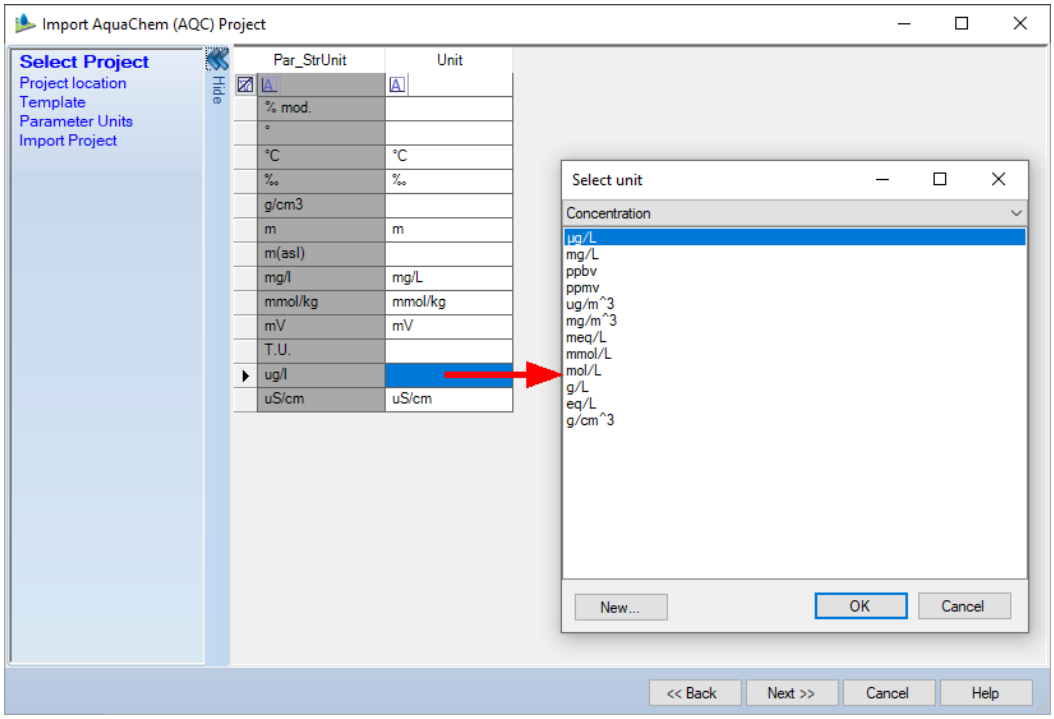
You can now proceed to the Parameter Units mapping step by clicking the  button.

Parameter Units

The Parameter units step allows you to define measurement units and link them to a specific unit category so that you can take advantage of the dynamic unit conversion available in AquaChem. The original measurement units from the AquaChem 2014 project are shown in the left "Source unit" column and you must map these units to equivalent "Target units" in AquaChem 10.0.



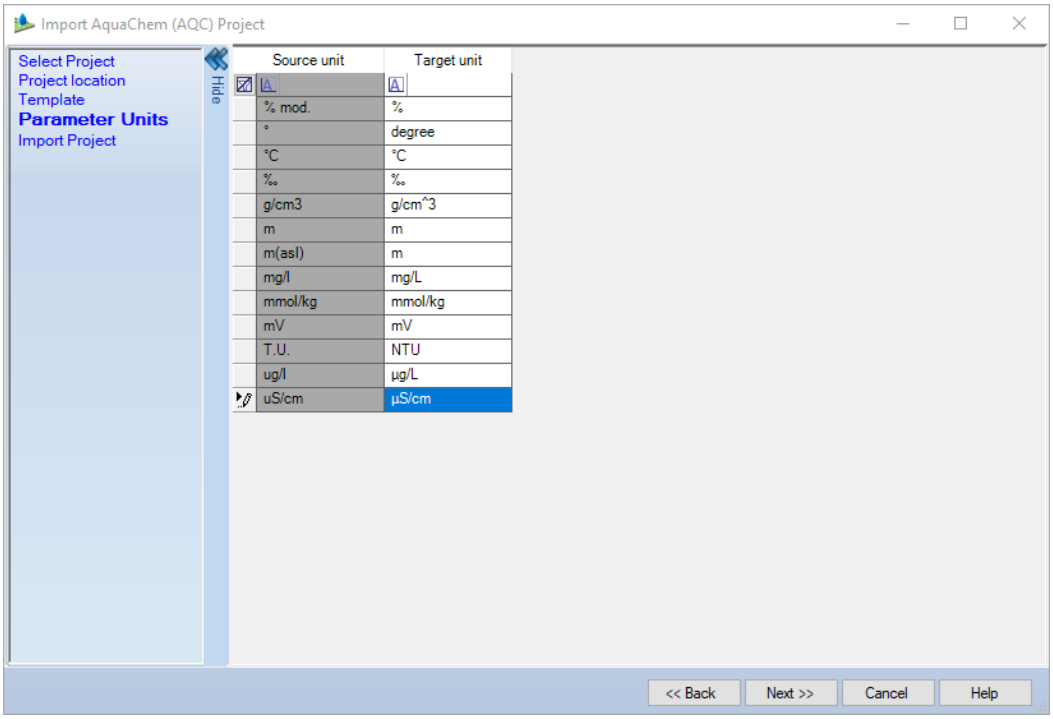
To map units, simply click the empty cells under the 'Units' column. A 'Select Unit' window will open, allowing you to choose from available unit categories using the dropdown menu at the top. Available units for the selected category will then be displayed, allowing you to choose the desired unit:



Spend a moment mapping the following units:

- **% mod** should be mapped to '%" under the **Fraction** unit category
- **°** should be mapped to degrees under the **Angle** unit category
- **g/cm3** should be mapped to **g/cm^3** under the **Concentration** unit category
- **m(asl)** should be mapped to **m** under the **Length** unit category
- **T.U.** should be mapped to **NTU** under the Turbidity unit category
- **ug/L** should be mapped to **µg/L** under the **Concentration** unit category
- **uS/cm** should be mapped to **µS/cm** under the **Electrical Conductivity** unit category

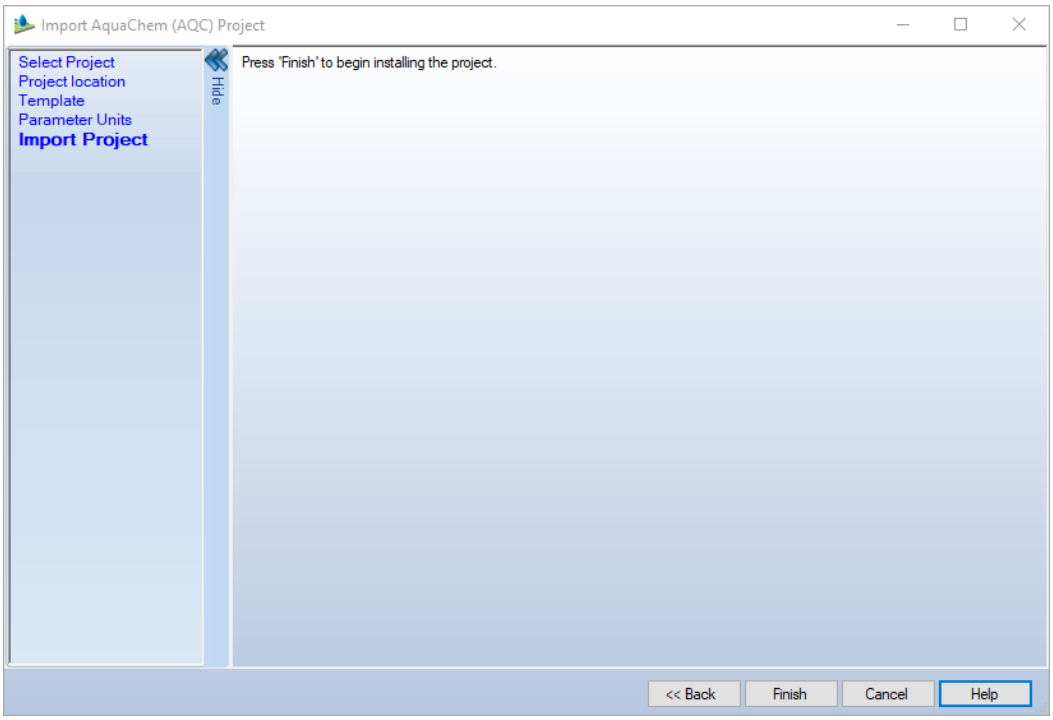
The Parameter Units step should look like the image below before you proceed:



Click the Next >> button to proceed to the final step of the import process.

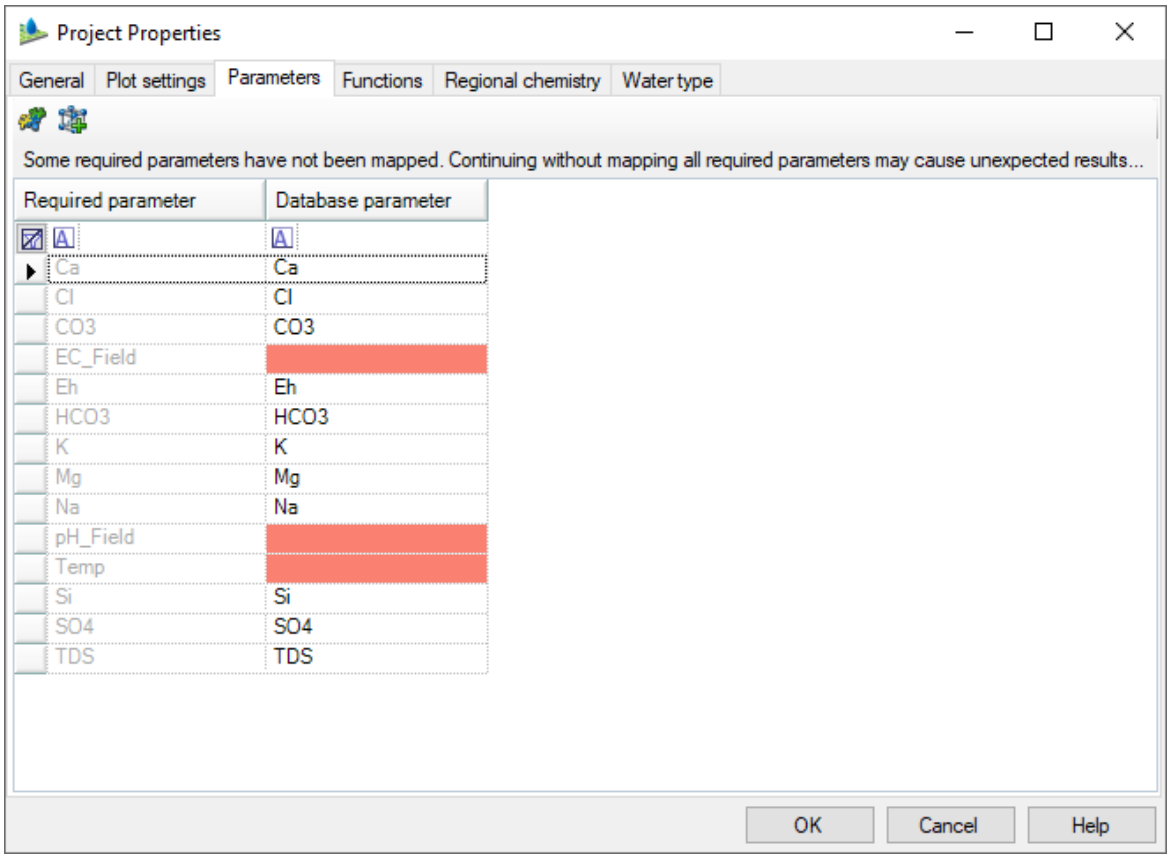
Import Project

The final step in the import process is to simply click the Finish button and initiate the import process:



When you click the Finish button, AquaChem 10.0 will generate the new AquaChem project database based on the contents and structure of the AquaChem 2014 original project and the settings you have selected in the previous steps. Database tables, fields and records will be recreated faithfully in the new project. When the import process is finished, the 'Import AquaChem (AQC) Project' window will close, and the project will be loaded.

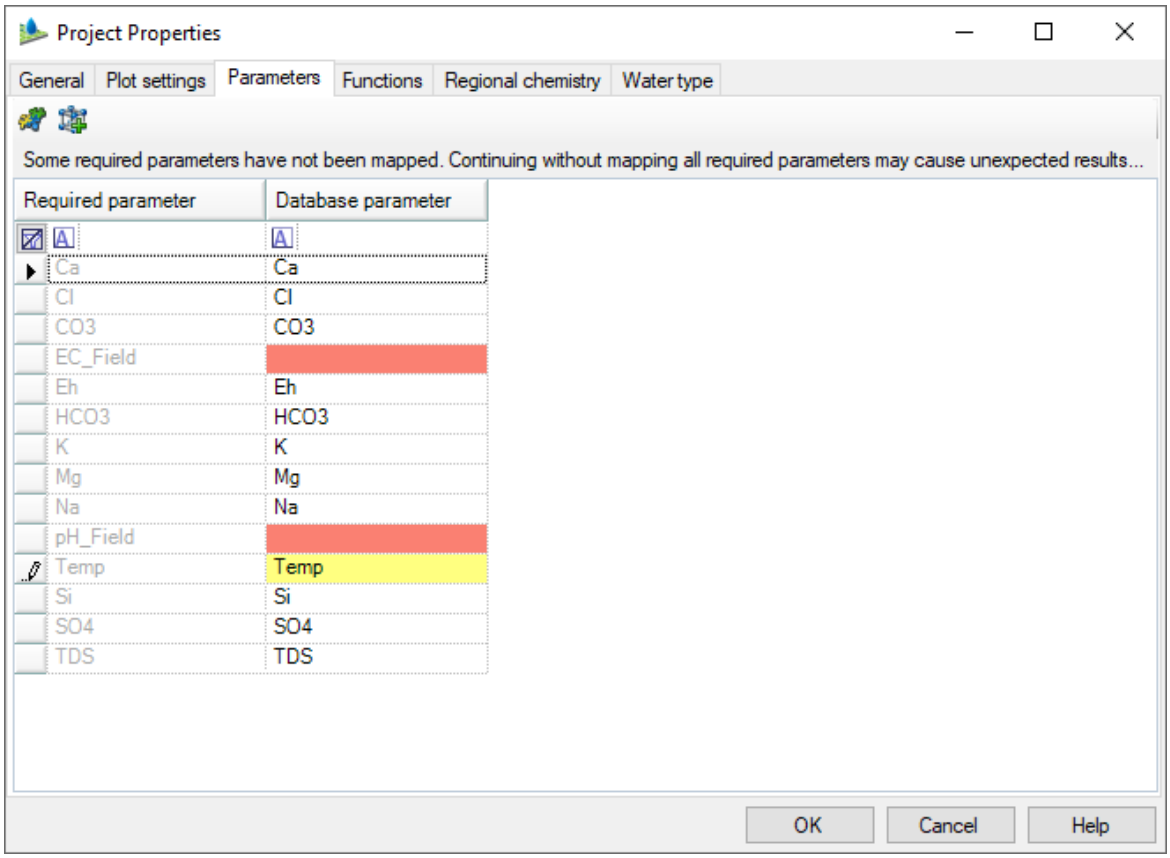
If any of the required parameters from the AquaChem 2014 project have not been automatically mapped, then the Project Properties window may appear, as shown below. Please note that the project imported for this tutorial (i.e. 'Demo_Basic.aqc') should have all parameters mapped, but this may not be the case for all projects imported from AquaChem 2014.



Please Note: in this tutorial all parameters should be mapped automatically. The image above and the following paragraphs are simply provided as a reference.

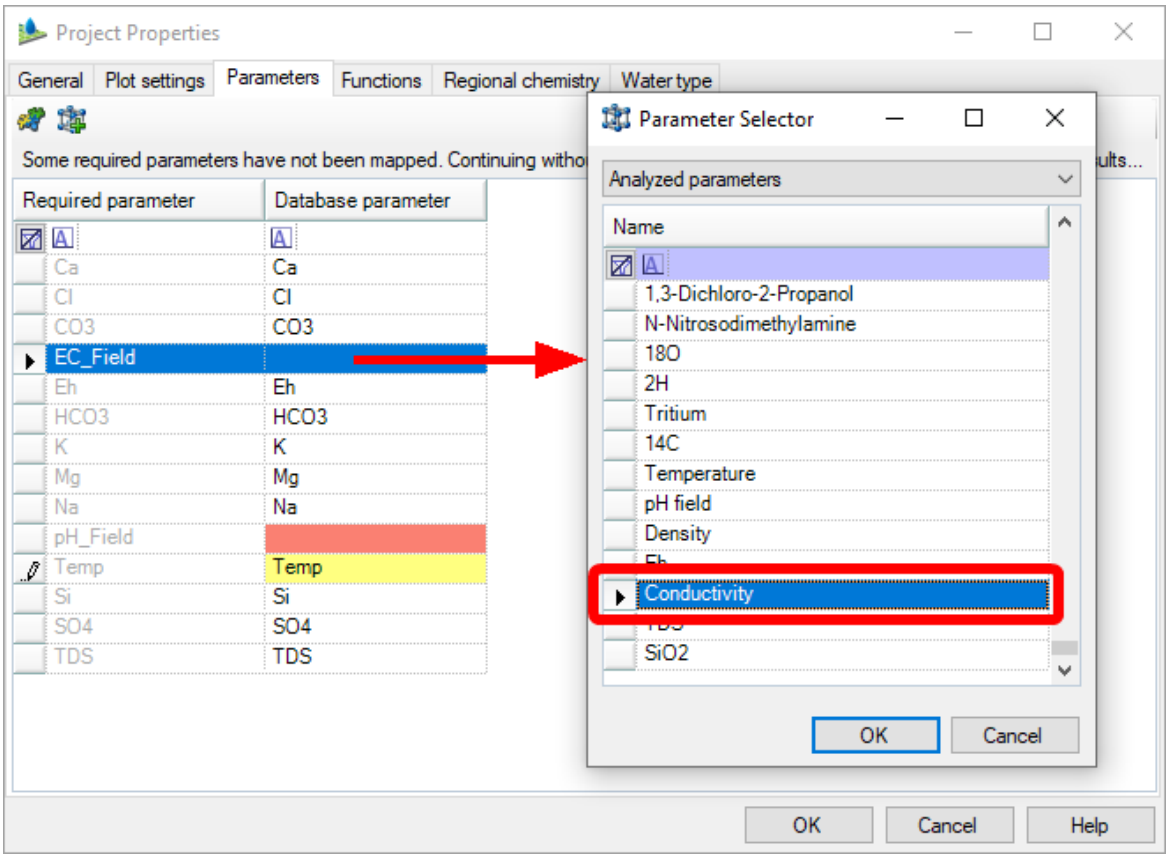
In both versions of AquaChem, there are a number of parameters which must be included in your project and mapped to required parameters to enable a variety of functions (e.g. hardness, scaling, and agricultural functions) and plots. If the window above appears, you can use the toolbar buttons to quickly map the existing database parameters to the required parameters (i.e. indicate to AquaChem 10.0 which of the available parameters represents the required parameters).

The 'Auto-map' button [] will automatically match any unmapped parameters from the original project to the new database structure based on matching parameter names. Click the 'Auto-map' button now to map most of the parameters. After clicking the 'Auto-map' button [] the Project Properties window may look like the image below:

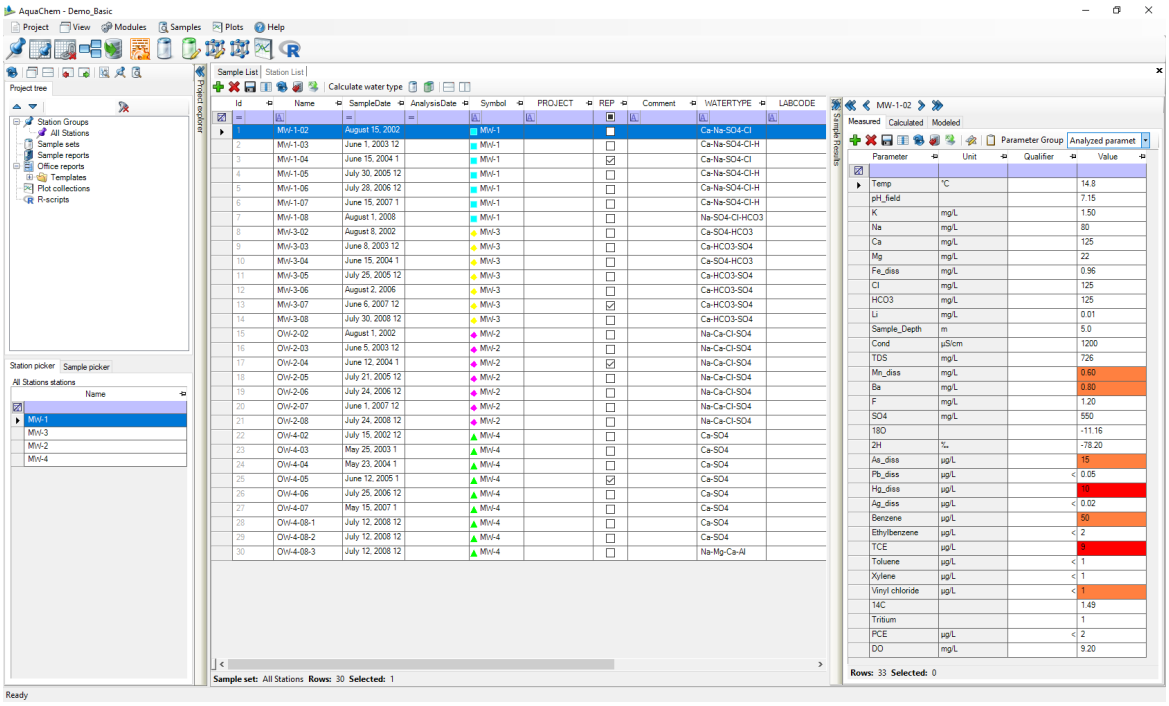


The Conductivity and ph_Field parameters have not been mapped automatically, since the form label/name for these parameters in the original project were different than the 'Required Parameters' listed here.

Click the red cells (■) next to 'EC_Field' to open a 'Parameter Selector' window which displays all parameters available in the project, scroll down until you find 'Conductivity' (near the bottom of the list) and select it. Then repeat the same procedure for 'ph_Field' (mapping to 'ph field').



After mapping the Conductivity parameter simply click OK to accept the changes and dismiss the Project Properties window. The AquaChem 2014 project has now been loaded. You can use the Station List, Sample List and Sample Details windows to review the imported data, and begin exploring the features offered in AquaChem 10.0.



- This concludes the 'Importing Projects from AquaChem 2014' tutorial -

Chapter 3 Fundamental Concepts

AquaChem is a desktop application that facilitates data management, plotting, mapping, and analysis of environmental water quality and hydrogeochemical data. This section provides you with an overview of the concepts that are fundamental to working with AquaChem. If you are new to AquaChem, you should read this section and work through the Quick Start Tutorials. Although the software was designed to be intuitive to environmental professionals, this will likely help you become more proficient with the software in less time.

Learning more

The Fundamental Concepts section provides an introduction to the following key concepts that will help you get the most out of AquaChem:

- See Data Structure
- See AquaChem Interface
- See Stations
- See Samples
- See Parameters
- See Projections
- See Chemical List
- See Measurement Units
- See Functions
- See Adjustable Windows
- See Data Entry

3.1 Data Structure

The AquaChem data structure is described below:

Data Concepts

The following concepts are fundamental to working with AquaChem:

- **Stations** are records that represent a single location with an X- and Y-coordinate, often including associated metadata. Examples of stations would include groundwater monitoring wells or fixed locations along a stream. These are designated by a unique identifying code (Station ID), such as MW-01 for a monitoring well, or SW-01 for a

surface water sampling location although for larger projects with multiple sites and/or long histories, longer codes are often required. The **Station Picker** can be found in the lower left quadrant of the interface (by default) and allows you to select which Station(s) and by extension which associated Samples are currently selected and used in various parts of the interface.

- **Samples** are records that represent unique events where one or more physical measurements and/or analytical samples have been collected at a given location. Samples must be associated with an existing Station (using the Station ID) and typically also include associated metadata, such as the sample collection date, time, and the name(s) of who collected the sample. Samples must be identified using a unique identifying code (Sample ID); however, a given Sample will often be associated with multiple physical samples collected from the same location (Station) during the same sampling event. For example, when collecting physical samples from a given location, different analyses will often require different collection and preservation methods: samples may include measurements from hand-held devices for pH and temperature in addition to physical samples collected for metals analyses, which are typically pre-filtered to plastic sample containers and preserved with acid or physical samples collected for organic compound analyses, which are typically not-filtered and filled into glass containers with no head-space. These individual physical samples should share a common Sample ID so that the results for the various measurements and analytical results can be correlated. The **Sample Picker** can be found in the lower left quadrant of the interface (by default) and allows you to select which Station(s) and by extension which associated Samples are currently selected and used in various parts of the interface.

- **Results** are records that represent the value and associated data for a single parameter and associated metadata such as quality assurance/quality control flags, data validation flags, method detection limits, etc.

- **Parameters** are the types of measurements and observations that are included included in the project (for example: temperature, pH, and the concentration of Calcium are individual parameters). Each parameter must be uniquely named and has a designated measurement unit. AquaChem also stores other optional metadata about parameters, including molecular weights, valence, and CAS numbers.

- **Standards** are threshold values that indicate parameter results may be be present at levels that may pose an unacceptable risk to the health of receptors or the environment, require some action or further evaluation. Multiple standards can apply to the same parameter such as the case of different criteria between federal and state/provincial criteria or different criteria for different receptors (e.g. human health vs. aquatic biota).

AquaChem Relational Database and Simplified Data Model

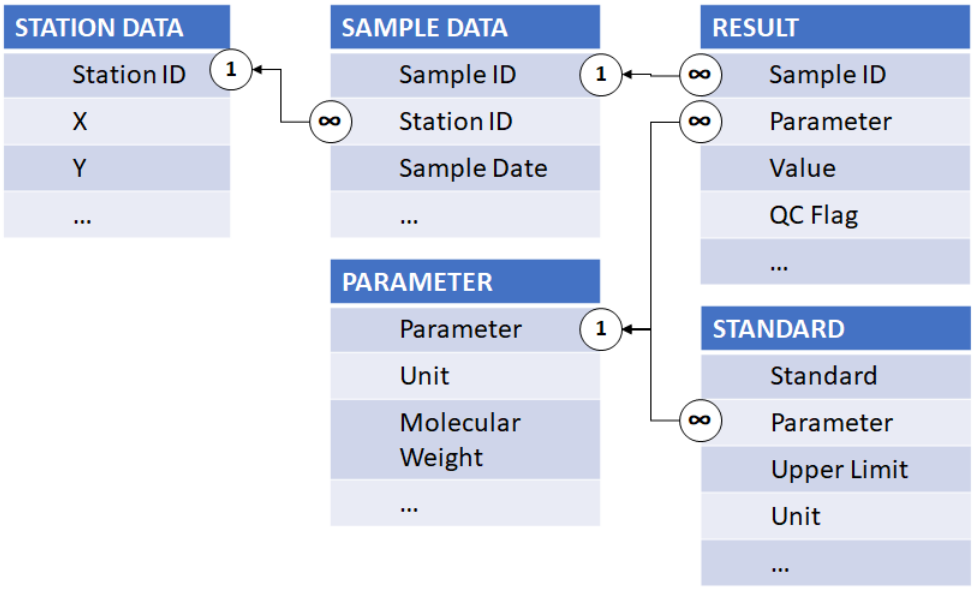
The information described above is stored in AquaChem using a structured format in a Microsoft Access relational database. The relational database organizes data into several tables consisting of columns and rows, with a unique key (e.g. a unique sample ID) that

identifies each row. Rows in a data table are typically called records; while columns are typically called fields.

- **Tables** store information about specific entity types with common data attributes. For example, separate tables store information about stations, samples, and results.
- **Records** represent individual entities (e.g. a specific environmental sample).
- **Fields** store specific attributes about each record in that table (e.g. sample collection date).
- **Keys** are fields that store a unique attribute that is used to identify a record (e.g. sample ID) that allow you to retrieve information about that record.

One table can can be related to a second table by including the key of the first table as an attribute in the second (For example, the sample table includes the unique Station ID). A simplified version of the tables and their relationships is shown below:

Simplified Data Structure of AquaChem

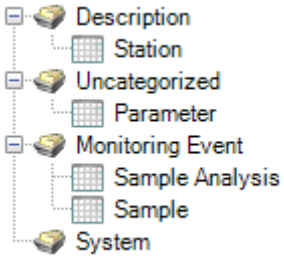


Template Manager

If you are comfortable working with databases, you can explore the complete data structure using the Template Manager module. You can also explore the data structure in MS-Access; however, this is not recommended for all but the most experienced users to avoid corrupting the AquaChem data structure. If you chose to work in Access as well, it is strongly recommended that you first backup your data so you can recover your project in case it is corrupted.

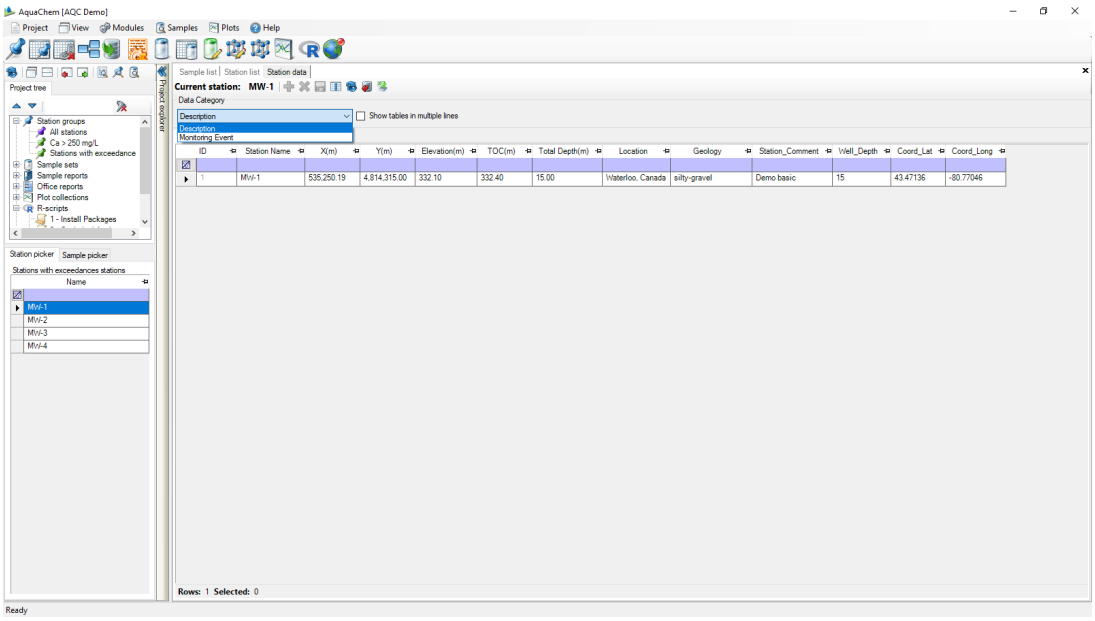
Data Categories

The tables in an AquaChem database can be organized into a logical grouping by placing them into a data categories. The number, names, and organization of the categories is defined using the Template Manager. The default template in AquaChem provides the following data categories:



These are related to the primary function of AquaChem, namely the hierarchical relationship between Stations, Samples, Parameters, and Results. You can create as many categories as you wish using the Template Manager. In this way, you can completely customize how the tables are organized within AquaChem. However, if your project includes a lot of additional data, particularly other monitoring events, borehole logs, well completion details, and geophysics, you may wish to consider converting your project to use Hydro GeoAnalyst which supports additional functionality such as borehole profiles, cross-sections, mapping, 2D/3D interpolation, and 3D scene views.

Categories of tables that are linked to the Stations using the Station ID, can be accessed by selecting the Station Data tab and selecting the Data Category combo box (ensure that one or more stations are selected in the Station List tab):



After a Data Category has been selected, the appropriate tables and fields belonging to this category will be displayed in the Station Data tab.

All of the data categories may be renamed and used differently if desired. For example, a category named Geology could be renamed to Surface Water and tables such as Catchments, Surface Water Monitoring Locations, Rivers, etc. could be organized under it. Placing tables under any one of these categories does not have any effect on how the tables are stored in the database.

File Format

AquaChem projects must be stored in their *own file folder* (i.e. you should not have more than one and consist of the following:

- **Project File:** stores information about the AquaChem project and has a ***.aqcx*** file extension
- **Database**: an MS-Access database that stores project data in the ***.accdb*** file format
- **Lockfile:** a temporary file generated by MS-Access with a ***.laccdb*** file extension that locks tables to prevent multiple users from modifying the same information at the same time.
- **Module Folders:** a series of folders that store and organize module-specific input and output data:
  - Plots Collections,
  - Reports, and
  - Scripts

When copying, moving, sharing, or archiving an AquaChem project, all of these files described above must be copied, moved, or otherwise transferred to a common empty folder.

3.2 AquaChem Interface

This section describes the layout of AquaChem and how to navigate in it.

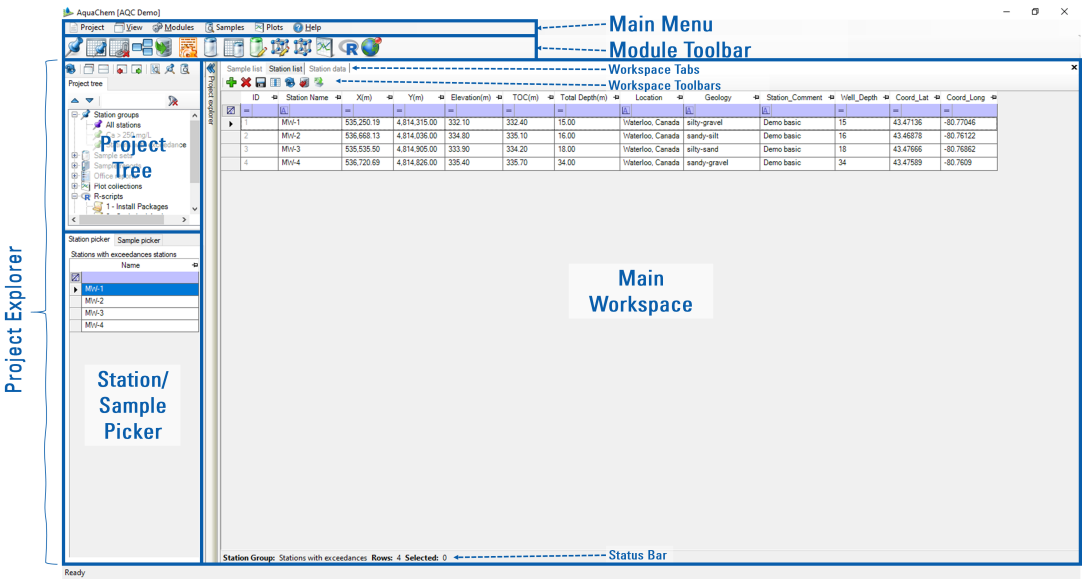
AquaChem Layout

The AquaChem interface is composed of several controls:

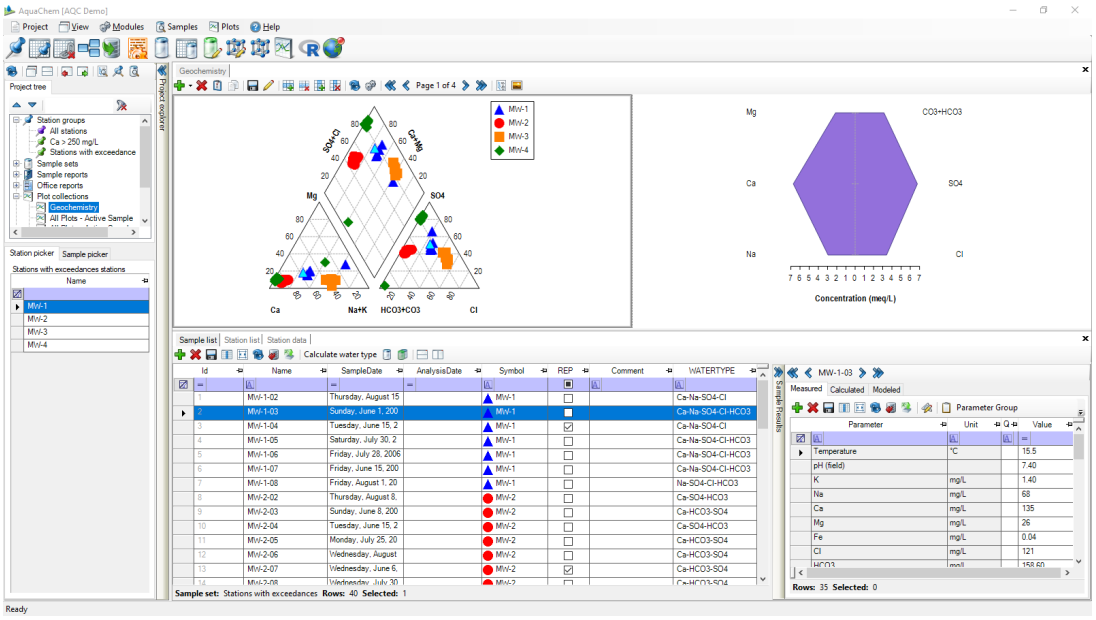
- **Menu Bar**: Contains menu commands with access to most features that are available in AquaChem.
- **Module Toolbar**: A toolbar that contains short-cut buttons for the most frequently used features in AquaChem.
- **Project Explorer**: Hosts the Project Tree view listing the major components of your project as well as the Station Picker and Sample Picker.
- **Station & Sample Picker**: Allows you to select groups of station(s) or sample(s) that are used to display and work with data in other modules, tabs, and plots.

- **Workspace Tabs**: Provides access to the various views, modules, and components of AquaChem projects including: the Station List, Sample List, Plot Collections, and R-Console.
- **Main Workspace**: Contains the workspace for the current view.
- **Workspace Toolbars**: Contain icons for the main options you can perform with the current view in the workspace.
- **Status Bar**: Displays the program status.

Once a project is loaded, the main window will appear; the AquaChem demo project is displayed below.



You also have the option to move tabs around and place them where you like. The default configuration is to have one tab group for the Project Tree and one tab group with the rest of the tabs (station list, station data, etc.). However, you can have more tab groups – vertical or horizontal. You can find these options by right clicking on a tab. Then you can just drag and drop the tabs where you prefer them! Here is an example configuration that you might like to use. You can also undock tabs so that you can make use of multiple monitors.



Project Explorer

The Project Explorer is one of the main navigation tools in the AquaChem interface. It is composed of the Project Tree, the Station Picker and the Sample Picker. The main toolbar of the Project Explorer contains the following commands:

- refreshes the Project Explorer from the project database
- combines the Project Tree tab with the Station and Sample Picker tabs
- separates the Project Tree tab from the Station and Sample Picker tabs
- docks the Project Explorer to the left of the main workspace
- docks the Project Explorer to the right of the main workspace
- toggles the visibility of the Project Tree
- toggles the visibility of the Station Picker
- toggles the visibility of the Sample Picker

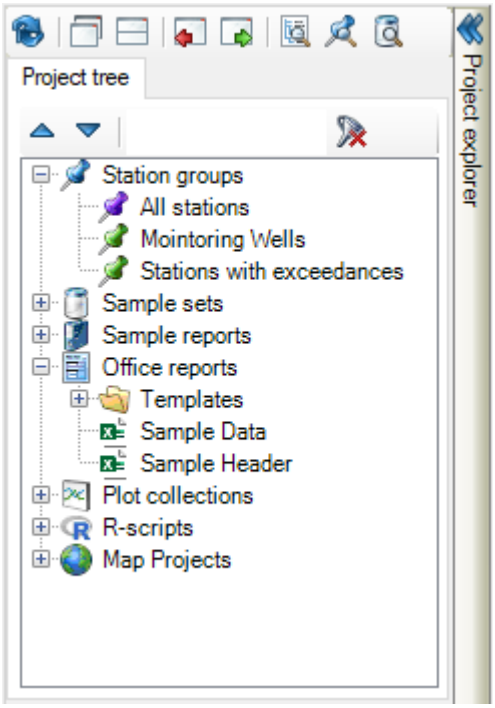
You can hide/show the Project Explorer by selecting the double blue arrows ( ) located between the Project Explorer and the Main Workspace.

Project Tree

The project tree allows you to organize and navigate through the data and related components in your project:

- Station Groups,
- Sample Sets,

- Sample Reports,
- Office Reports,
- Plot Collections,
- R-scripts, and
- Map Projects



Each item is organized as a branch in the tree view with one or more items under each branch. By double-clicking an item in the Project Tree you will either activate the appropriate tab or launch appropriate module to view this item. The following options are available in the Project Tree Toolbar:

collapses all branches in the Project Tree.

expands all branches in the Project Tree.

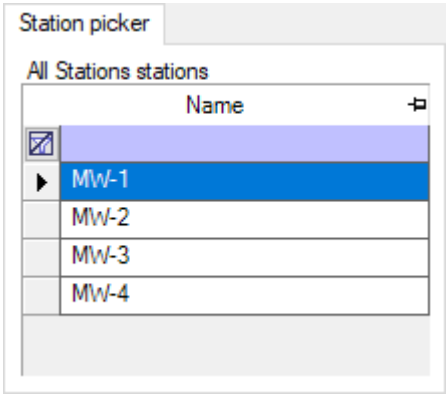
the search bar filters the project tree to items (and their parents) that *contain* your search string.

clears the search filter.

You can organize any of the branches of the Project Tree (except for the Reports branch as it has it requires its own structure) by creating folders to group the items under the branch. Simply right click the branch and select *Add Folder...* . Provide a name for the folder and then you can drag and drop items from that branch into the folder.

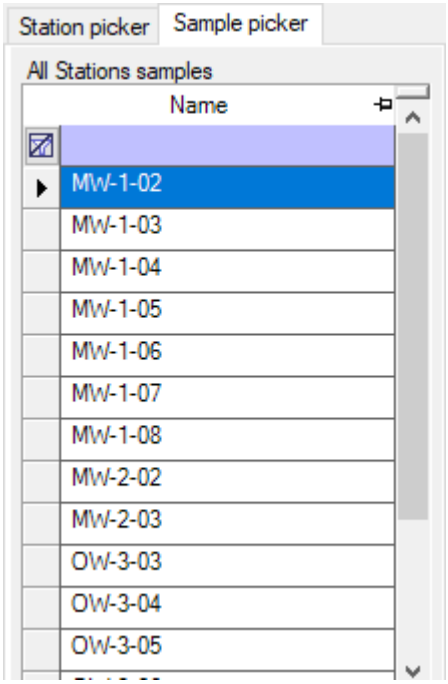
Station Picker

The Station Picker displays a list of the stations in the currently active station group and allows you to select the active station to display in relevant tabs (e.g. the Station List and Station-Data Tab). The active station is highlighted in blue and denoted by the ▸ symbol, while selected stations are highlighted in blue. The active station and selected stations are set by clicking on a station in the station picker (or in the Station List). Only one station can be active at a time; however you can select multiple stations using the left mouse button with the <SHIFT> or <CTRL> keys. To change the active station group double-click on the station group or sample set in the Project Tree.



Sample Picker

The Sample Picker displays a list of the samples in the currently active sample set and allows you to select sample(s) to display in relevant tabs (e.g. Sample List View and Plot Collections). The active sample is highlighted in blue and denoted by the ▸ symbol, while selected samples are highlighted in blue. The active sample and selected samples are set by clicking on a sample in the sample picker (or in the Sample List). Only one sample can be active at a time; however you can select multiple samples using the left mouse button with the <SHIFT> or <CTRL> keys. To change the active sample set, double-click on a sample set or station group in the Project Tree.



Station Groups

In AquaChem, stations can be sorted into groups allowing for efficient management and quick retrieval of data stored in the database. All station groups created for a project are listed in the Project Tree under the Station Groups node. Double clicking on any of the branches corresponding to a station group will load the Station List tab, and display the appropriate stations belonging to that group. There are three kinds of Station Groups in AquaChem:

All Stations: A list of the all stations in the project database. The station group is in all projects and all stations that are added (either manually or by import) to the project will be found in this station group. You can not delete or rename this station group.

Static: A fixed list of stations. To build a static station group, select one or more stations directly in the Station List tab, right-mouse click, and select the Add to [New/Existing] Station Group option from the pop up menu.

Dynamic: A variable list of stations that meet applicable condition(s) specified in the Sample Set Editor. This list is built on-demand by AquaChem each time it is activated or refreshed by a workspace tab (e.g. the Station List).

Once the stations in a group are displayed, a number of operations can be applied based on the selection. To find out more about Station Groups please refer to Station Groups section of the manual.

Sample Sets

Similarly, samples can be grouped into Sample Sets allowing you to easily manage, retrieve, and work with specific and meaningful groups of samples. Sample sets created for a project are listed under the Sample Sets node in the Project Tree. Double clicking on any of the branches corresponding to a station group will load the Station List tab. There are three kinds of Sample Sets in AquaChem:

 **Static:** A fixed list of samples. To build a static sample set, select one or more samples directly in the Sample List tab, right-mouse click, and select the Add to [New/Existing] Sample Set option from the pop up menu.

 **Dynamic:** A variable list of samples that meet applicable condition(s) specified in the Sample Set Editor. This list is built on-demand by AquaChem each time it is activated or refreshed by a workspace tab (e.g. the Sample List).

 **Stations**: Station groups are also implicitly sample sets as they also refer to all of the samples collected at the stations within that station group. **Note** that by definition, the  *All Stations* station group includes all samples in your project.

Once the samples in a set are displayed, a number of operations can be applied based on the selection. To find out more about Sample Sets please refer to Sample Sets section of the manual.

Modules

The AquaChem interface is organized into modules, which are core components of the application that help you perform specific tasks. For example: that Data Import module allows you to import data, the Plot Collection module allows you to build plots, etc. A complete list of modules and links to their relevant topics is presented in the Modules section of the manual.

Toolbars

There are different tool bars available within the program - the Module Toolbar which provides quick access to AquaChem Modules and the Workspace Toolbar which provides access to common tools and features within each module.

Module Toolbar

The top toolbar with the larger buttons is the main toolbar and provides quick access to the various views and modules available in AquaChem. The default toolbar is shown below; however, the main toolbar is configurable via the Module Manager options in the AquaChem Settings:

	Station List Tab
	Station Data Tab
	Non Station Data Tab
	Template Manager
	Import Data
	List Editor
	Sample List
	Sample Analysis Viewer
	Sample Set Editor
	Parameter Editor
	Parameter Group Editor
	Plot Collections
	R-Console
	Map Viewer

Workspace Toolbar

There are also toolbars available on the individual tab groups specific to the actions you may wish to perform on the data contain within the tab group. Below is the general tool bar found on most tab groups:

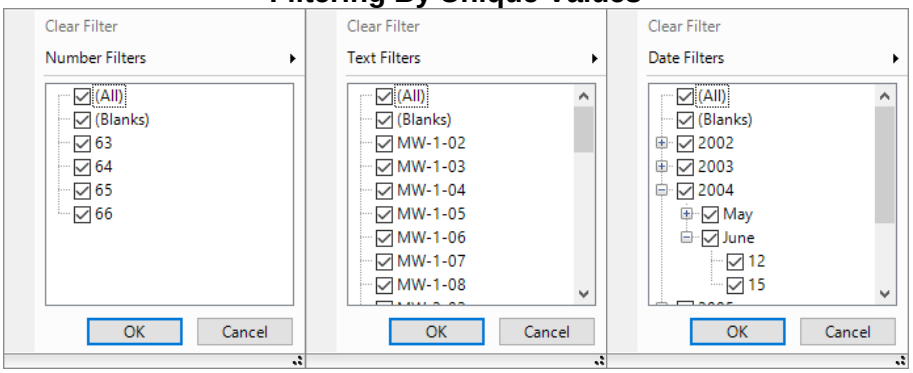
It provides options to add a record and delete items (typically a record) as well as save any edits made by committing changes to the database. There is also typically an option to show/hide columns, refresh the data from the database, export data (usually as a table), or print the data to a formatted template file.

By placing your cursor over any of the icons in the tool bars you will find a tooltip indicating what the button does.

Data Filtering

AquaChem has many tabs, windows, and views that includes data tables and provides helpful options allowing you to filter your data so that you can quickly find the information that you need - the first row on any data grid is the filter row (shown in light blue). You can filter by unique values; if the field contains date values, the values will additionally be filterable by groups of year, month, or day:

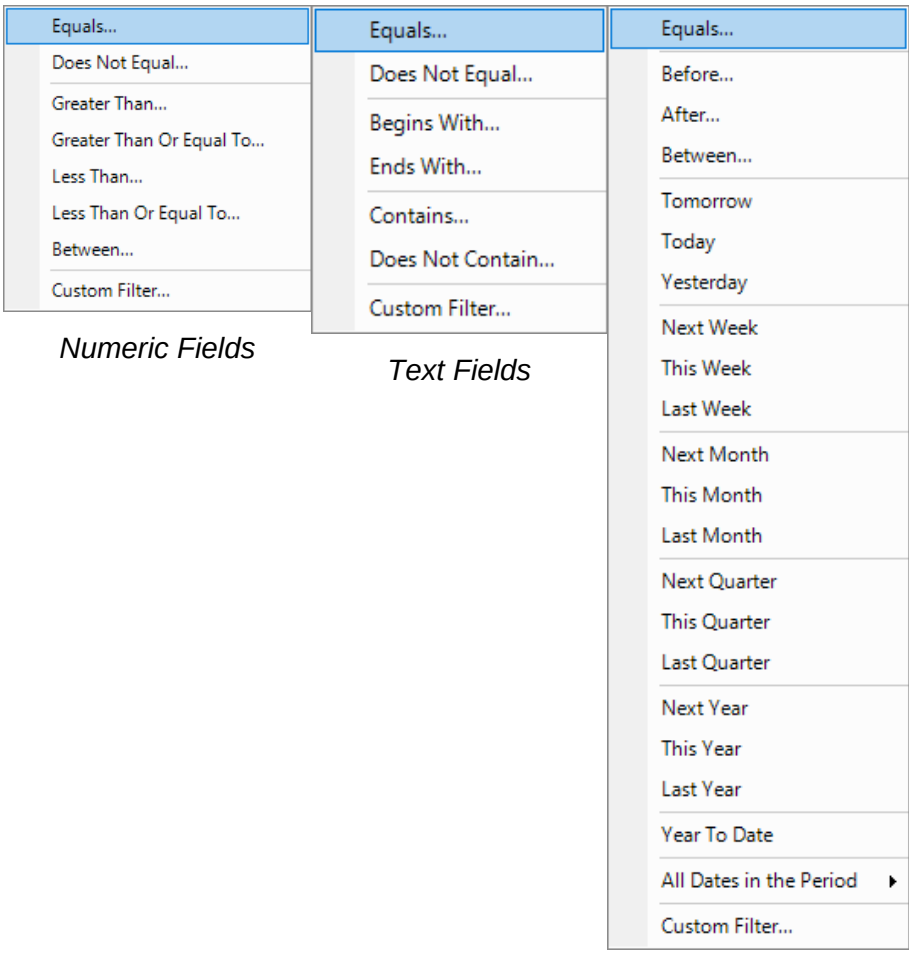
Filtering By Unique Values



Numeric Field *Text Field* *Date Fields*

You can also filter by using a relational condition, as shown below:

Filtering by Relational Conditions



Numeric Fields

Text Fields

Date Fields

3.3 Stations

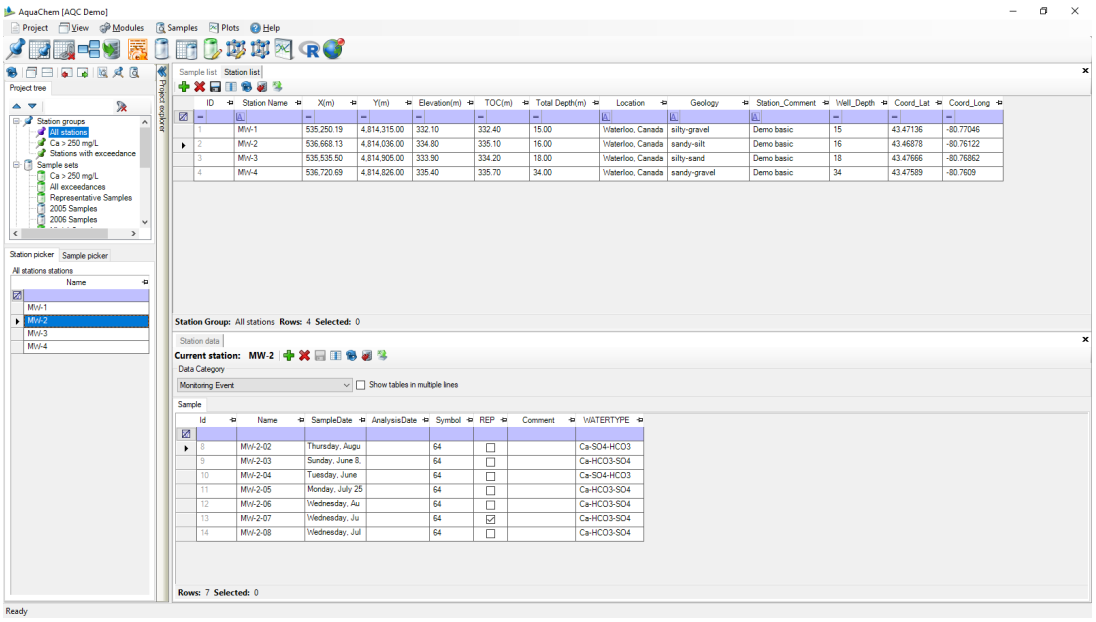
Stations are records that represent a single location with an X- and Y-coordinate, often including associated metadata. Examples of stations would include groundwater monitoring wells or fixed locations along a stream. These are designated by a unique identifying code (Station ID), such as MW-01 for a monitoring well, or SW-01 for a surface water sampling location although for larger projects with multiple sites and/or long histories, longer codes are often required. The **Station Picker** can be found in the lower left quadrant of the interface (by default) and allows you to select which Station(s) and by extension which associated Samples are currently selected and used in various parts of the interface.

Station Table

The Station Table stores all the station location information for all projects residing in the database. The Station Table may contain an unlimited number of fields. Though, as a minimum, the Station Table must contain the following fields:

- Station ID (ID) - *must be unique*
- Station Name (Name)
- Station Coordinate (X)
- Station Coordinate (Y)

Stations can be added, modified, or deleted through the Station List tab. The Station List Tab displays information about the station; whereas the Station Data Tab can be used to show additional information that links back to the current station (e.g. all samples collected at that station), as shown below:



Station Groups

Many operations in AquaChem require the selection of one or more stations. An example of such an operation is data entry. One or more stations for which you would like to add, view, and/or modify data need to be selected so that the Station Data Tab is accessible (activated).

The complete list of stations that comprise a project can be viewed in the Station List tab by selecting the All Stations item, under the Station Group node in the project tree. By default, all projects will contain a station group named All Stations that lists all stations in the database belonging to the project. However, for some of the tasks commonly performed in AquaChem, retrieving the complete list of stations in the project may not be necessary.

Moreover, retrieving all the stations when only few of them are needed may be a time-consuming process especially for large databases containing hundreds or thousands of stations.

The solution is to create Station Groups. Grouping stations into their logical groups allows efficient management and quick retrieval of data stored in the database. For instance, all stations which contain isotopic sampling data can be grouped together under a group named as Isotope Sample Locations. Whenever these stations need to be updated with a new groundwater sampling round, selecting the Isotope Sample Locations group displays only those stations that belong to this group.

Station groups can be created based on any criteria. Common examples include:

- Locations of the stations (e.g. locations categorized by City, Project Site, watershed, etc.)
- Station type (e.g. Surface/Groundwater Monitoring Locations, Boreholes, etc.), or
- Purpose of Study (e.g. remediation, site monitoring)

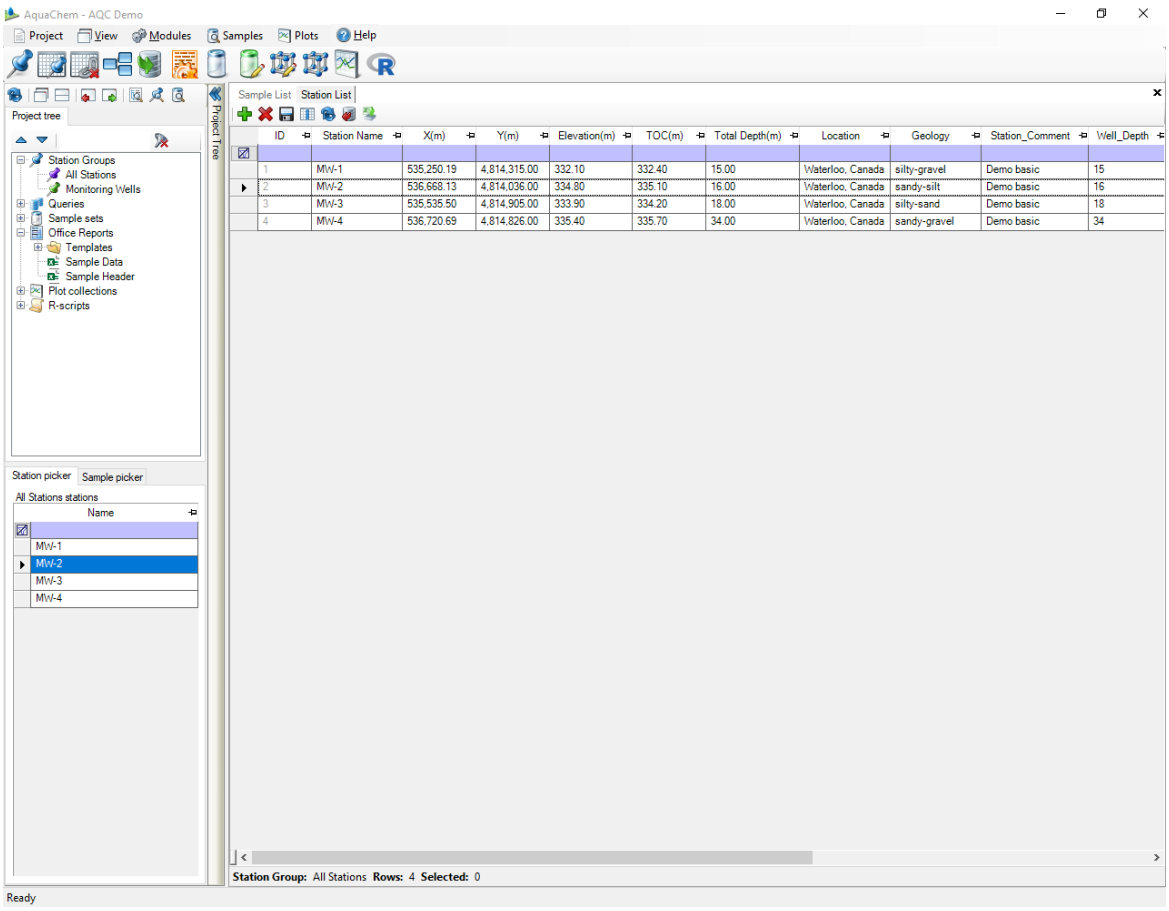
There are three kinds of Station Groups in AquaChem:


All Stations: A list of the all stations in the project database. The station group is in all projects and all stations that are added (either manually or by import) to the project will be found in this station group. You can not delete or rename this station group.


Static: A fixed list of stations. To build a static station group, select one or more stations directly in the Station List tab, right-mouse click, and select the Add to [New/Existing] Station Group option from the pop up menu.


Dynamic: A variable list of stations that meet applicable condition(s) specified in the Sample Set Editor. This list is built on-demand by AquaChem each time it is activated or refreshed by a workspace tab (e.g. the Station List).

All Station Groups created for a project are listed in the Project Tree under the Station Groups branch. Double-clicking on any of the sub-branches corresponding to a Station Group will load the Station List tab, and display the appropriate stations belonging to that group. An example is shown below.



If desired, selected stations can be removed from a static station group or the Station Group can be deleted as a whole (unless it is the *All Stations* group). To remove stations from a static station group simply select the station(s) by highlighting the desired row(s) and then selecting the remove stations [] button - this will remove the station from the station group - but will not delete the station from the database. To delete a station from the database, select the delete [] button.

To delete an entire station group right click on the station group in the Project tree and select delete.

3.4 Samples

Samples are records that represent unique events where one or more physical measurements and/or analytical samples have been collected at a given location. Samples must be associated with an existing Station (using the Station ID) and typically also include

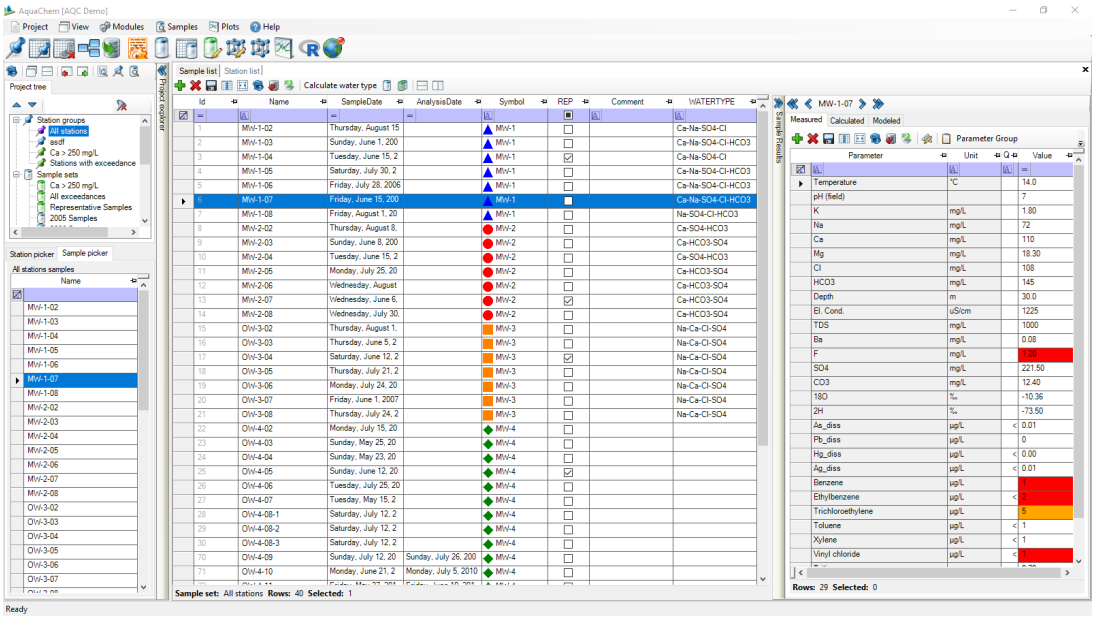
associated metadata, such as the sample collection date, time, and the name(s) of who collected the sample. Samples must be identified using a unique identifying code (Sample ID); however, a given Sample will often be associated with multiple physical samples collected from the same location (Station) during the same sampling event. For example, when collecting physical samples from a given location, different analyses will often require different collection and preservation methods: samples may include measurements from hand-held devices for pH and temperature in addition to physical samples collected for metals analyses, which are typically pre-filtered to plastic sample containers and preserved with acid or physical samples collected for organic compound analyses, which are typically not-filtered and filled into glass containers with no head-space. These individual physical samples should share a common Sample ID so that the results for the various measurements and analytical results can be correlated. The **Sample Picker** can be found in the lower left quadrant of the interface (by default) and allows you to select which Station(s) and by extension which associated Samples are currently selected and used in various parts of the interface.

Sample Table

The Sample Table stores all of the sample information in the database. The Sample Table may contain an unlimited number of fields. Though, at a minimum, the Sample Table must contain the following fields:

- Sample ID (ID) - *managed as an automatic sequential number by AquaChem*
- Sample Name (Name) - *must be unique*
- Station Name (Station)
- Sample Date (SampleDate)

Samples can be added, modified, or deleted through the Sample List. The Sample List displays information about the currently active sample set on the left side of the workspace and the results for the active Sample (as denoted by a black triangle in the leftmost column of the sample table) on the right side of the workspace.



Sample Sets

Many operations in AquaChem require the selection of one or more samples. One example of such an operation is data entry. One or more samples for which you would like to add, view, and/or modify data need to be selected so that the Sample List is accessible (activated). Another such example is plotting: most of the plots you will likely want to create in AquaChem will be based on a specific subset of your samples.

The complete list of samples that comprise a project can be viewed in the Sample List tab by selecting the *All Stations* item, under the Station Group node in the project tree. By default, all projects will contain a station group named All Stations that includes all samples for every station in the database. However, for some of the tasks commonly performed in AquaChem, retrieving the complete list of samples in the project may not be necessary or even desired. Moreover, retrieving all the samples when only few of them are needed may be a time-consuming process especially for large databases containing hundreds or thousands of samples.

The solution is to create Sample Sets. Grouping samples into logical sets allows efficient management and quick retrieval and plotting of data stored in the database. For instance, you may wish to find all samples that:

- were collected within a certain period of time,
- exceed some water quality standard,
- belong to a certain group of stations, or
- a combination of the above.

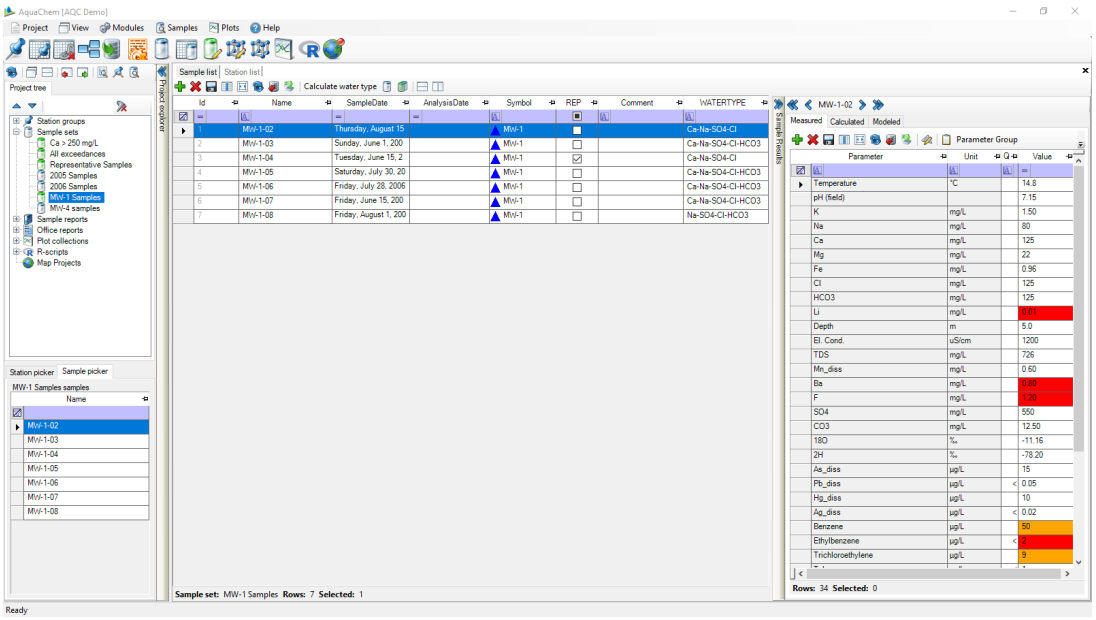
There are three kinds of Sample Sets in AquaChem:

Static: A fixed list of samples. To build a static sample set, select one or more samples directly in the Sample List tab, right-mouse click, and select the Add to [New/Existing] Sample Set option from the pop up menu.

Dynamic: A variable list of samples that meet applicable condition(s) specified in the Sample Set Editor. This list is built on-demand by AquaChem each time it is activated or refreshed by a workspace tab (e.g. the Sample List).

Stations: Station groups are also implicitly sample sets as they also refer to all of the samples collected at the stations within that station group. **Note** that by definition, the *All Stations* station group includes all samples in your project.

All sample sets created for a project are listed in the Project Tree under the Sample Sets branch. Double clicking on any of the sub-branches corresponding to a Sample Set will load the Sample List tab, and display the samples belonging to that set. An example is shown below.



If desired, selected samples can be removed from a static sample set or the samples set can be deleted as a whole. To remove samples from a sample set simply select the samples(s) by highlighting the desired row(s) and then select the remove samples [ ] button - this will remove the sample(s) from the sample set - but will not delete them from the database. To delete a sample from the database, select the delete [ ] button.

To delete an entire sample set, right-click on the sample set in the Project tree and select delete.

3.5 Parameters

Parameters are those properties whose values describe the state of a particular station or sample. There are three general kinds of parameters in AquaChem:

- **Station parameters** are those parameters that describe a station and its properties. All of the fields in the Station Table are station parameters; for example: station name, x- and y-coordinates, and site description.

- **Sample parameters** are those parameters that describe a sample and its properties. Similarly, all of the fields in the Sample Table are sample parameters; for example: sample ID, station, and sample date.

- **Analytical parameters** are associated with sampling results and describe the value or measurement of a particular constituent (e.g. calcium concentration, pH, temperature, etc.).

Generally in AquaChem, unless otherwise specifically stated, the term *parameter* refers to analytical parameters. Analytical parameters may be further subdivided into various groups as discussed below.

Viewing Parameters and Results

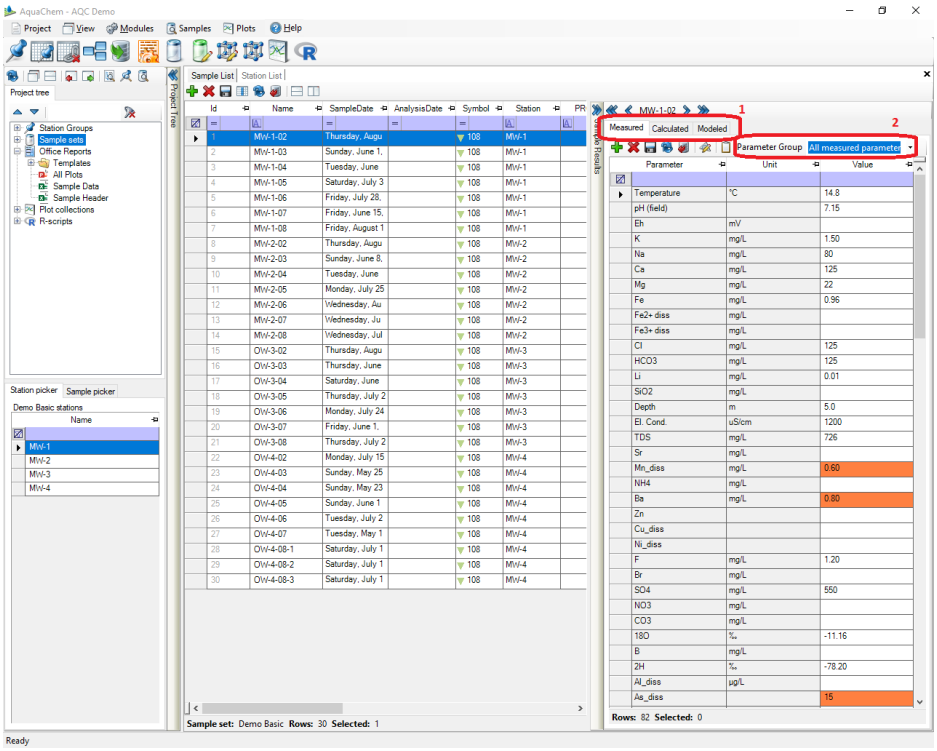
When viewing the Sample List, results for the selected sample are shown in the Results pane. Results are shown by parameter type in the tab at the top of the results pane (as denoted by circled area 1):

- **Measured parameters** are those values that are explicitly stored in the database and typically have been measured either in the field or in an analytical laboratory.

- **Calculated parameters** are those values that have been calculated using AquaChem's built-in functions. These are calculated dynamically and are not stored in the database.

- **Modeled parameters** are those values that have been estimated using PHREEQC in an imported AquaChem 2014 project. This tab is only shown for projects that used PHREEQC and have been imported into the current version AquaChem. Note that support for PHREEQC in AquaChem is planned for a subsequent release.

Measured parameters can be filtered in the Results tab using the parameter group dropdown (as denoted by circled area 2), discussed below.

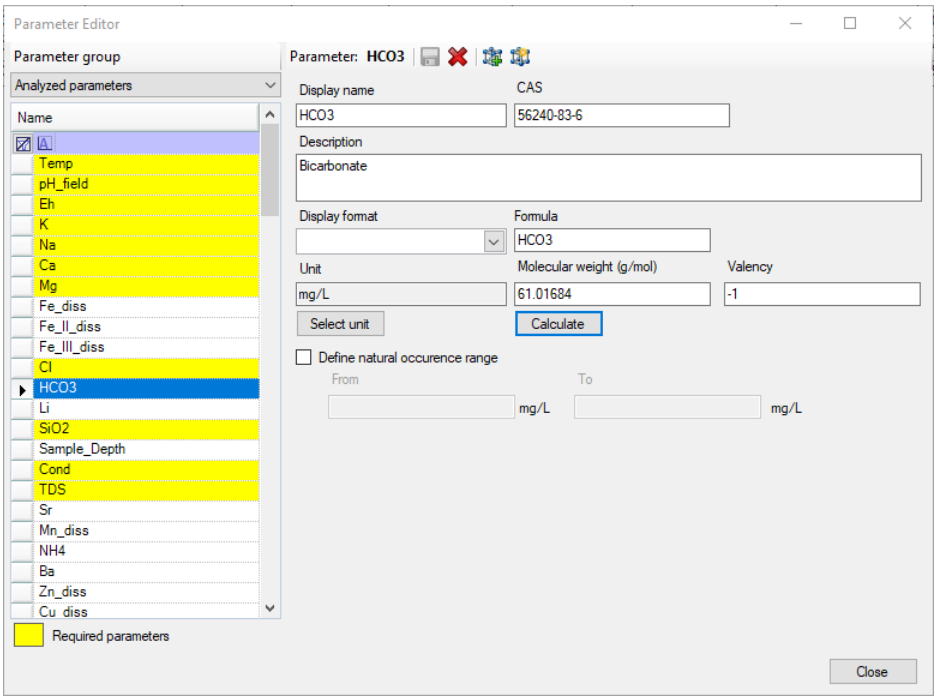


Parameters and the Parameter Editor

Information about all measured parameters is stored in the Parameter Table, and includes the relevant chemical and descriptive attributes as follows (using bicarbonate as an example):

- **Short Name**: a unique, typically short or abbreviated, name that is easily recognizable (e.g. HCO3) and used as a look up name and a primary key.
- **Display Name**: a longer descriptive name (e.g. bicarbonate) used for labeling in plots and tables.
- **CAS**: Chemical Abstracts Service (CAS) Registry number (e.g. 56240-83-6), a unique number assigned by CAS, a division of the American Chemical Society
- **Description**: typically a more descriptive name that may include a list of alternate names (e.g. bicarbonate; hydrogencarbonate)
- **Formula**: chemical formula (e.g. HCO3)
- **Molecular Weight:** combined atomic weights of all constituent atoms that compose the parameter (e.g. HCO3 = 1x1.00794 + 1x12.0107 + 3x15.9994 = 61 g/mol)
- **Valency:** the ionic/electric charge of the parameter in solution (e.g. -1).

For more information, see the Parameter Editor section.



Parameter Groups

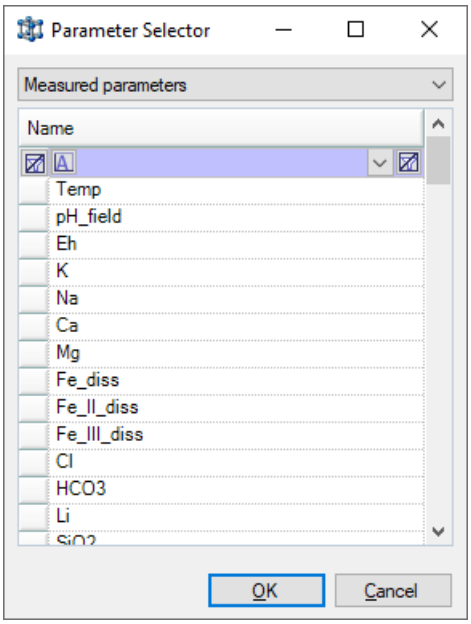
Measured parameters may be grouped into categories called parameter groups to facilitate viewing, analyzing, plotting, and tabulating your data. Some parameter groups are automatically created for you by AquaChem, including:

- **All Measured Parameters:** all of the measured parameters in your project
- **Analyzed Parameters:** parameters with results for the active sample(s)
- **Ions:** parameters with a non-zero valence
- **Cations:** parameters with a positive valence
- **Anions:** parameters with a negative valence
- **Required Parameters**: parameters that are used in a supported formula and are required
- **Used in Standard**: parameters in your project that are present in an *active* Water Quality Standard.

Custom Parameter Groups may be created in the Parameter Group Editor.

Parameter Selection Window

The parameter selection window is used throughout AquaChem to allow you to easily find and select one or more parameters:



The main portion of the window displays a list of parameters that can be selected. In many cases, you can select more than one parameter by holding the <CRTL> key to add individual items to your selection or the <SHIFT> key to add a range of items to your list.

You can filter the list in one of two ways:

- **Parameter Group dropdown menu**: which will restrict the listed parameters to the selected parameter group or
- **Filter bar**: allows you to filter the parameter list using a search term

3.6 Projections

A projection is a system that is used to reference geographic locations. Projection systems, sometimes called coordinate reference systems (CRS) are typically comprised of the following components:

- **Projection (Type)**: a coordinate system that transforms the 3D surface of the earth into a 2D coordinate system. Some of the more commonly used projections include:
  - the so-called geographic system which consists of a longitude (east/west x-coordinate) and a latitude (north/south y-coordinate);
  - Universal Transverse Mercator (UTM), and
  - Lambert conformal conic projection which is used by the U.S. National Geodetic Survey for the State Plane CRS's.

- **Horizontal Datum**: a reference frame that includes a reference ellipsoid or geoid that models the shape of the Earth, an origin tied to a know location, and associated control points. Two of the more commonly used datums include:
  - **WGS-84** used for global maps and by many national jurisdictions
  - **NAD-83** used in the United States and Canada

- **Units:** measurement units for the coordinate system. Typically, decimal degrees, meters, or feet.

There are hundreds of well-known CRS that are identified using numeric EPSG codes developed by the Euro European Petroleum Survey Group and maintained at https://spatialreference.org/. For example EPSG:4326 represents a CRS with a geographic system, using the WGS-84 horizontal datum and decimal degrees. Many geographic information system (GIS) applications store the CRS information in projection (.prj) files that accompany spatial layers such as those used in the Map Viewer Module (e.g. shapefiles and images). When creating a map, the map and each layer within it must either have a common CRS or each component and the map itself must have a specified CRS that allows the map to correctly position each layer.

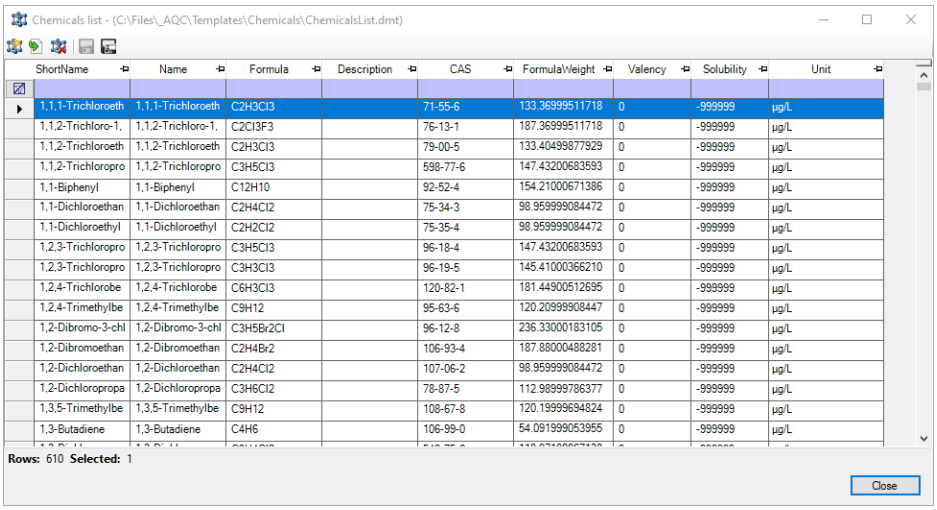
By default, maps in your Map Viewer maps will use the CRS defined when you create a new project or import an existing project from AquaChem. 2014.

For more information, please refer to:
https://docs.qgis.org/3.16/en/docs/gentle_gis_introduction/coordinate_reference_systems.html

3.7 Chemical List

The Chemical List is a database of parameters and their properties that is external to your AquaChem projects. This is a common resource that is shared across all of your projects and can be centrally or collectively managed by your organization. Data fields in the Chemical list table are aligned with the data entry fields in the Parameter Editor, which allows you to use the Chemical list as a reference for adding parameters.

The default Chemical list is located in the AquaChem install folder, typically: *C:\Program Files (x86)\AquaChem 10\ChemicalList.dmt* and is read-only; however, you can save editable copies of the Chemical List to other locations, including network drives to which you have access, so that you can share and centrally manage/curate the list with colleagues.



Commands

The following commands are available in the Chemicals list:

New: allows you to create a new chemical with a (short) name, display name, CAS, description, formula, measurement unit (mg/L or µg/L), formula weight, and valency.

Import: allows you to import a list of chemicals from an Excel file.

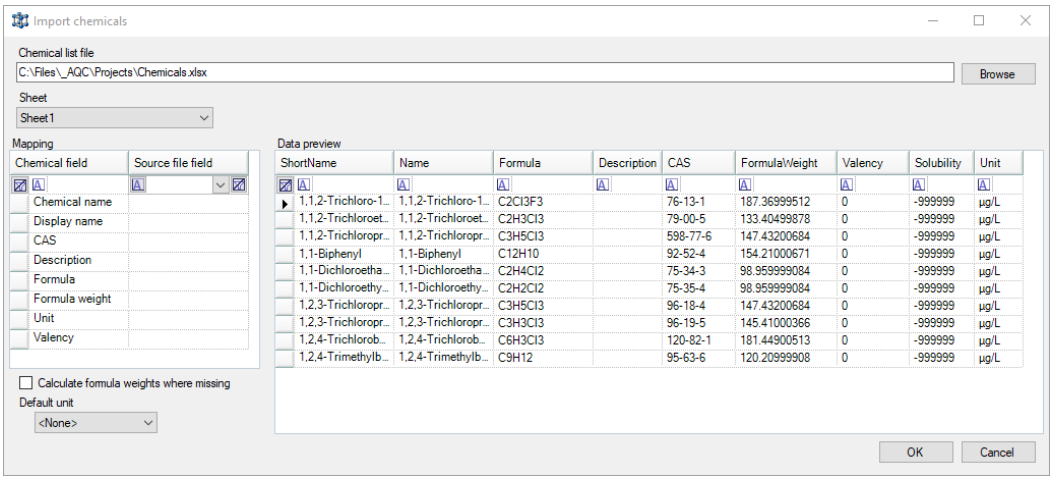
Delete: removes the selected parameter(s) from the Chemical List.

Save: saves the Chemical List in its current location; enabled once you edit the list.

Save As: saves a copy of the Chemical List to a new location.

Importing Chemicals into the Chemical List

You can import chemicals into the Chemical list by specifying an Excel file and selecting the appropriate worksheet containing the data.

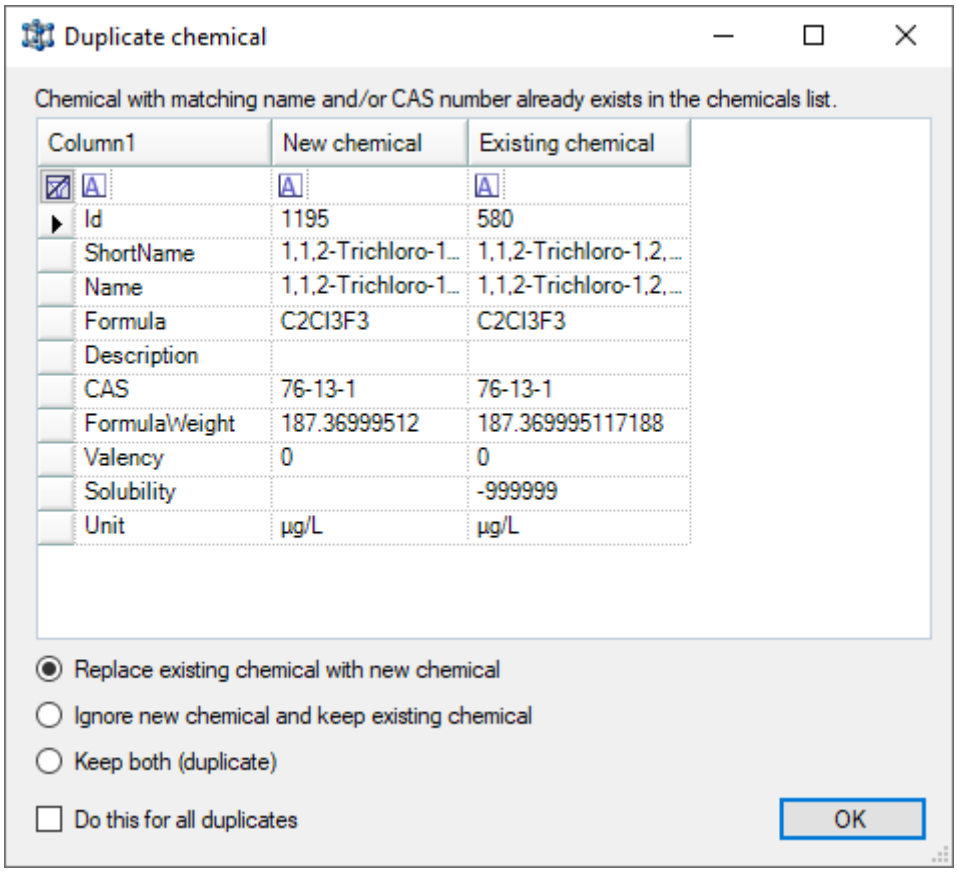


The Import Chemicals window contains the following controls:

- **Chemical list file:** allows you to specify the Excel file containing the list of chemicals to be imported
- **Sheet:** allows you to specify the worksheet containing the list of chemicals to be imported
- **Mapping:** allows you to map fields from the source file to the Chemical List fields. The Chemical field (left) column contains the list of fields from the Chemical List. The Source file field (right) column allows you to map data fields from the source file to the Chemical List fields.
- **Data Preview:** provides a preview of the source Excel file
- **Calculate formula weights where missing:** calculates the FormulaWeight field based on a supplied formula, if none is otherwise supplied in the source file
- **Default Unit:** allows you to select a concentration unit that will be used if none is otherwise supplied in the source file

Duplicates

If one or more of the Chemicals to be included contain duplicate values of the Short Name, Name, or CAS, then the duplicate chemical window will be presented to facilitate managing the conflicts:



You can manage duplicate values by selecting one of the following options:

- Replace existing chemical with new chemical
- Ignore new chemical and keep existing chemical
- Keep both (duplicate)

You can select the option to apply the same choice to all subsequent duplicates to be imported.

3.8 Measurement Units

In AquaChem, measurement units are grouped into categories and many of the views and modules will automatically perform unit conversions on demand.

In order for this to work, parameter values stored in the underlying database use consistent units. For example, all sodium results stored in the sample results will be stored using one common unit, typically milligrams per liter (mg/L), while PCE results may be stored in micrograms per liter (µg/L), and temperature is stored in degrees Celcius (°C).

Unit Categories

In many situations in AquaChem, such as the viewing the Sample List, creating plots in a Plot Collection, or generating a Sample Report, it may be preferable to work with or report values using units other than the measurement unit stored in the database. In these cases, you may be provided with controls to select a different unit of measurement. In order to correctly convert units, AquaChem relies on unit categories. Unit categories consist of units of measurement that share dimensionality - that is, they share the same dimension of base units: length (L), mass (M), time (T), and temperature (K). For example, the concentration (by volume) category is based on a dimensionality of M/L^3 and includes the milligrams per liter, micrograms per liter, and milligrams per cubic meter. Furthermore, concentration units also include molar concentrations (e.g. moles per liter [mol/L] and milli-moles per liter [mmol]) for parameters with a specified formula molecular weight and equivalent concentrations (e.g. equivalents per liter [eq/L] and milli-equivalents per liter [meq/L]) for parameters with a specified formula molecular weight and valence.

Unit Conversion

Each unit category has one designated primary reference unit; all other units in the same category have conversion factors relative to this primary unit. For example, in AquaChem the primary reference unit for the Time unit category is seconds and it has a unit conversion multiplier of 1 - all other units have conversion multipliers relative to seconds, as shown in the table below:

Units	Name	Multiplier	Offset	Base
s	**second**	**1**	**0**	**TRUE**
min	minute	60	0	FALSE
hr	hour	3600	0	FALSE
day	day	86400	0	FALSE
yr	year	31557600	0	FALSE

Note the offset field is present to facilitate conversions for units with linear offsets such as the conversion from degrees Celcius to degrees Fahrenheit (i.e. °F = 5/9 x ° C + 32).

Units and Importing Data

When importing data, you must also include specifications on the measurement unit of each parameter to be imported. If the units are recognized by AquaChem, the values to be imported will be automatically converted into the units associated with the parameter in the project (as specified in the Parameter Editor). If the units are not recognized, you will be asked to map the unrecognized unit to an existing one or add a new unit and conversion factors. Once a unit is added at the import step, it will be saved in the project for future use.

3.9 Functions

The Functions tab in the Project Properties window lists all of the internal calculations performed by AquaChem, with reference information for each calculation provided in the discussion below. All of the active functions (as indicated by a checkmark) will be available as "calculated parameters" which can be included in statistical comparisons and for plotting data. In this dialogue, you may manage which calculations should appear in the lists and in what order. For example, if you never use the enthalpy calculations, you may deactivate them here. In addition, you may define the units in which some of the functions are reported.

The calculated values of functions are displayed in the Calculated tab of the Sample Details window.

The calculated parameters are treated by AquaChem as regular database parameters with respect to plotting, searches, or statistical calculations. However, in order for the built-in calculations to work, their corresponding database parameters must be included in the database and mapped to the required parameters in the Project Properties window. For example, the database must include calcium and magnesium in order to calculate hardness, and both of these parameters must be identified with an internal name of `Ca' and `Mg' respectively.

You may edit the name of the function or hide/show a function. Hidden functions will not appear in the list of functions within AquaChem. To edit the name of the function, press **Project > Properties**, select the appropriate function in the Functions tab and edit the Label input. For functions that can be expressed in different units (e.g. hardness as meq/L, mmol/L $CaCO_3$, or mg/L $CaCO_3$) you may specify a default unit.

AquaChem includes a number of common calculations for determining common geochemical parameters. Each of the available calculations (functions) is explained below.

Ions, Hardness, and Alkalinity Calculations

- Sum of Ions
- Electroneutrality
- Non-Carbonate Hardness
- Sum of Anions
- Total Hardness
- Calculated Alkalinity
- Sum of Cations
- Carbonate Hardness
- Calculated TDS

Agricultural and Irrigation Calculations

- Magnesium Hazard (MH)
- Residual Sodium Carbonate (RSC)

tic Factic (SAR)

Scaling and Corrosion Calculations

- Langelier saturation index (LSI)
- Ryznar
- Larson-Skold Index (LSkI)
- Puckorius Scaling Index (PSI)

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Organic Calculations

- Calculated Total Organic Halides (TOX)

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Isoptope Infiltration Calculations

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- T
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- T(18O)
- z(2H)

Enthalpy Calculations

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- Calculated Total Organic Halides (TOX)

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Exceedances and Comparisons

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- Exceeds Natural Occurrence

Date Time Calculations

- Year
- Season
- Month

Ions, Hardness, and Alkalinity Calculations

Note: Ions, Cations, and Anions in AquaChem

Ions, Anions, and Cations are specified in AquaChem using the Valency value in the Parameter settings:

- Ions are any parameter with a *non-zero* parameter valency
- Anions are any parameter with a *negative* parameter valency
- Cations are any parameter with a *positive* parameter valency

Valencies are always integer values. New parameters are assumed to have a valency of zero and are therefore not considered Ions unless/until otherwise specified.

Sum of Ions:

Sum of the concentration of all measured ion concentrations in the sample, given by the equation:

$$Sum\ of\ Ions = \sum [X_i]$$

where: X_i is the volumetric concentration in units of meq/L [Default], mmol/L, or mg/L

Sum of Anions:

Sum of the concentration of all measured anion concentrations in the sample, given by the equation:

$$Sum\ of\ Anions = \sum [A_i]$$

where: A_i is the volumetric concentration of the ith anion parameter measured in the solution in units of meq/L [Default], mmol/L, or mg/L

Sum of Cations:

Sum of the concentration of all measured anion concentrations in the sample, given by the equation:

$$Sum\ of\ Cations = \sum [C_i]$$

where: C_i is the volumetric concentration of the ith cation parameter measured in the solution in units of meq/L [Default], mmol/L, or mg/L

Electroneutrality

The principal of electroneutrality is one of the foundations of aquatic chemistry. This principle states that the sum of positive and negative charges within a solution must balance to zero. The electroneutrality ratio (E.N.) is the relative difference in the ionic charge of the solution and is given by the following equation:

$$Electroneutrality = \frac{\sum[C_i] - \sum[A_i]}{\sum[C_i] + \sum[A_i]} \times 100\%$$

Electroneutrality is expressed in terms of percent. According to Appelo and Postma (1994), electroneutrality differences of up to ±2% are nearly inevitable but differences of more than

±5% mean that sampling and analytical procedures should be reviewed as this may indicate that:

- the sample was subjected to sampling and/or analytical procedural errors, or
- there are other (less common/unanalyzed) major ions in the solution

Total Hardness

The sum of ions that can precipitate from water as calcite or dolomite. Generally, the sum of Ca^{2+} and Mg^{2+}, expressed in meq/L or mg/L CaCO3, or mol/L CaCO3.

$$TH = 2[Ca^{2+}] + 2[Mg^{2+}]$$

where: *TH* is in units of meq/L
$[Ca^{2+}]$ is the concentration of calcium ions in solution in mmol/L
$[Mg^{2+}]$ is the concentration of magnesium ions in solution in mmol/L

TH unit conversion ⟶ 1 meq/L [$CaCO_3$] = 50 mg/L [$CaCO_3$] = 0.5 mmol/L [$CaCO_3$]

Carbonate (Temporary) Hardness:

Carbonate Hardness (CH) is the portion of total hardness that is balanced by carbonate [CO_3^{2-}] and bicarbonate [HCO_3^-] and thus can precipitate as calcium carbonate, magnesium carbonate, or related minerals.

$$CH = \mathbf{max}\left(TH - [HCO_3{}^-] + 2\left[CO_3{}^{2-}\right], 0\right)$$

where: CH is in units of meq/L
TH is total hardness in units of meq/L
$[CO_3^{2-}]$ is the concentration of carbonate ions in solution in mmol/L
$[HCO_3^-]$ is the concentration of bicarbonate ions in solution in mmol/L

CH unit conversion ⟶ 1 meq/L [$CaCO_3$] = 50 mg/L [$CaCO_3$] = 0.5 mmol/L [$CaCO_3$]

Non Carbonate (Permanent) Hardness:

Non carbonate hardness (NCH), also known as permanent hardness, is the portion of calcium and magnesium hardness in excess of carbonate [CO_3^{2-}] and bicarbonate [HCO_3^-].

$$NCH = TH - CH$$

where: NCH is in units of meq/L
TH is total hardness in units of meq/L
CH is carbonate hardness in units of meq/L

NCH unit conversion ⟶ 1 meq/L [$CaCO_3$] = 50 mg/L [$CaCO_3$] = 0.5 mmol/L [$CaCO_3$]

Calculated Alkalinity

Alkalinity Is a measure of the acid neutralizing capacity of the solution. Alkalinity is most commonly measured by titration, but can be estimated using the following equation:

$$Alk = [HCO_3^-] + 2[CO_3^{2-}] + 10^{-pOH} - 10^{-pH}$$

where: Alk is in units of meq/L
pH = $-\log_{10}[H^+]$
pOH = $-\log_{10}[OH^-] \approx 14 - pH$ (@ 25°C, 1 atm)
Alk unit conversion ⟶ 1 meq/L [$CaCO_3$] = 50 mg/L [$CaCO_3$] = 0.5 mmol/L [$CaCO_3$]

Calculated Total Dissolved Solids (TDS)

TDS is a measure of the evaporation residue at a given temperature. It can also be thought of as the mass of all ions in solution. TDS is calculated as the sum of all ions plus dissolved silica less the amount of bicarbonate that will outgas under the following reaction (Hounslow, 1995, p 57):

$$2 \cdot HCO_3^- \rightarrow CO_3^{2-} + CO_{2(g)} + H_2O_{(g)}$$

So, the formula to estimate total dissolve solids is as follows:

$$TDS = Sum\ of\ Ions + SiO_2 - (HCO_3^-)\left(\frac{FMW\ H_2CO_3}{2 \cdot FMW\ HCO_3^-}\right)$$

$$= Sum\ of\ Ions + SiO_2 - (HCO_3^-)\left(\frac{62.02}{2 \cdot 61.016}\right)$$

$$= Sum\ of\ Ions + SiO_2 - 0.5082 \cdot HCO_3^-$$

where: TDS is in units of mg/L
FMW = formula molecular weight (mg/mmol)

Please Note: calculated TDS is only an approximation; it is always better to have a measured value

Agricultural and Irrigation Calculations

Sodium Adsorption Ratio (SAR)

The sodium adsorption ratio is an empirical water quality criterion that is important for irrigation waters. It is used in the Wilcox Plot.

$$SAR = \frac{Na^{+}}{\sqrt{\frac{Ca^{2+} + Mg^{2+}}{2}}}$$

where: SAR is in units of $(meq/L)^{0.5}$, but the units are not traditionally reported
Inputs are in units of meq/L

Magnesium Hazard (MH)

Magnesium is considered to be harmful for plants, but the effect is reduced by the presence of calcium. Magnesium Hazard was proposed by Szabolcs and Darab (1964) and is calculated as follows:

$$MH = \frac{Mg^{2+}}{(Ca^{2+} + Mg^{2+})} \times 100$$

where: MH is dimensionless.
Inputs are in units of meq/L

Waters with values of MH that exceed 50 are generally considered to be harmful for use in irrigation.

Residual Sodium Carbonate (RSC)

Residual sodium carbonate (RSC) is similar to the SAR in that it expresses the sodium content in relation with calcium and magnesium (Richards, 1954). This value may appear in some water quality reports, although it is not frequently used. Residual sodium carbonate (RSC) has the following equation:

$$RSC = \left(HCO_3^{-} + {CO_3}^{2-}\right) - (Ca^{2+} + Mg^{2+})$$

where: RSC is in units of meq/L

Waters are categorized using RSC as follows:

RSC Value	Significance

< 1.25 meq/L	waters are generally considered safe for irrigation, although some crops may require lower values
1.25 – 2.5 meq/L	waters are considered are considered marginal
> 2.5 meq/L	waters are generally not appropriate for irrigation without treatment

Scaling and Corrosion Calculations

Please Note: The scaling and corrosion indices presented below are only approximations of the real saturation state and should only be used in preliminary analyses. Modeled (e.g. PHREEQC) saturation index values of calcite or dolomite will generally provide more reliable results since they are based on a thermodynamic dataset and include more corrosion/scaling-relevant minerals and parameters such as Eh, Mn, Fe, iron hydroxides, etc.

Langelier Saturation Index (LSI)

The Langelier index is a popular way of expressing the equilibrium state of a solution in respect to calcite (Langelier, 1936) and is given by:

$$LSI = pH - pH_s$$

where: LSI is in standard pH units
pH is the measured pH
pH_s is the estimated pH at calcite saturation

The value of pH_s is estimated using temperature, alkalinity, hardness and total dissolved solids values as follows:

$$pH_s = 9.3 + \left(\frac{log(TDS - 1)}{10}\right) + \left(34.55 - 13.12 \cdot log(T)\right) - \left(log(Ca^{2+}) - 0.4 + log(Alk)\right)$$

where: TDS is total dissolved solids in units of mg/L
T is temperature in units of Kelvin
Ca is the concentration of calcium in mg/L-$CaCO_3$
Alk is the alkalinity in mg/L-$CaCO_3$

Waters are categorized using LSI as follows (Belitz *et al.*, 2016):

LSI Value	Significance
< -0.5	potentially corrosive

-0.5 – +0.5	indeterminate
> +0.5	potentially scale-forming

Larson-Skold Index (LSkI)

The Larson-Skold Index (LSkI) is used to describe the corrosivity of water towards mild steel and was developed based on *in situ* measurements of corrosion in steel lines transporting Great Lakes water (Larson and Skold, 1958). The index describes the ratio of concentration of chloride and sulfate ions to the concentration of bicarbonate and carbonate ions. Because the LSkI is an empirical correlation, its utility for describing corrosion for other types of water is questionable. The following equation is used to calculate the LSkI:

$$LSkI = \frac{[Cl^-] + [SO_4{}^{2-}]}{[HCO_3{}^-] + [CO_3{}^{2-}]}$$

where: LSkI is dimensionless
All inputs are concentrations in meq/L

The following table describes the criteria for evaluating values of L&SkI (Larson and Skold, 1958):

LSkI Value	Significance
< 0.8	Chloride and sulfate concentrations will not interfere with natural film formation
0.8 – 1.2	Chloride and sulfate concentrations may interfere with natural film formation; corrosion may occur
> 1.2	High corrosion rates are anticipated

Ryznar Stability Index (RSI)

The Ryznar stability index (RSI) attempts to correlate an empirical database of scale thickness observed in municipal water systems to water chemistry (Ryznar, 1944). Like the LSI, the RSI has its basis in the concept of saturation level. Ryznar attempted to quantify the relationship between calcium carbonate saturation state and scale formation. The Ryznar stability index is calculated as follows:

$$RSI = 2pH_s - pH$$

where: LSI is in standard pH units
pH_s is the pH at calcite saturation
pH is the measured pH in standard units

The value of pH_s is estimated from temperature, alkalinity, hardness and total dissolved values using the following empirical formula:

$$pH_s = 9.3 + \left(\frac{log(TDS - 1)}{10}\right) + \left(34.55 - 13.12 \cdot log(T)\right) - \left(log(Ca^{2+}) - 0.4 + log(Alk)\right)$$

where: TDS is total dissolved solids in units of mg/L
T is temperature in units of Kelvin
Ca is the concentration of calcium in mg/L-$CaCO_3$
Alk is the alkalinity in mg/L-$CaCO_3$

The empirical correlation of the Ryznar Stability Index can be summarized as follows:

RSI Value	Significance
< 6	the scale tendency increases as the index decreases
> 7	the calcium carbonate formation probably does not lead to a protective corrosion inhibitor film
> 8	mild steel corrosion becomes an increasing problem

Puckorius Scaling Index (PSI)

The Puckorius Scaling Index (PSI) is based on estimates of the maximum quantity of precipitate that can form and the buffering capacity of the water. The PSI index is calculated in a manner similar to the Ryznar Stability Index, described above, except that it incorporates the equilibrium pH and is calculated as follows:

$$PSI = 2pH_s - pH_{eq}$$

where: PSI is in standard pH units
pH_s is the estimated pH at calcite saturation
pH_{eq} is the estimated pH at equilibrium

The value of pH_s is estimated using temperature, alkalinity, hardness and total dissolved solids values as follows:

$$pH_s = 9.3 + \left(\frac{log(TDS - 1)}{10}\right) + \left(34.55 - 13.12 \cdot log(T)\right) - \left(log(Ca^{2+}) - 0.4 + log(Alk)\right)$$

where: TDS is total dissolved solids in units of mg/L
T is temperature in units of Kelvin

Ca is the concentration of calcium in mg/L-$CaCO_3$
Alk is the alkalinity in mg/L-$CaCO_3$

The value of pH_{eq} is based on the buffering capacity of the solution and is estimated using alkalinity:

$$pH_{eq} = 1.465 + log(Alk)$$

where: pHeq is in standard units
Alk is alkalinity in mg/L $CaCO_3$

The empirical correlation of the Puckorius Scaling Index can be summarized as follows:

PSI Value	Significance
< 6	the scale tendency increases as the index decreases
> 7	the calcium carbonate formation probably does not lead to a protective corrosion inhibitor film
> 8	mild steel corrosion becomes an increasing problem

Organic Calculations

Calculated Total Organic Carbon (TOC)

This function calculates the total carbon associated with organic parameters. Organic carbon is assumed to be present in parameters with a molecular formula containing carbon and excluding the following specific inorganic species: HCO_3, CO_3, and CO_2. Values are reported in mg/L or µg/L.

Calculated Total Organic Halogens (TOX)

This function estimates the total halogens associated with organic parameters. Organic halogen are assumed to be those parameters with a molecular formula containing halogens (i.e. Cl, Br, I) and excluding inorganic species containing only halogens (thus, chloride mass from Cl^- and Cl_2 is excluded). Values are reported in mg/L or µg/L.

Isotope Infiltration Calculations

AquaChem includes functions to estimate infiltration elevation and temperature based on linear relationships with the measured fractionation of oxygen-18 (18O) and deuterium (2H)

isotopes. The slope and intercept fitting parameters are valid only for a very limited zone that must be established for your area of interest using empirical data and are specified in AquaChem using the project settings for Regional Chemistry.

z(18O)

Average infiltration height as a function of oxygen-18 isotopic composition.

$$z_{infiltration} = m \cdot [18O] + b$$

where: $z_{infiltration}$ is a length unit in meters or feet, depending on the fitting parameter values

18O is the fractionation of oxygen-18, usually expressed in units of permille (‰).

m and b are regression fitting parameters based on regional/site-specific data

T(18O)

Average temperature of infiltration zone as a function of oxygen-18 isotopic composition.

$$T_{infiltration} = m \cdot [18O] + b$$

where: $T_{infiltration}$ is a temperature unit in ^{o}C or ^{o}F, depending on the fitting parameter values

18O is the fractionation of oxygen-18, usually expressed in units of permille (‰).

m and b are regression fitting parameters based on regional/site-specific data

z(2H)

Average infiltration elevation of the infiltration zone as a function of deuterium (2H) isotopic composition.

$$z_{infiltration} = m \cdot [2H] + b$$

where: $z_{infiltration}$ is a length unit in meters or feet, depending on the fitting parameter values

2H is the fractionation of deuterium, usually expressed in units of permille (‰).

m and b are regression fitting parameters based on regional/site-specific data

T(2H)

Average temperature of infiltration zone as a function of deuterium isotopic composition.

$$T_{infiltration} = m \cdot [2H] + b$$

where: $T_{infiltration}$ is a temperature unit in °C or °F, depending on the fitting parameter values

2H is the fractionation of deuterium, usually expressed in units of permille (‰).

m and b are regression fitting parameters based on regional/site-specific data

Enthalpy Calculations

Temp > H H2O(l)

The enthalpy (H) of liquid water as a function of temperature (T) in Kelvin is approximated using the following function:

$$H_{(H_2O_{(l)})}(T) = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 + a_6T^5 + a_7T^{-1} + a_8T^{-2} + a_9log_{10}(T)$$

where: temperature is in units of Kelvin
a_1 = 418.84
a_2 = 10.286
a_3 = -0.05092
a_4 = 0.00026309
a_5 = -0.00000069303
a_6 = 0.00000000074566
a_7 = -1209.8
a_8 = 11.99
a_9 = -353.76

For more details please refer to Fournier and Potter (1972).

Temp > H H2O(v)

The enthalpy (H) of water vapor as a function of temperature (T) in Kelvin is approximated using the following function:

$$H_{(H_2O_{(v)})}(T) = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 + a_6T^5 + a_7T^{-1} + a_8T^{-2} + a_9log_{10}(T)$$

where: temperature is in units of Kelvin
a_1 = 2035
a_2 = -5.0499
a_3 = 0.057399
a_4 = -0.00030426
a_5 = 0.00000079095
a_6 = -0.00000000086968
a_7 = 1342.4
a_8 = -13.298

a_9 = 396.29

For more details please refer to Fournier and Potter (1972).

SiO2 > H H2O(l)

The enthalpy (H) of liquid water as a function of dissolved silica in mmol/L is approximated using the following function:

$$H_{(H_2O_{(l)})}(T) = a_1 + a_2 SiO_2 + a_3 {SiO_2}^2 + a_4 {SiO_2}^3 + a_5 log_{10}(SiO_2)$$

where: SiO2 is the concentration of dissolved silica in units of mmol/L
a_1 = -42.198
a_2 = 0.28831
a_3 = -0.00036686
a_4 = 0.00000031665
a_5 = 77.034

For more details please refer to Fournier and Potter (1972).

SiO2 > H H2O(v)

The enthalpy (H) of water vapor as a function of dissolved silica is approximated using the following formula:

$$H_{(H_2O_{(v)})}(T) = a_1 + a_2 SiO_2 + a_3 {SiO_2}^2 + a_4 {SiO_2}^3 + a_5 log_{10}(SiO_2)$$

where: SiO2 is the concentration of dissolved silica in units of mmol/L
a_1 = -3.5532
a_2 = 0.146
a_3 = -0.0004927
a_4 = 0.0000012305
a_5 = -0.00000000049421

For more details, please refer to Fournier and Potter (1972).

Exceedance Calculations

Exceeds Natural Occurrence Range (NO)

Returns the number of measured parameters in a given sample that fall outside of a specified natural occurrence range. The natural occurrence range can be defined for a given parameter using the Parameter Editor.

Exceeds Standard

Returns the number of measured parameters in a given sample that exceed the active standard(s) as specified in the Water Quality Standards view.

Date Calculations

Year

Returns the calendar year of the sample collection date.

Season

Returns a season index number (1-4) for the sample collection date, based on the time of year as follows:

Index	Date Range	Season	
		Northern Hemisphere	Southern Hemisphere
1	Mar 21 - Jun 20	Spring	Fall
2	Jun 21 - Sep 20	Summer	Winter
3	Sep 21 - Dec 20	Fall	Spring
4	Dec 21 - Mar 20	Winter	Summer

The season index is a convenient metric to find and select samples that were sampled in the same season but in different years.

Month

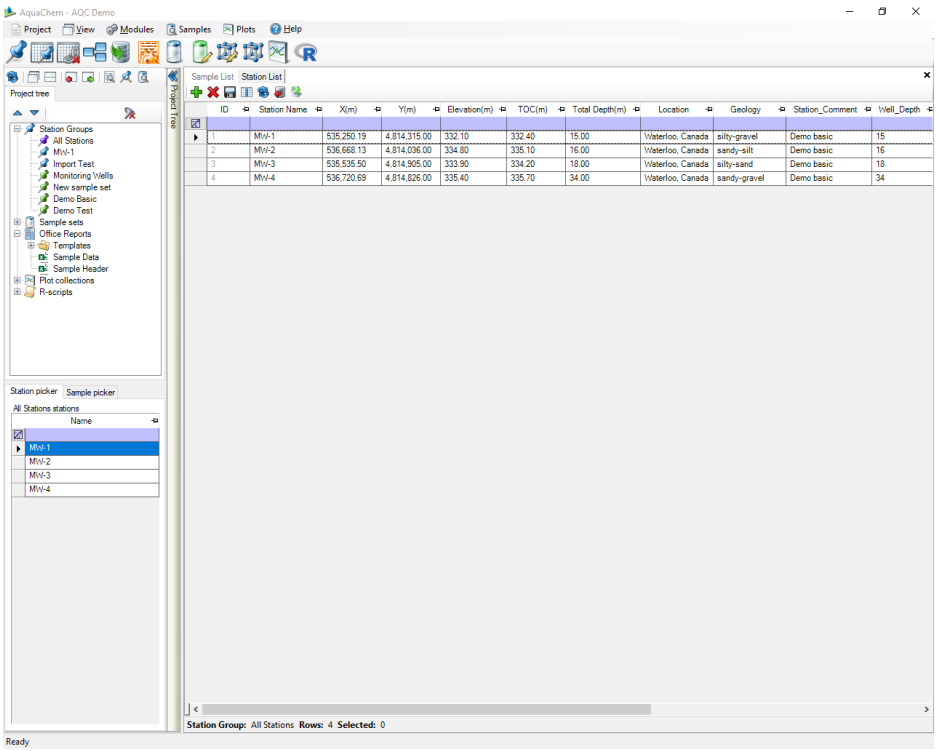
Returns the index of the month of the sample collection date, where the index is the ordinal number of the month (i.e. January=1, February=2, March=3, etc.). Using this function is a convenient metric to find and select sample data for calculating month-based statistics over several years.

3.10 Adjustable Windows

When opening an AquaChem project for the first time, the default window displays will appear. There are two groups, one with the Project Tree tab (on the left) and the main group area with the following two tabs:

- Station List
- Sample List

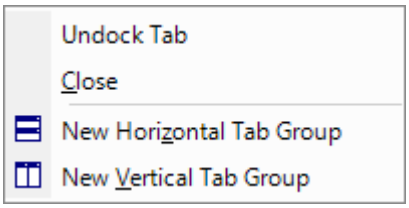
The Start Page may also be shown.



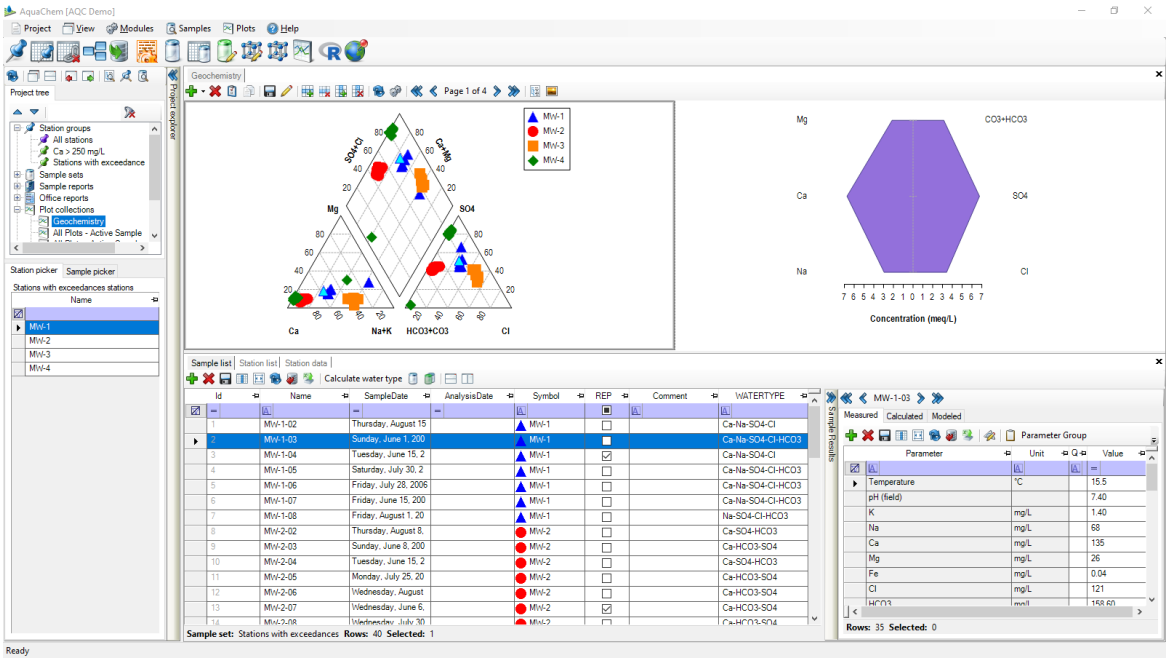
You have several options to adjust the view of these groups. You can add additional groups (right-click on any existing tab) either vertical or horizontal. Several of the modules within AquaChem will launch as a tab (e.g. Query Builder, List Editor, Parameter Group Editor, etc.)

You can rearrange tabs in the following ways:

- rearrange the order of a tab within a group by simply dragging and dropping it
- move a tab to a new or different group or a new undocked window by dragging and dropping it
- right-click to create a new horizontal or vertical group



Here is an example of another way to organize your windows so that you can view plots and corresponding tabulated sample data simultaneously:



3.11 Data Entry

Manual Data Entry

You can manually enter and edit data in the following tabs:

- Station List Tab
- Sample List
- Station Data Tab
- Non Station Data Tab

You can use the add button (➕) to add a new record (row) within one of the above tabs. New records will be highlighted by a yellow row, and the new record must be saved using the Save button (💾) before they are committed to the database. Furthermore, you must save records from a parent table before related data can be entered into any child tables. For example, you must save a new station record before you can add new samples to the station, and new sample records must also be saved before result data can be added to that

sample. You can also delete data by selecting the delete button () in one of the above tabs.

Import Data Module

It may be more efficient to import the data using the Import Data module. The Data Import module provides you with several options for importing your data: Chemical Samples, General, and Image. For more details on how to import data using the Import Data module, please refer to the Import Data section.

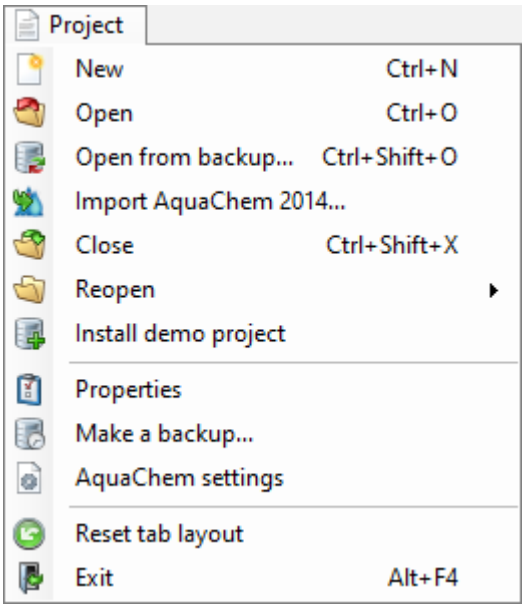
Chapter 4 Menu Bar

The AquaChem menu items have been specifically designed for optimal flexibility and ease of use. The items in the menu bar are context sensitive; this means that one or more menu items may be greyed out if a specific feature is not applicable for a particular view.

The following sections describe the items which appear in the menu bar.

4.1 Project

The Project menu contains options for project level actions as described below.



New

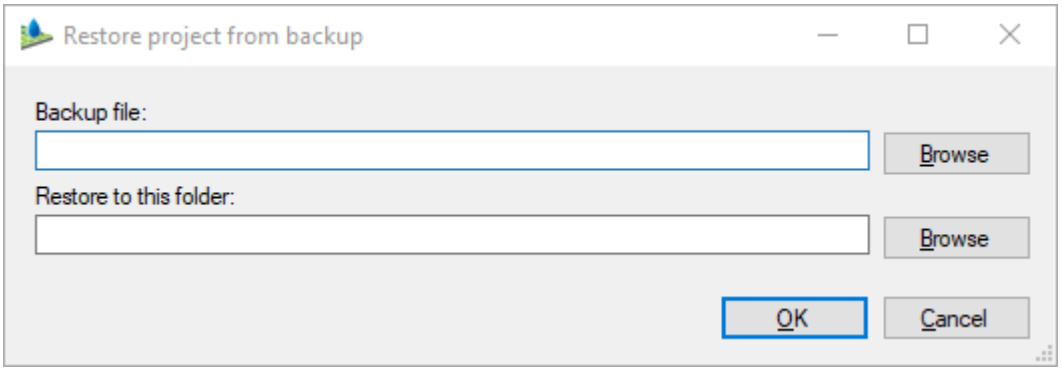
This option launched the New Project wizard which is described further in the section: Creating New Projects.

Open

The Open menu item is used to open existing AquaChem projects by selecting the *.aqcx file. The *.aqcx file contains basic information for the project, including a connection string to the AquaChem database (*.accdb).

Open from Backup

Use this option to open a backup copy of the AquaChem project and database. This is useful if receiving a copy of someone else's project and database. Simply enter or browse to the location of the backup AquaChem project file (*.bak) and specify a restore folder.



Import AquaChem 2014...

Use this option to import an AquaChem 2014 project (*.aqc). Note that if the .aqc file was developed using an older version of AquaChem, you may need to upgrade it using AquaChem 2014.2 before to importing it into AquaChem 10.0. For more information, see the topic on Importing AquaChem 2014 Projects or the tutorial for Importing Projects from AquaChem v2014.2.

Close

Close the project which is currently open.

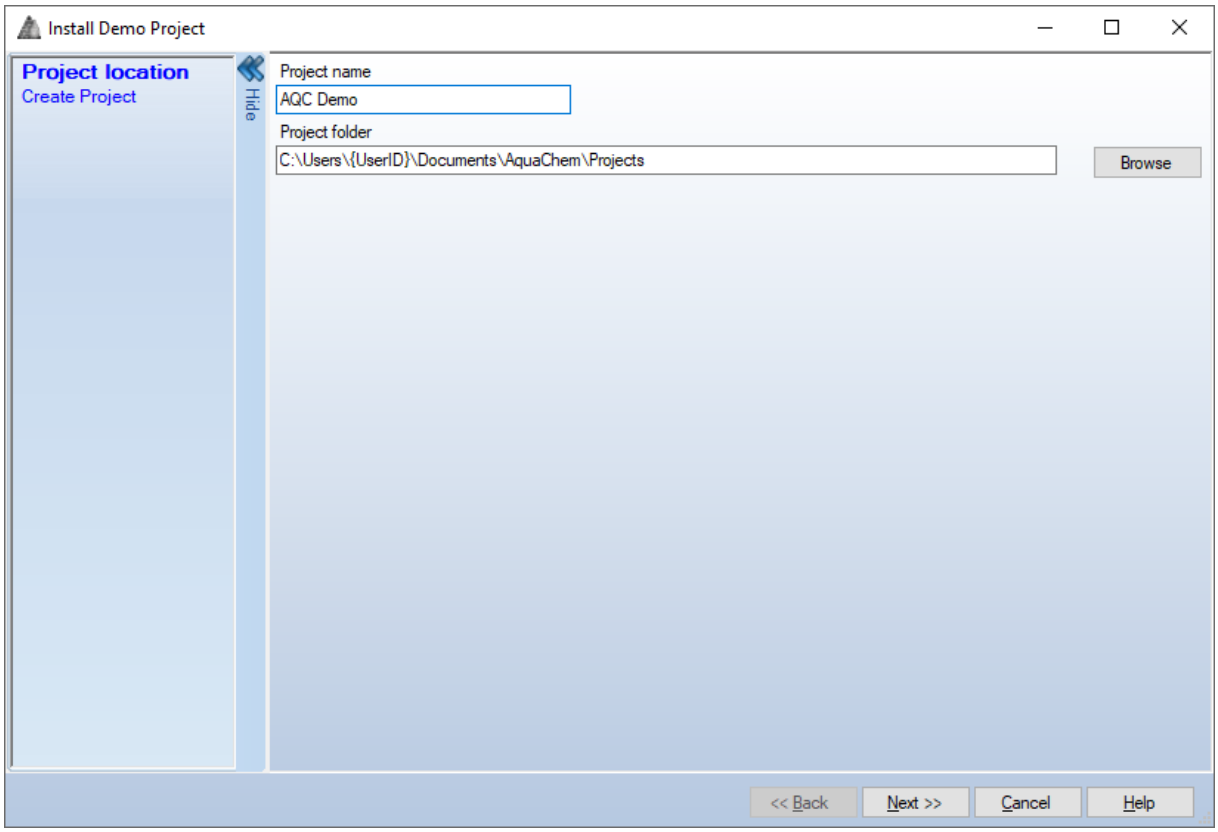
Reopen

This menu item provides a sorted list of projects that have been recently opened, with the most recent project appearing at the top and older projects at the bottom. Simply select the desired project, and it will be reloaded.

Install the Demo Project

You can install the Demo Project from within the program by selecting Project / Install the Demo Project (Note that there is also an option to do this from the Start Page.

The Default option will install the Demo Project to your specified projects folder. Simple select Next and then Finish to Install the Demo Project.



However, if you prefer, you can install the Demo Project to an alternative location.

Properties

This menu item will load a window displaying the Properties for the current project.

Make a Backup

This menu item will prompt you to chose a backup location and filename. A backed-up project can be restored using the Open from Backup command in this menu.

AquaChem Settings

This option opens the Settings for AquaChem. For more information, see the sub-section on AquaChem Settings.

Reset Tab Layout

The Reset Tab Layout option will restore your AquaChem based on your Module settings. Tabs and modules included in the Startup settings will be docked and merged into the main workspace and all other tabs will be closed.

Exit

This menu item will close AquaChem and all related windows (if any are open).

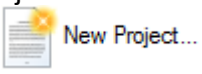
4.1.1 Creating New Projects

This section presents information on how to create new projects, and modify the properties of existing projects. A new project is usually created with a completely new database; however, AquaChem is designed to also allow for managing multiple projects on a single database.

The most common workflow is to create a new database for each new project and that workflow is documented here.

Starting the New Project Wizard

The New Project Wizard can be launched in two ways:

- Select Project / New from the Main Menu; OR
- Click the 

button on the Start Page.

The New Project Wizard will then appear. The Project Wizard contains various steps, each step appearing in a new window, with the various settings for a new project. It is designed in

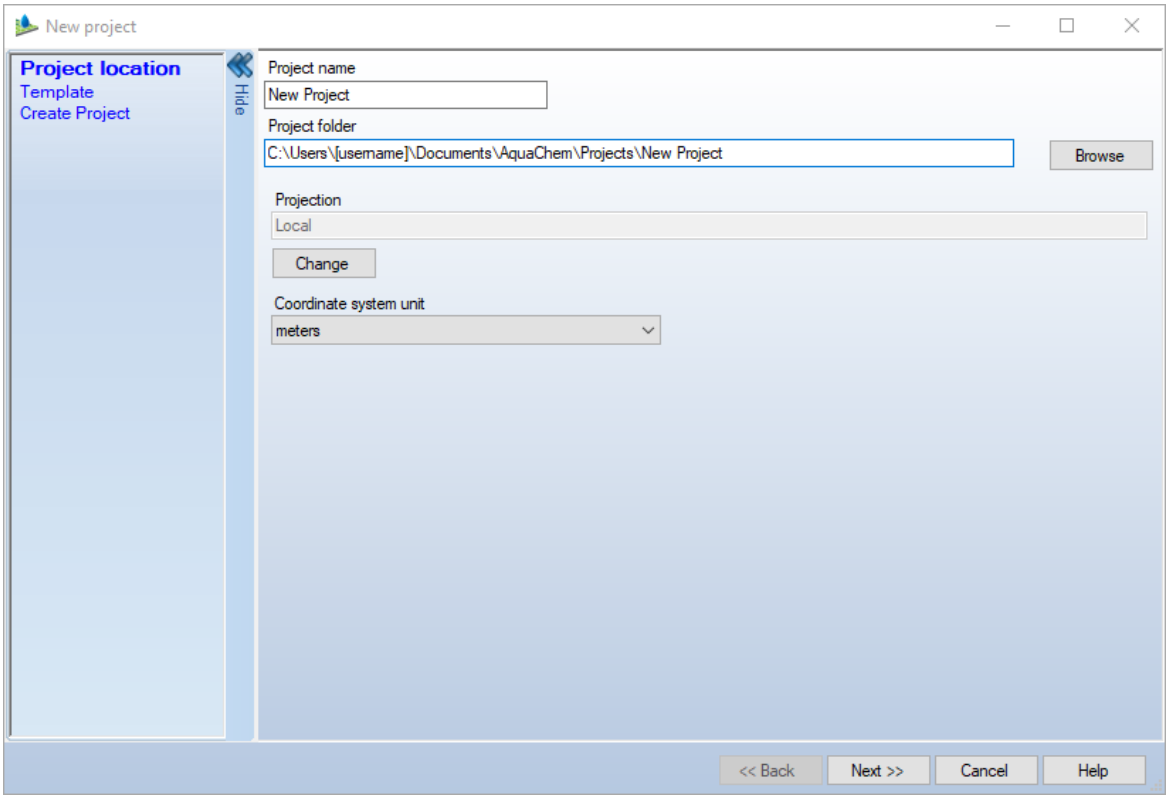
a sequential fashion; after defining the necessary inputs in each window, press the Next button to proceed. The Next button will only become activated after the necessary fields have been defined.

The Wizard includes the following steps:

- Select Project Location
- Select Template
- Create Project

Project Location

The first step in the New Project Wizard provides the data source settings options.

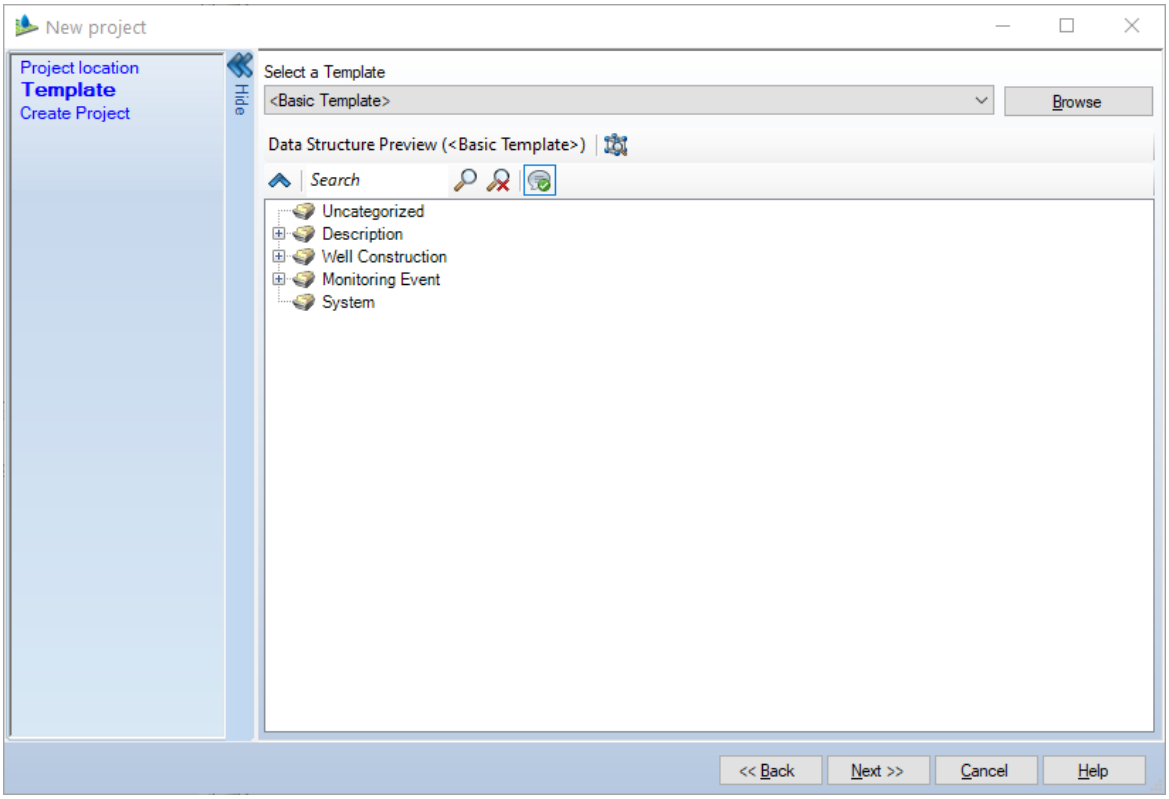


Select the Next >> button to proceed to the next step in the New Project wizard.

Select Template

This step in the New Project wizard allows you to select which database template to use for your project. A <Basic Template> that can be extended is provided with AquaChem.

When you select a template from the drop down list you can review the database structure in the preview below.

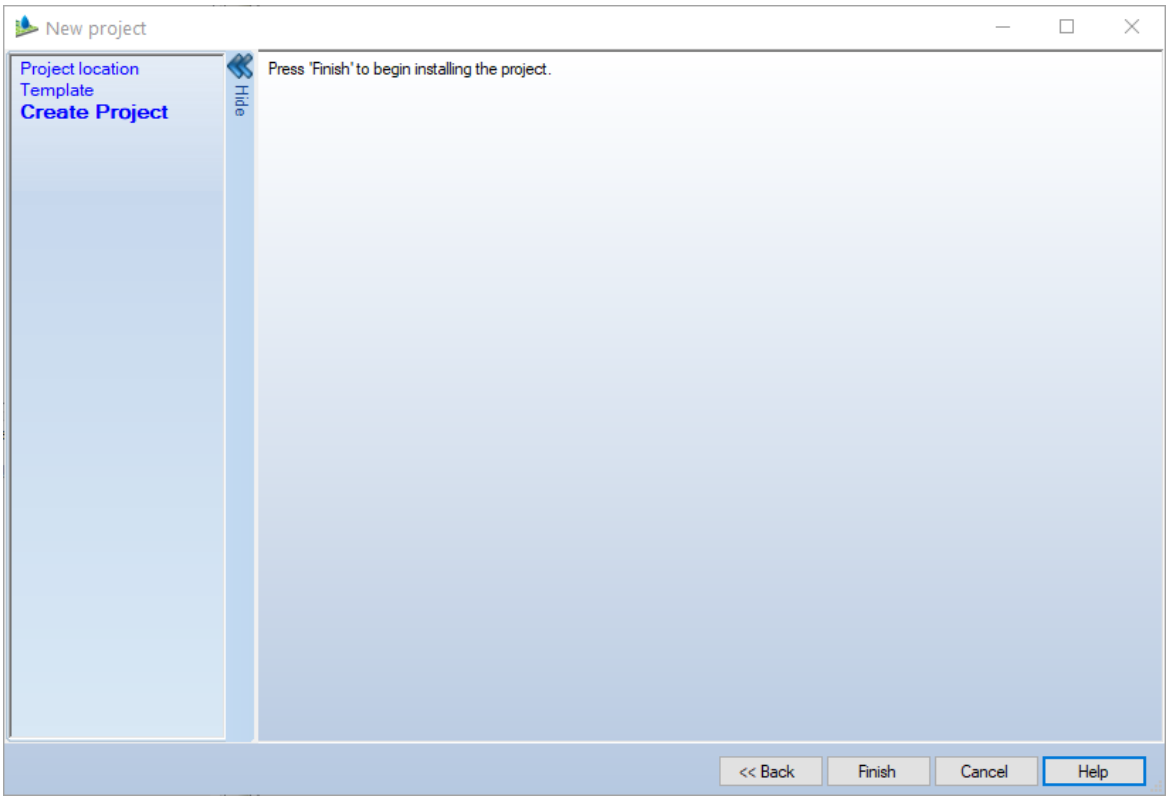


If you have exported a database template from another project and would like to use it to create a new project, select the browse button and browse to the location of your template (*.hgat).

Select the Next >> button to proceed to the next step in the New Project wizard.

Create Project

At this final step in the process, click the Finish button to finish the setup of the new project.



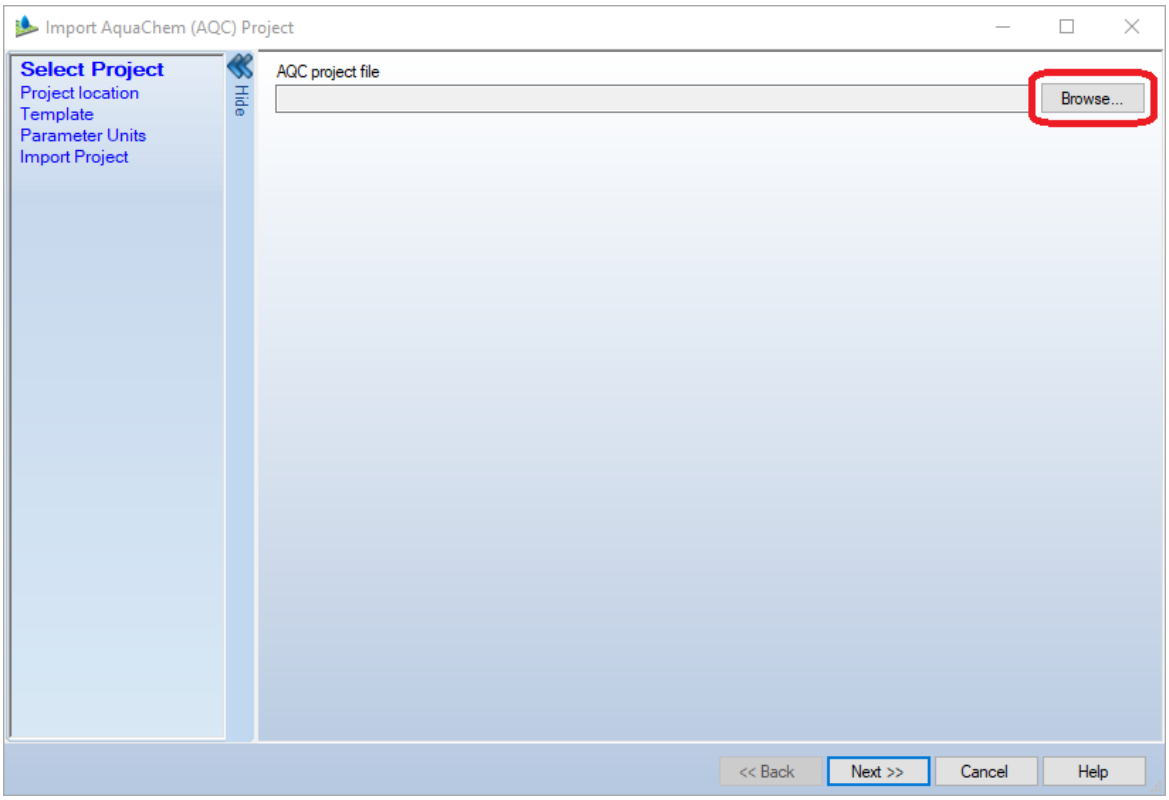
4.1.2 Import 2014 Project

To starting importing an AquaChem 2014 project, you can select '**Project > Import AquaChem 2014...**' from the main menu or select Import AquaChem 2014... from the Start Page, which opens the Import AquaChem (AQC) Project wizard, which includes four major steps:

- Select Project
- Project Location
- Template
- Parameter Units
- Import Project

Select Project

In the first step of the import process, you select the project to be imported; simply use the Browse... button and navigate to the AquaChem 2014 project you wish to import:



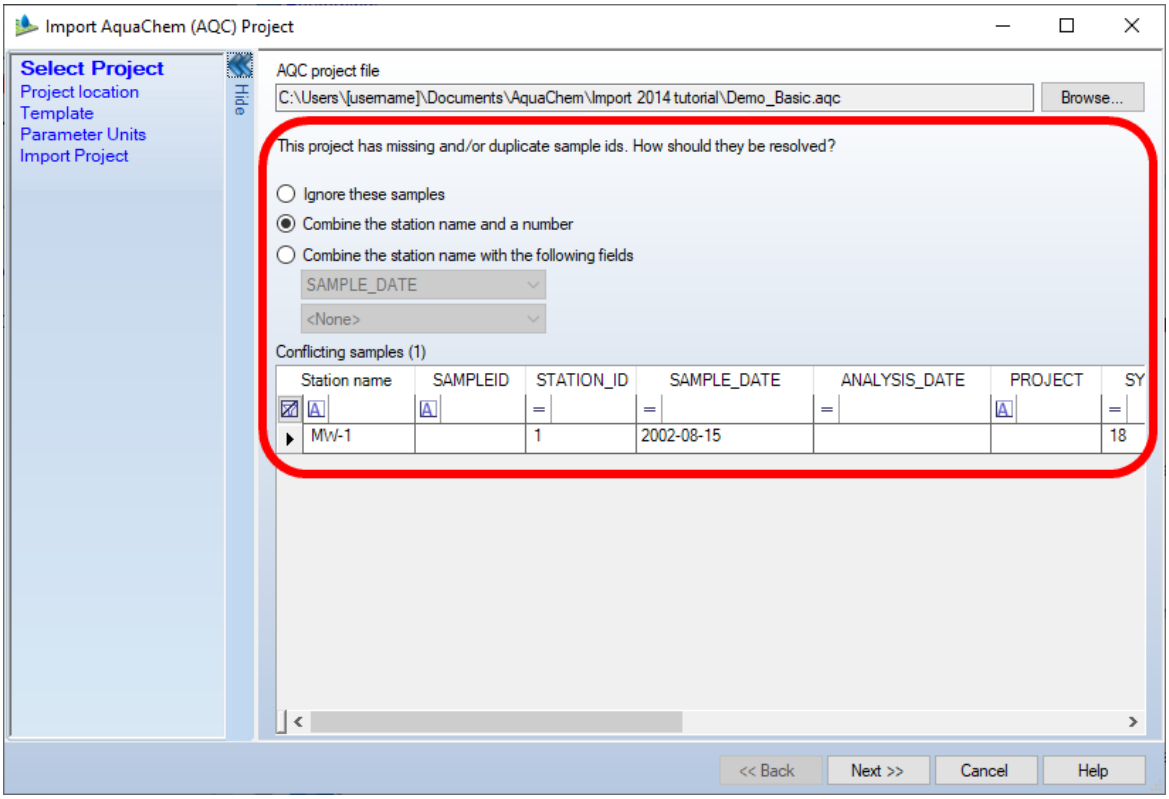
Once you have selected the AquaChem 2014 project to be imported, AquaChem will scan the project to verify that the sample IDs are unique. If the project is ready to be imported without further action, you may select Next >> button to proceed to the **Project Location** step. If missing or duplicate sample IDs are encountered in your project, you will be prompted with some options for this to be resolved.

Resolving Missing or Duplicate Sample IDs

If samples in the original project file do not contain unique a SampleID (e.g. Sample IDs are missing or there are duplicate values), you will be shown a preview of the relevant records in the Sample table and prompted with the following options:

- **Ignore these samples:** samples with missing or duplicate ids will be skipped and not included in the project import
- **Combine the station name and a number:** samples IDs will be generated for the non-unique records by appending a sequential number to the station name. In the example below, the sample ID would be "MW-1-1", subsequent samples would be "MW-1-2", "MW-1-3", etc.
- **Combine the station name with the following fields:** sample IDs will be generated for the non-unique by appending the station name and one or two selected fields. In the example below, the sample ID would be appended with the Sample Date: "MW-1-2002-08-25". Note that you will receive a warning if duplicate records would result from

your selection (e.g. if you collected more than one sample at the same station on the same date).

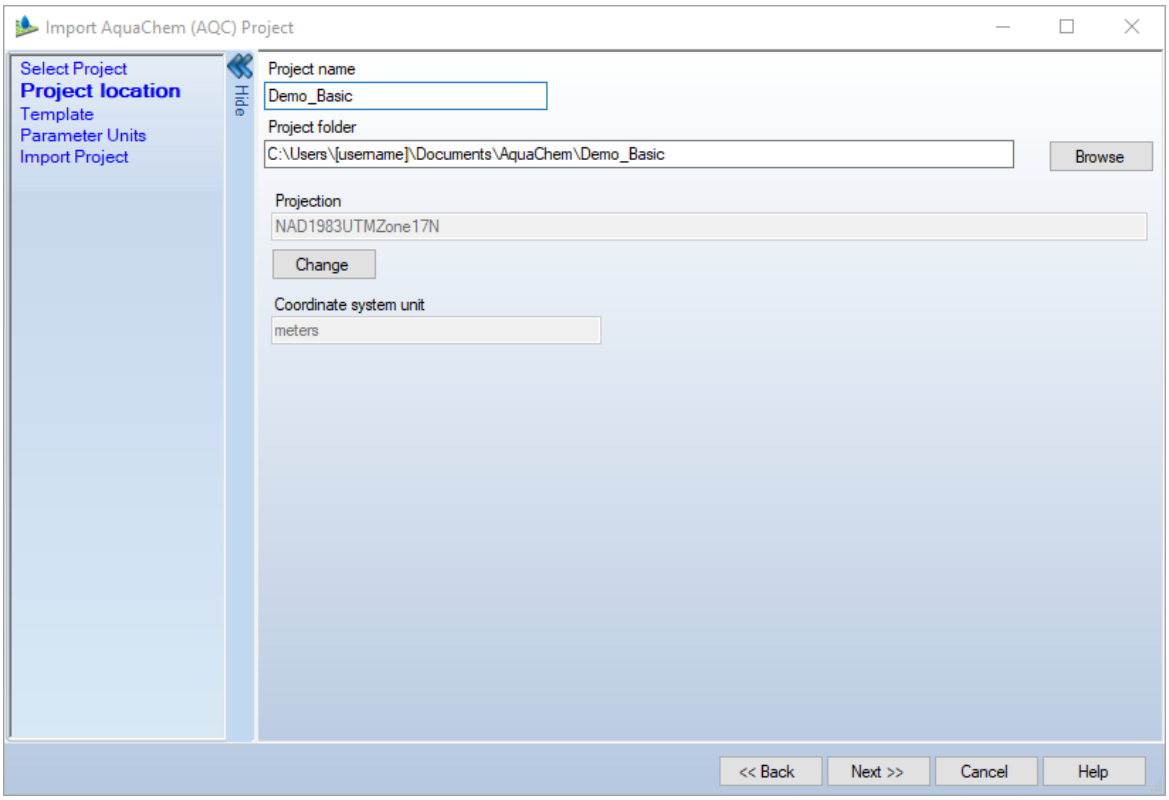


These options ensure that each sample in the imported project contains a unique SampleID; which is a strict requirement in AquaChem 10.0.

Once the unique sample IDs ensured in the imported project, you can proceed to the next step by clicking the Next >> button to proceed to the **Project Location** step.

Project Location

In the second step of the import process, you select the name of the AquaChem 10.0 project, the destination folder and the coordinate system units. Simply use the Browse... button and navigate to the folder where you want to store the project and provide a Project Name, as shown below:

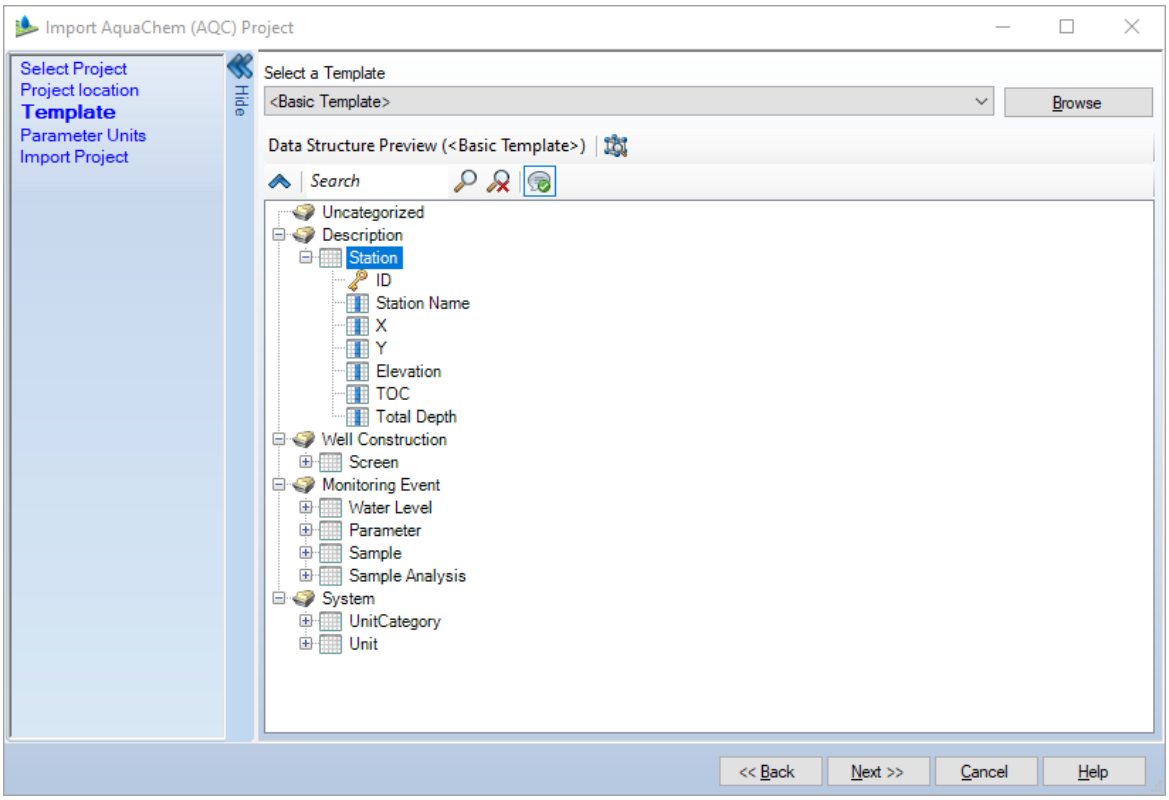


Here you can also select a Projection for your imported project. Select the Change button to select a projection system.

You can now proceed to the **Template** mapping step by clicking the Next >> button.

Template

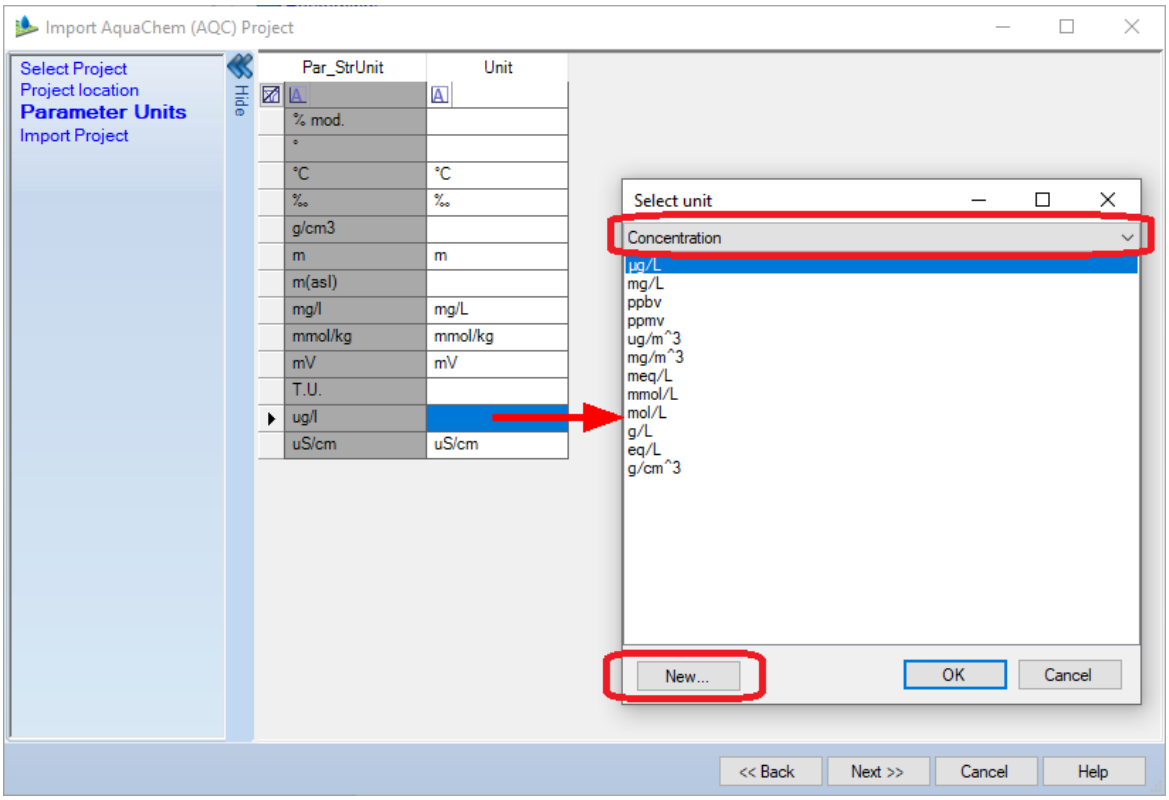
In the third step of the import process, you select a project template to migrate the data into. Simply use Select a Template dropdown to select an existing template in your templates folder or use the Browse... button to navigate to the desired template. You may review the data structure of the selected template using the Data Structure Preview pane. To further explore selected template, you can toggle the tooltips button on and hover over a field to see its description and browse the list of template parameters by clicking the button.



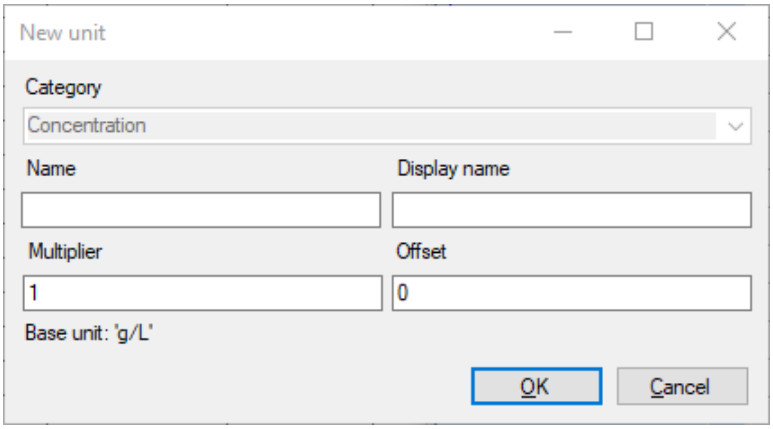
Parameter Units

At this fourth step, you will be prompted to map measurement units that are present in the original AquaChem v2014 project to equivalent units in AquaChem 10.0.

To map units, simply click unmapped (empty) empty cells under the 'Units' column. A '**Select unit**' window will then open allowing you to choose from available unit categories using the dropdown menu at the top of the window. Available units for the selected category will then be displayed, allowing you to choose the desired unit:



You can select the units using **Category** dropdown list; which will show all of the units for the selected unit category. Units in the same category can be converted to each other. If the unit is not available for the appropriate category, select New... button to create a new unit for the current unit category:



- **Name:** the name of the unit category. For example, micrograms per liter
- **Display Name:** the name that will be used for labels in AquaChem. For example, µg/L

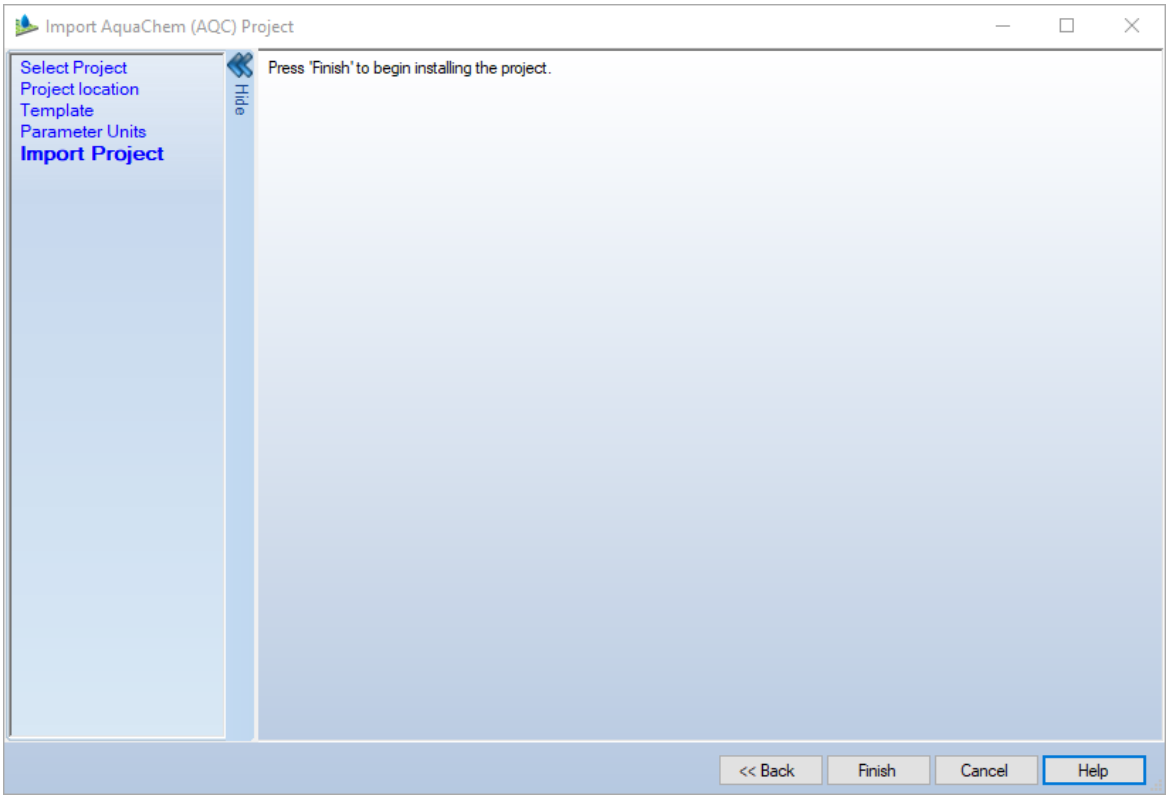
- **Multiplier:** the factor that converts the new unit to the base unit. For example, the conversion factor for µg/L to the base unit (g/L) is 1000.
- **Offset:** the unit offset that converts the new units to the base unit. Usually this is 0, but in some cases, for example: converting between the temperature units degrees Celcius to degrees Fahrenheit requires a linear offset.
- **Base Unit:** the base unit is the measurement unit that all other units of the same category are compared against (using the multiplier and offset).

If no units are specified for the unmapped units, parameters with these unmapped units will be imported with no units and corresponding values will be imported without any conversions. You can assign missing units after the import process using the Parameter Editor module.

Once you have mapped parameter units as desired, click the Next >> button to proceed to the final step of the import process: **Import Project**.

Import Project

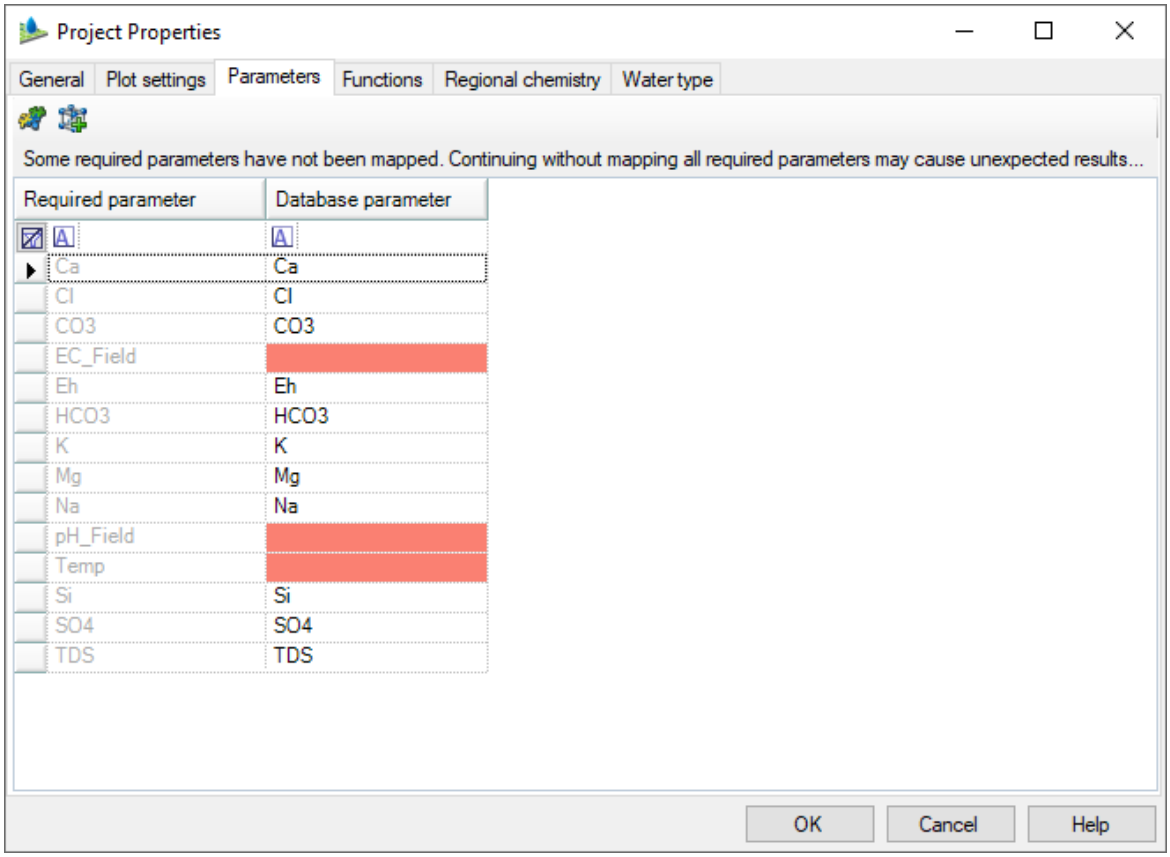
The final step in the import process, is to simply click the Finish button to initiate the import process:



When you click the Finish button AquaChem 10.0 will generate the new AquaChem project database based on the contents of the original project and populate it with the data from the AquaChem v2014 project. Database tables, fields and records will be recreated faithfully in the new project. When the import process is finished, the 'Import AquaChem (AQC) Project' window will close, and the project will be loaded.

Map Missing Required Parameters

If any of the required parameters from the AquaChem v2014 project have not been automatically mapped, then the Parameters tab of the Project Properties window will appear, as shown below:



In AquaChem there are a number of parameters which must be mapped/included in order to work with certain features built-into AquaChem, such as evaluating functions (e.g. hardness calculations) or adding plots (e.g. Piper plots) that require specific parameters. If the window above appears, you can use the toolbar buttons to quickly map the existing database parameters to the required parameters (i.e. indicate to AquaChem 10.0 which of the available parameters represents the unmapped required parameters):

- **Auto-map:** automatically matches unmapped parameters from the original project to the new database structure based on parameter names with similar names.

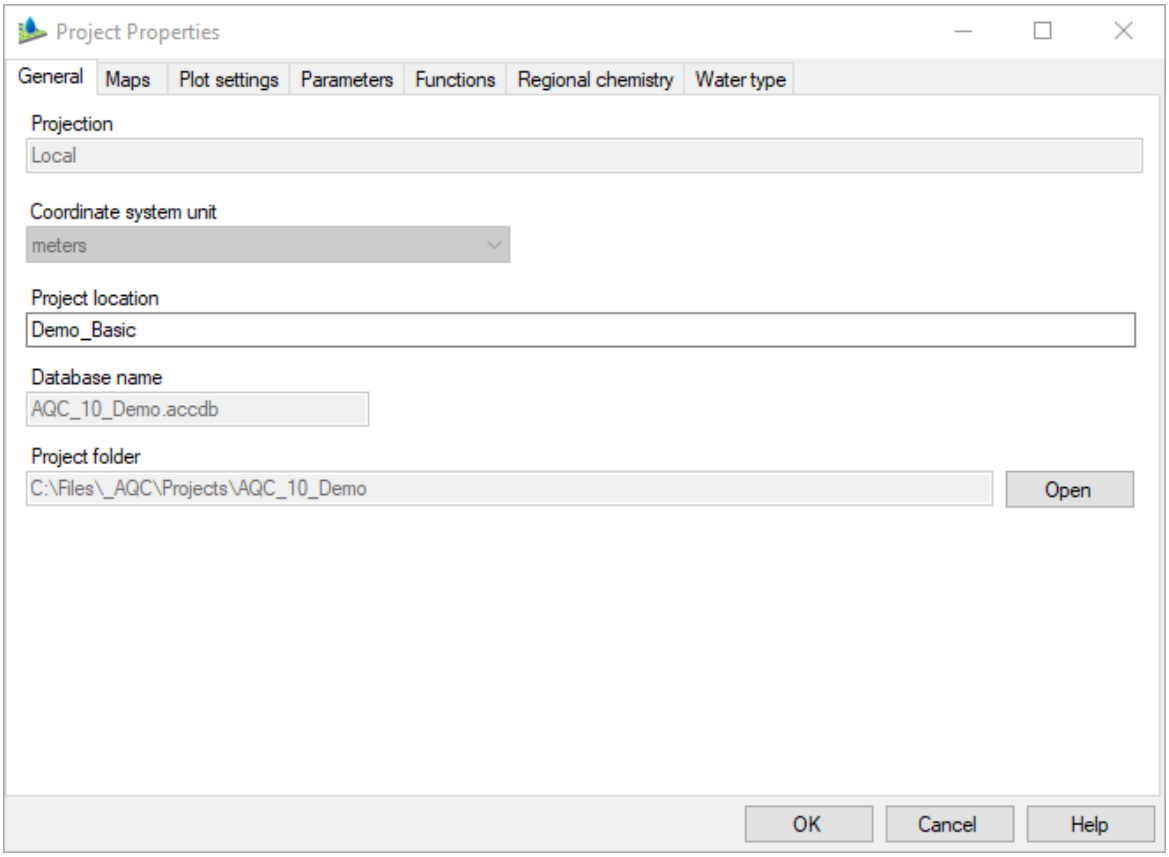
- **Create missing parameters:** creates new parameters for the unmapped parameters using the required parameter name. You will have to use the Parameter Editor to verify parameter properties (e.g. molecular weight and valence).

You can also click in the blank cells (highlighted) to use the Parameter Picker and select an existing parameter in your database.

After mapping the missing parameter(s) simply click OK to accept the changes and dismiss the Project Properties window.

4.1.3 Project Properties

This menu item will load a window displaying the properties for the current project.



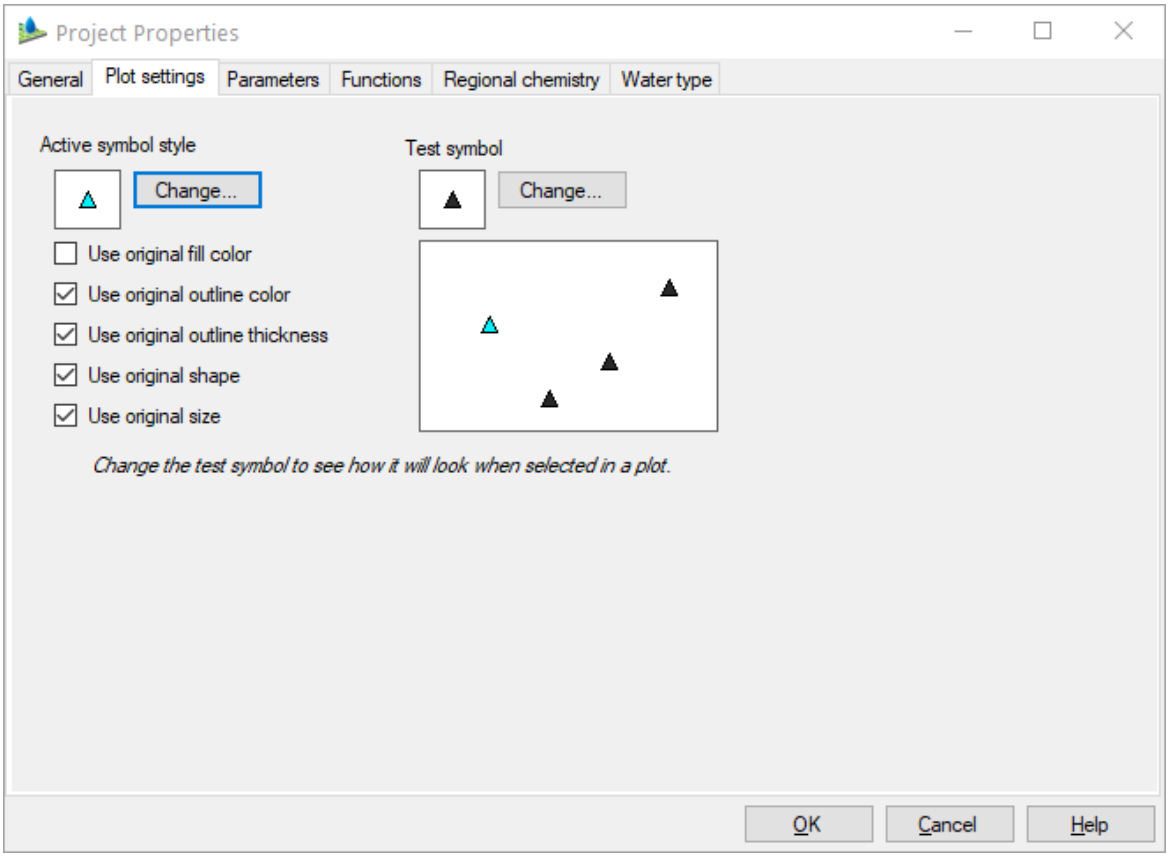
General Tab

On the General tab you can find the (read-only) settings selected during project creation including:

- **Projection:** the coordinate reference system (i.e. Projection) used as the default for Maps in the Map Viewer
- **Coordinate System Unit**: feet or meters
- **Project Location:** Description of the Project Location
- **Database Name:** File name of the associated Access database
- **Project Folder:** location of project files (e.g. output reports, associated images, EDD templates, plots, scripts, etc.)

Plot Settings

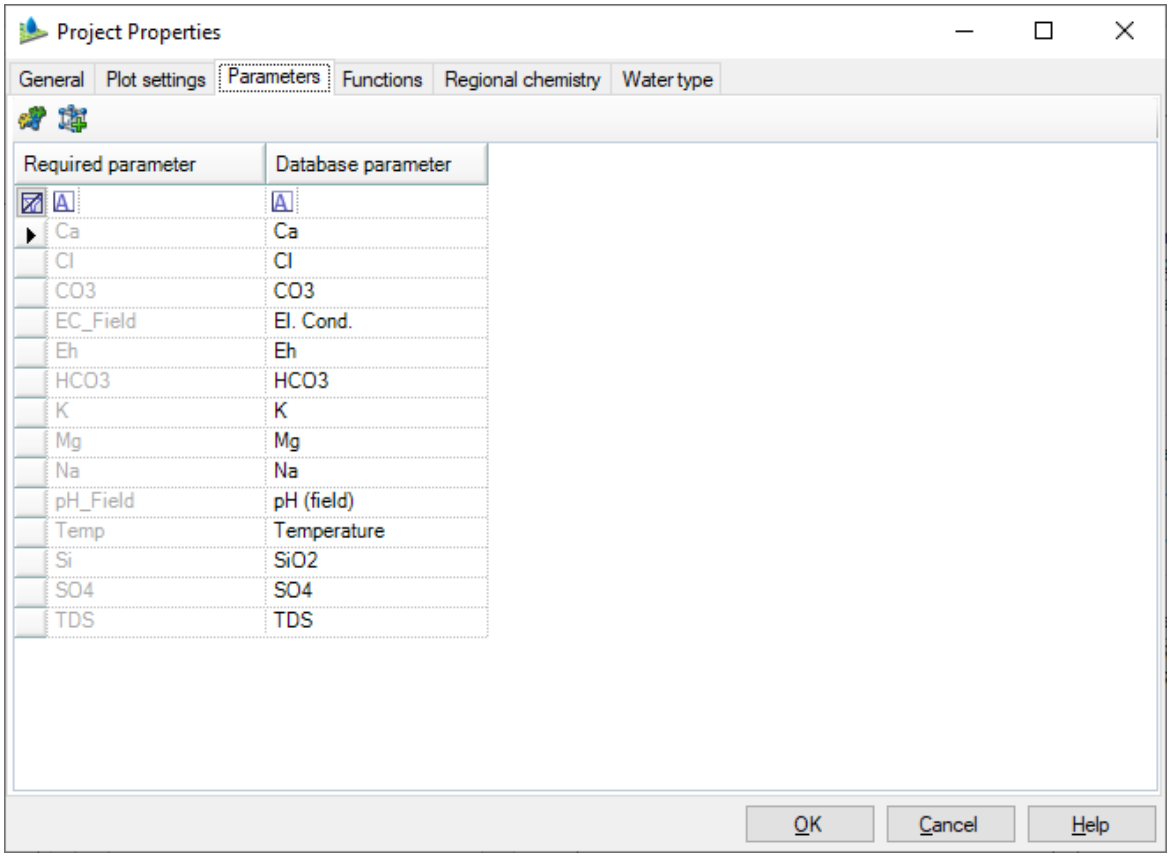
The Plot settings tab allows you to specify how active (selected) data points on interactive plots are displayed in AquaChem. The symbol(s) of the active data point(s) will be modified based on the settings of this tab. You can specify which properties are changed or not using the check marks. The Test symbol is shown to contrast how the active symbol will change based on the current active symbol style settings.



Parameters (Required)

The Parameters tab allows you to map Parameters in your database to the Parameters that are *required* by AquaChem to function. These parameters are required so that AquaChem can use them in built-in functions and calculations. If any of the Required Parameters are

unmapped when you create or open a project, AquaChem will prompt you to map the required fields using one of three options:



1. **Manual Selection:** You can manually map each missing parameter by clicking in the corresponding empty cell in the Database Parameter column. This will open the Parameter Selector and allow you to pick an existing parameter from the project database. Select an existing parameter from the database and Click OK.

2. **Auto-map:** you can select the Auto-map button in the upper left corner of the window and AquaChem will attempt to match the unmapped Required Parameter(s) to existing parameters in your project database with the same or similar spelling. If you don't agree with the match(es) that AquaChem suggests you can adjust the values or click the Cancel button and try again using a different method.

3. **Create missing parameters:** you can select the "Create missing parameters" button in the toolbar and AquaChem will create new parameters in the database.

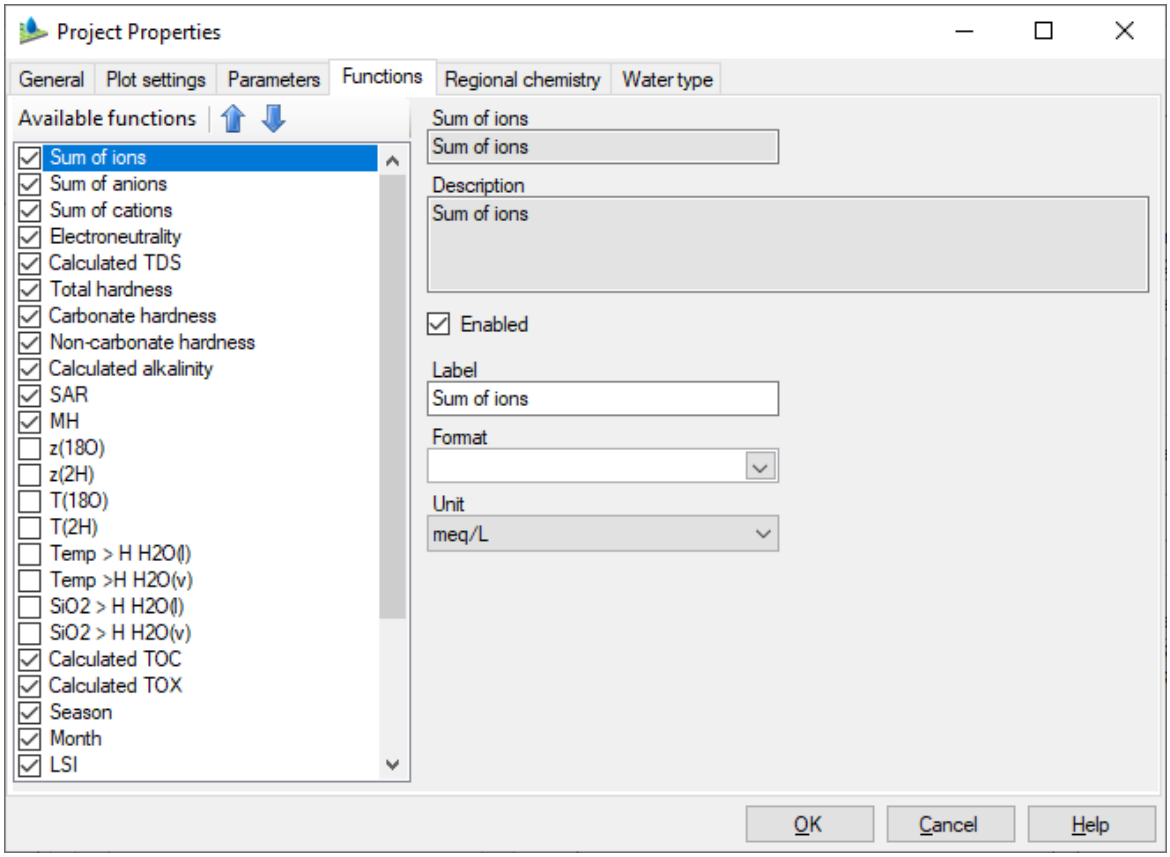
Please Note: if you create missing parameters, you may need to review the settings (e.g. molecular weight, CAS#, etc.) for the new parameters to ensure that they are used correctly in your project.

Functions

The Functions tab provides a list of the built-in functions supported in AquaChem and allows you to manage how they are shown in the Calculated tab of the Results pane in the Sample List View, including:

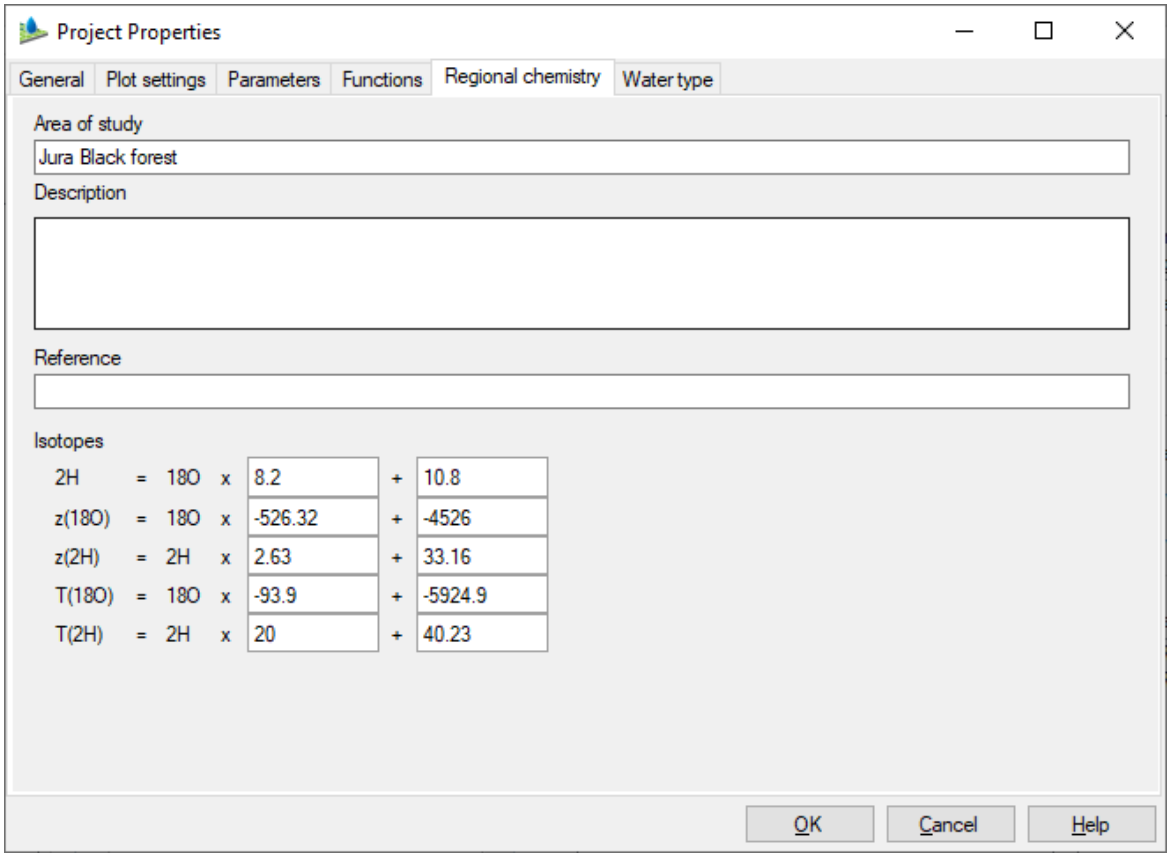
- **Order:** rearrange the order of functions in your project by selecting a formula and using the up and down arrows;
- **Label:** edit the label that will appear in the Results pane of the Sample List view for the selected function by editing the Label field;
- **Number Format:** set the format of function results using the standard formats that are available in Excel (e.g. #,##0.00; 0.00E+00; and 0); and
- **Output measurement units:** select one of the measurement units available for the selected function

Available functions are shown below and explained in detail in the Functions section.



Regional Chemistry

The Regional chemistry settings tab includes variable settings for empirical functions with parameters that vary regionally. These include the Meteoric Water Line and estimates of the infiltration elevation and infiltration temperature based on linear relationships with the measured fractionation of oxygen-18 (18O) and deuterium (2H) isotopes. The slope and intercept fitting parameters are typically valid only for very limited zones that must be established for your area of interest using published/empirical values. There are also settings that allow you to document the scope (i.e. Area of study and Description) and source (i.e. Reference) of the regional chemistry parameter values.

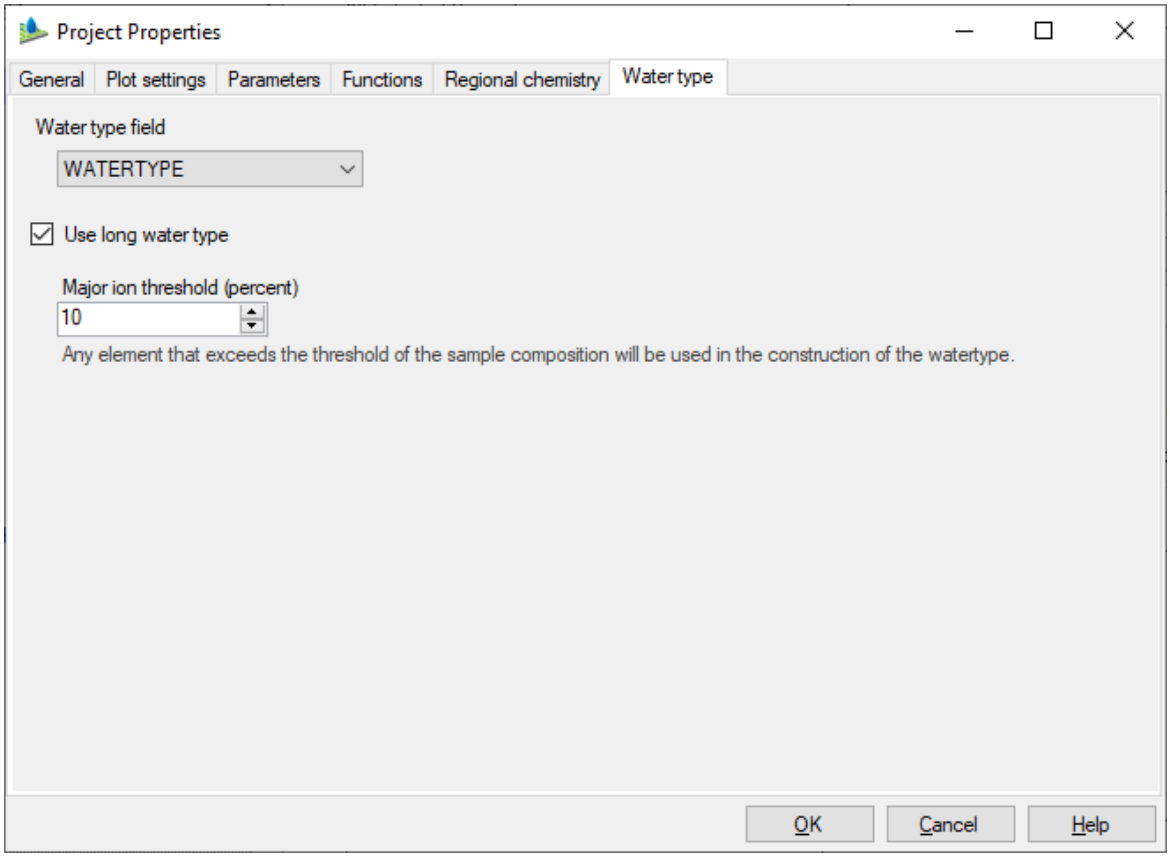


Water Type

The Water Type tab provides settings to facilitate and modify the calculation of water facies for samples in the project:

- **Water type field:** select the destination field in the sample table for water type calculations.

- ☑ **Use long water type:** if selected, the long facies name will be selected; otherwise, the water type will list only the anion and the cation with the highest concentration in the sample(s).
- **Major ion threshold (percent):** when calculating the long facies name, only ions that exceed the specified threshold of the total sample composition will be included in the construction of the water type.



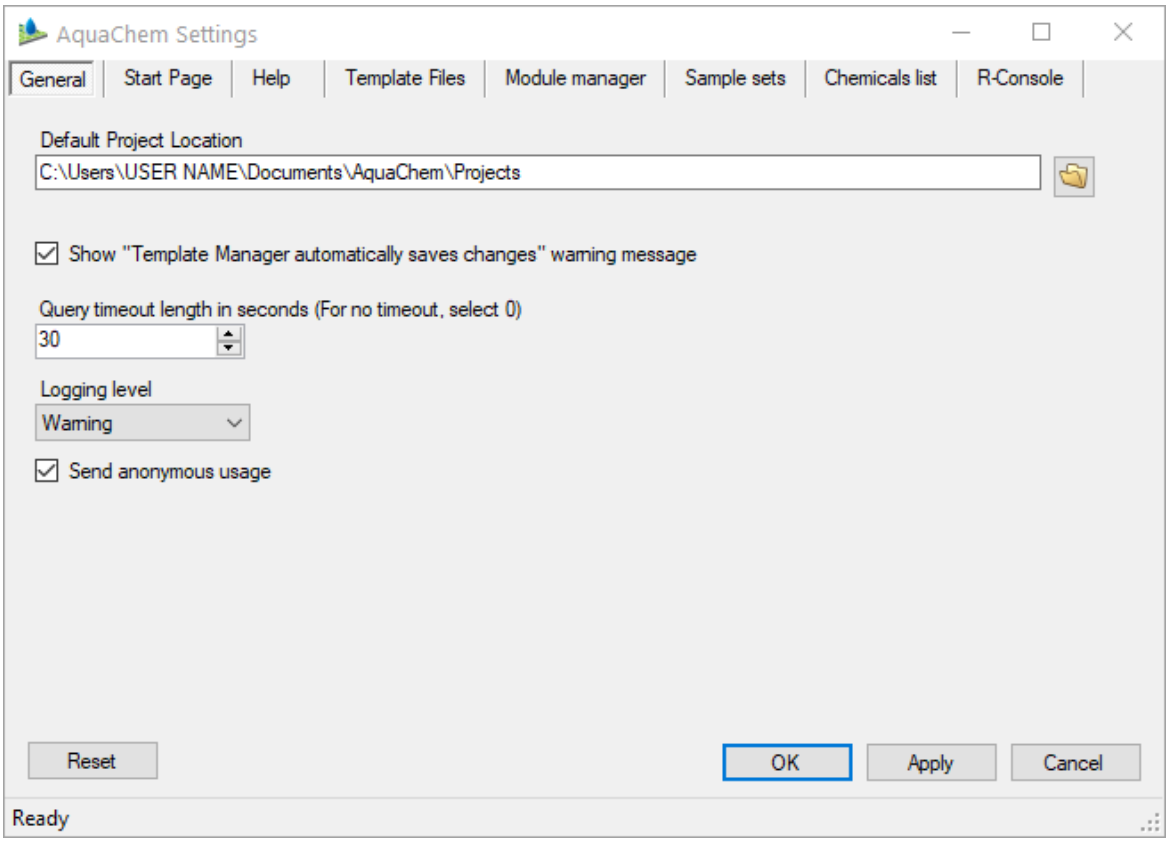
For more information, see the Calculate Water Type section.

4.1.4 AquaChem Settings

The AquaChem Settings dialog provides various settings for a number of options within the program.

General

The General settings tab allows you to specify the default save location for projects. These settings are taken into account when creating new projects or when installing the Demo project.



You can also turn the Template Manager warning message on or off. As well as find an option to set the Query timeout length and error logging Level.

Error Logging

AquaChem provides 4 levels of logging to track when/if AquaChem encounters unexpected issues and to facilitate related support requests:

- Error - this logs unexpected (bad) things
- Warning - this logs the errors as well as warning which might point to impending errors
- Information - this logs errors and warnings as well as other helpful things
- Verbose - this logs errors, warnings, information as well as debugging information

The Warning level is the default level; however if you are encountering errors and need support, our Technical Support may suggest that you increase the logging level and have you reproduce the issue and send the log file to help us better understand the problem.

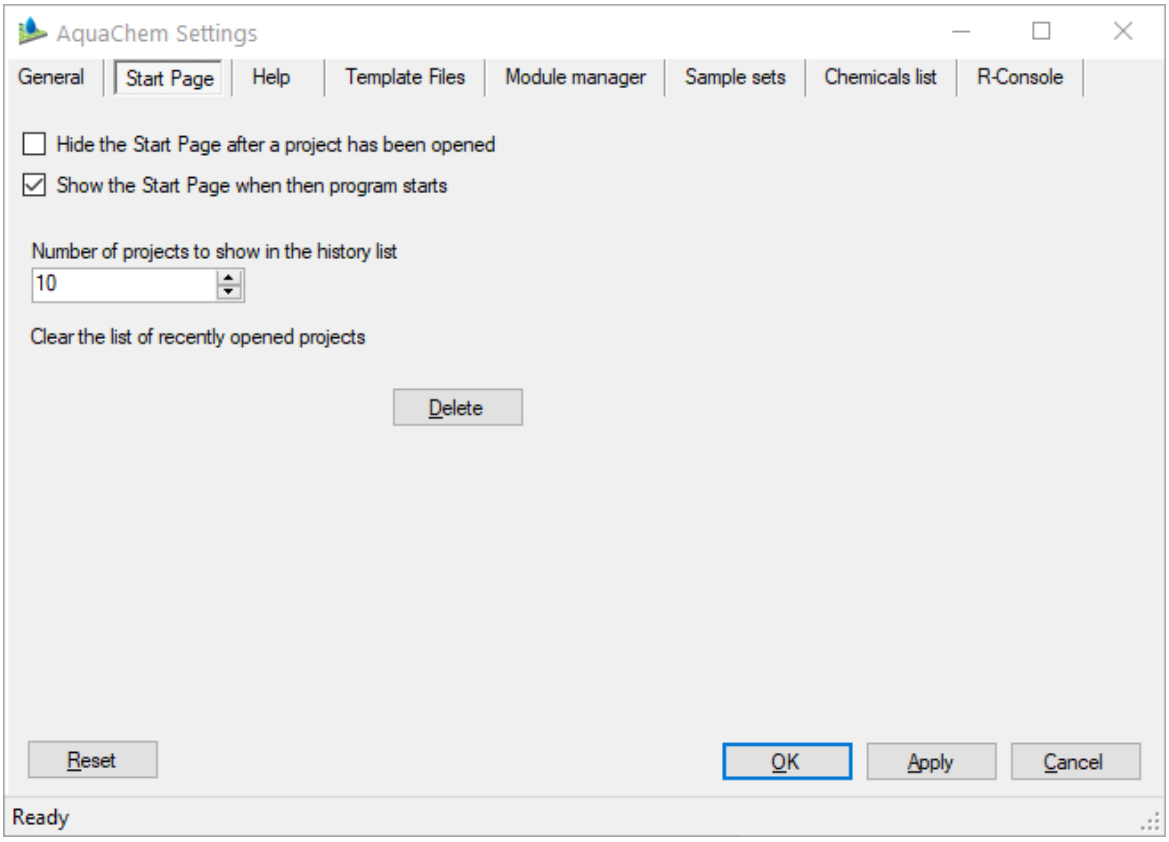
However, please be aware that changing the level to Verbose may have a negative impact on performance, so you might want to lower the level once you have provided Support with your log file!

Anonymous Usage

By default, AquaChem collects anonymous usage statistics. The data that we collect enables us (Waterloo Hydrogeologic) to get reliable statistics on which features are used (or not used) in AquaChem. This helps us better understand the needs of our users so we can build better applications. The information collected is completely anonymous – it is not traceable to any individual, project, or organization. You can always opt out by deselecting this option. For more information about our data collection policies, please see here.

Start Page

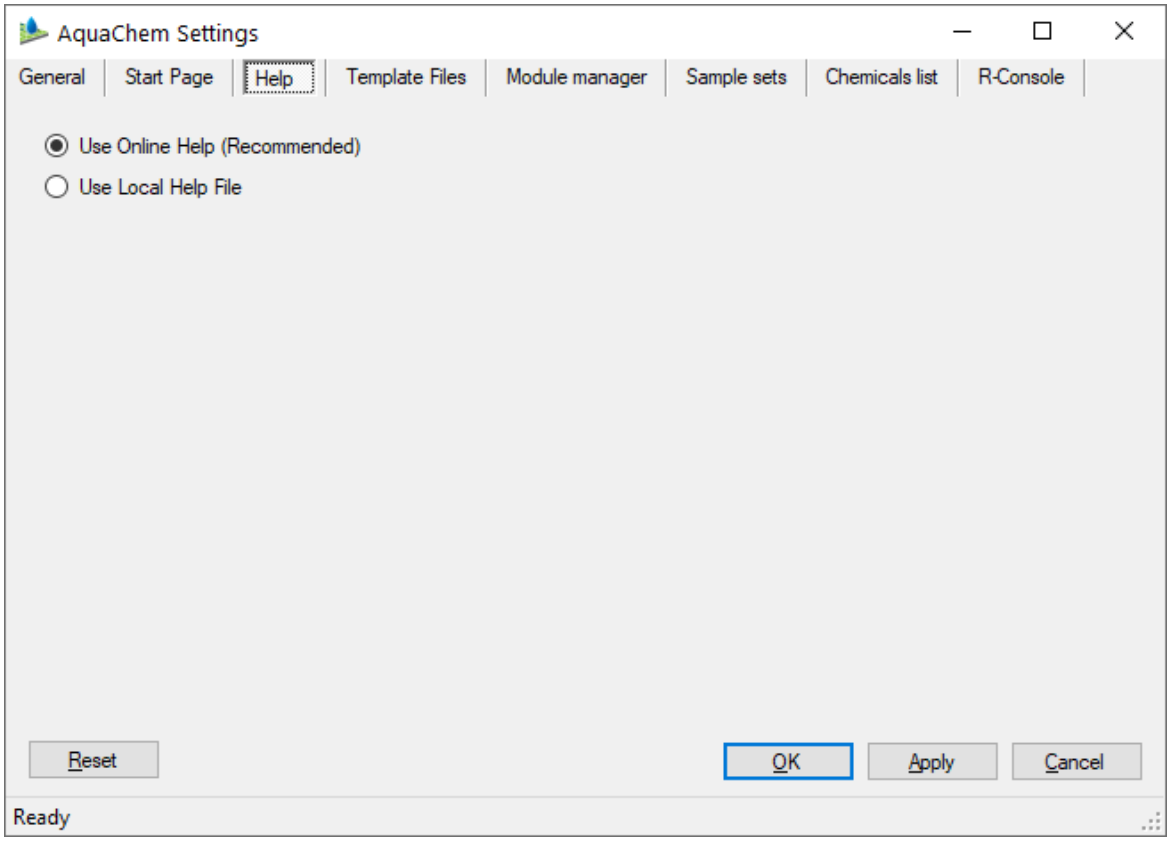
Here you can specify if you want the Start Page to be hidden after opening a project as well as if you want the Start Page to be shown when you start AquaChem.



Additionally, you can change the number of projects to show in the list of recently opened project - or even clear the list completely.

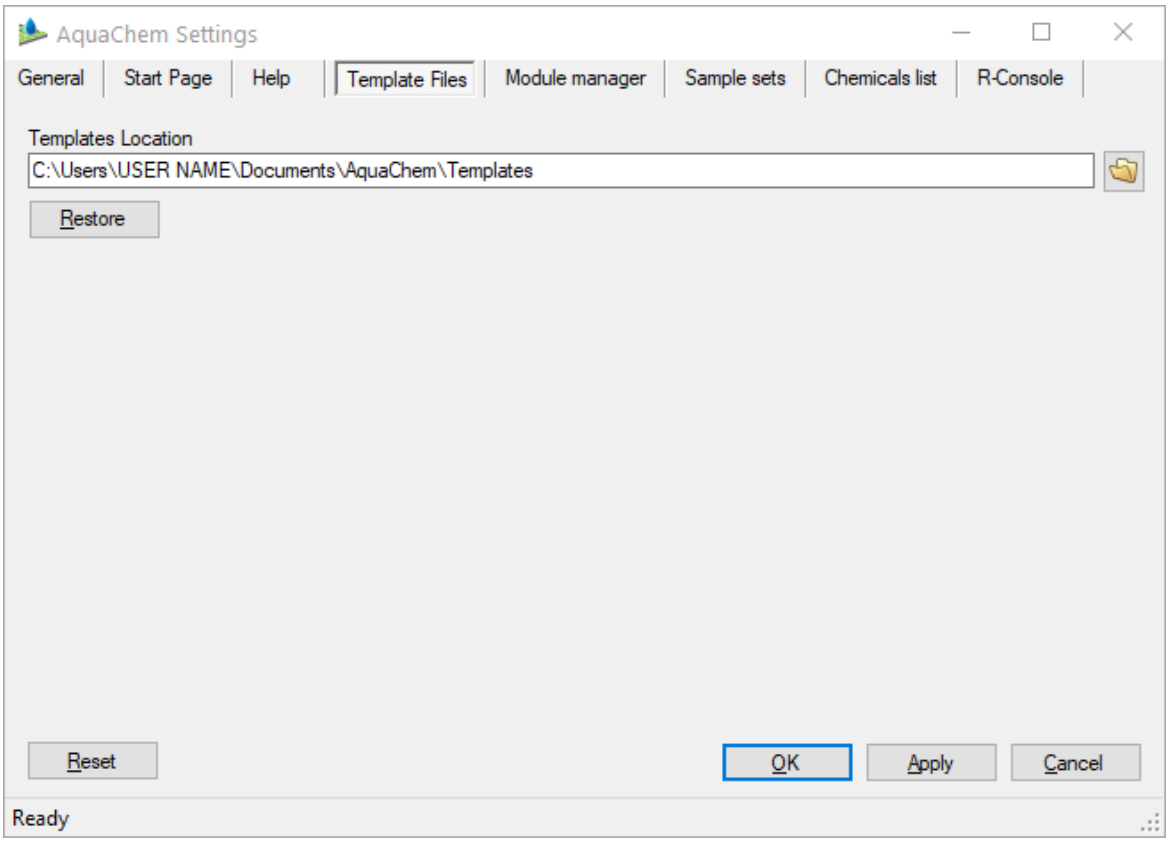
Help

Here you can specify if you want to use the Online Help (Recommended) or the Local (In Program) Help. We recommend the Online Help (if you are connected to the internet) as this set of documentation can be updated more frequently than the Local Help.



Template Files

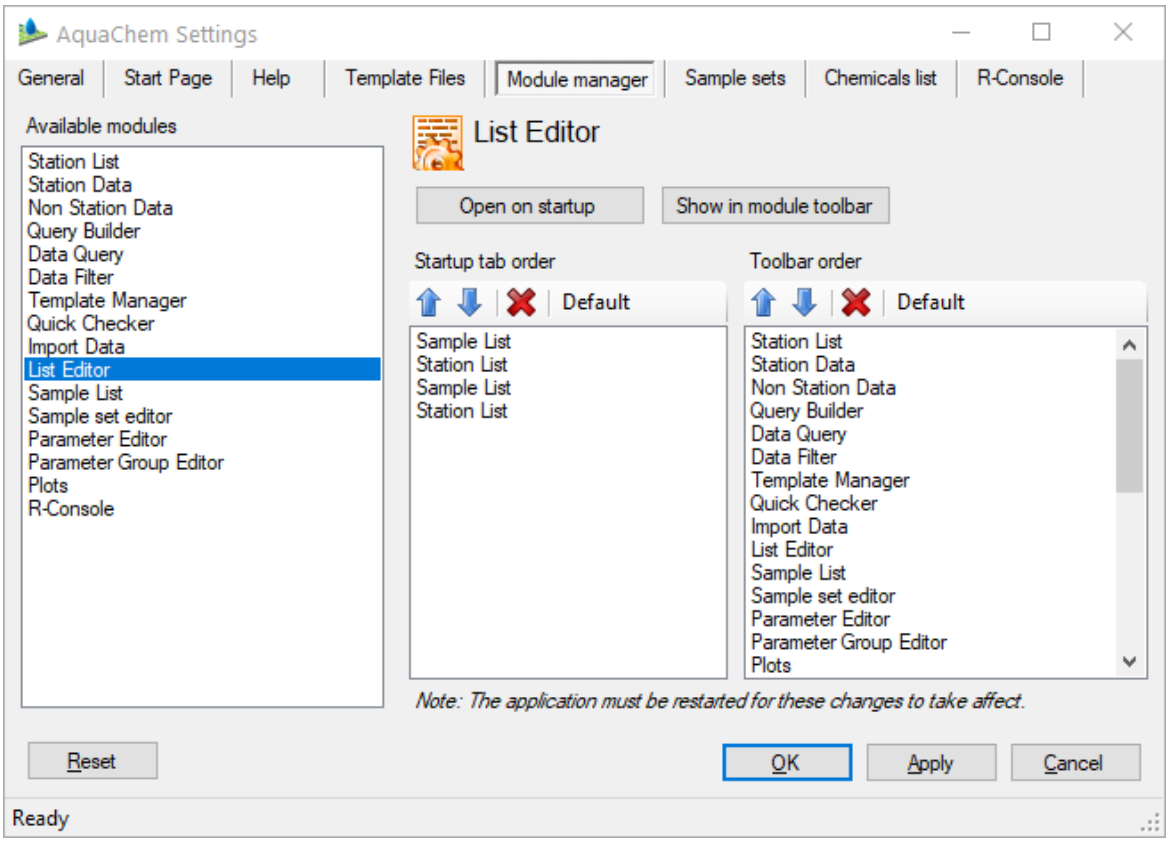
Here you can specify where you want to store AquaChem template files. These template files include the database template files used when creating a New Project as well as Microsoft Office template files for printing AquaChem data, reports, and plots to Excel and/or PowerPoint. The Office template files are organized into appropriately named folders. Do not adjust the folder names as this is how AquaChem knows which templates are available. Note, these can be stored on a shared or network drive so that you can use a consistent set of templates that is common to everyone in your organization.



You will also find the option to restore all of the templates - in case you have made changes to the original ones and want to revert back.

Module Manager

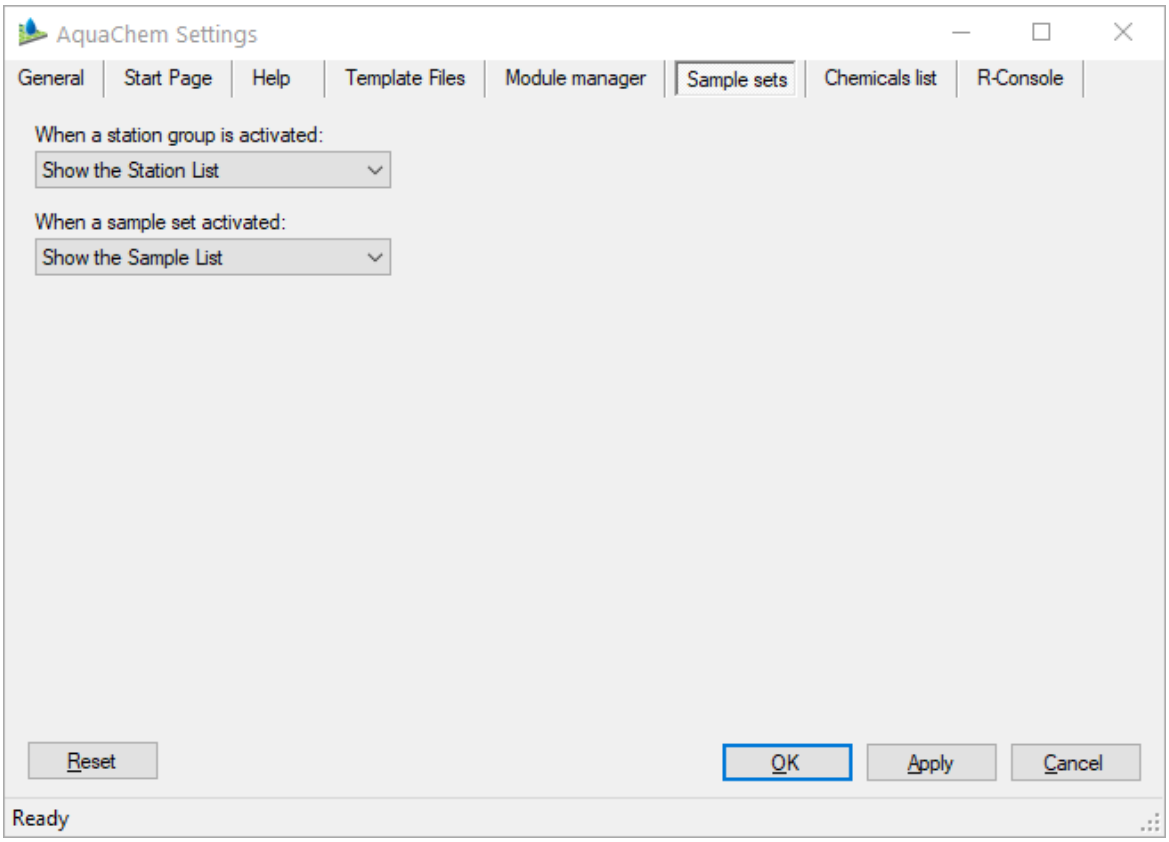
Here you can specify which modules are opened on Startup (with the exception of those modules that require specific items, e.g. R-scripts in the R-Console, Data Queries in the Query Builder) and which modules are shown in the Module Toolbar.



Sample Sets

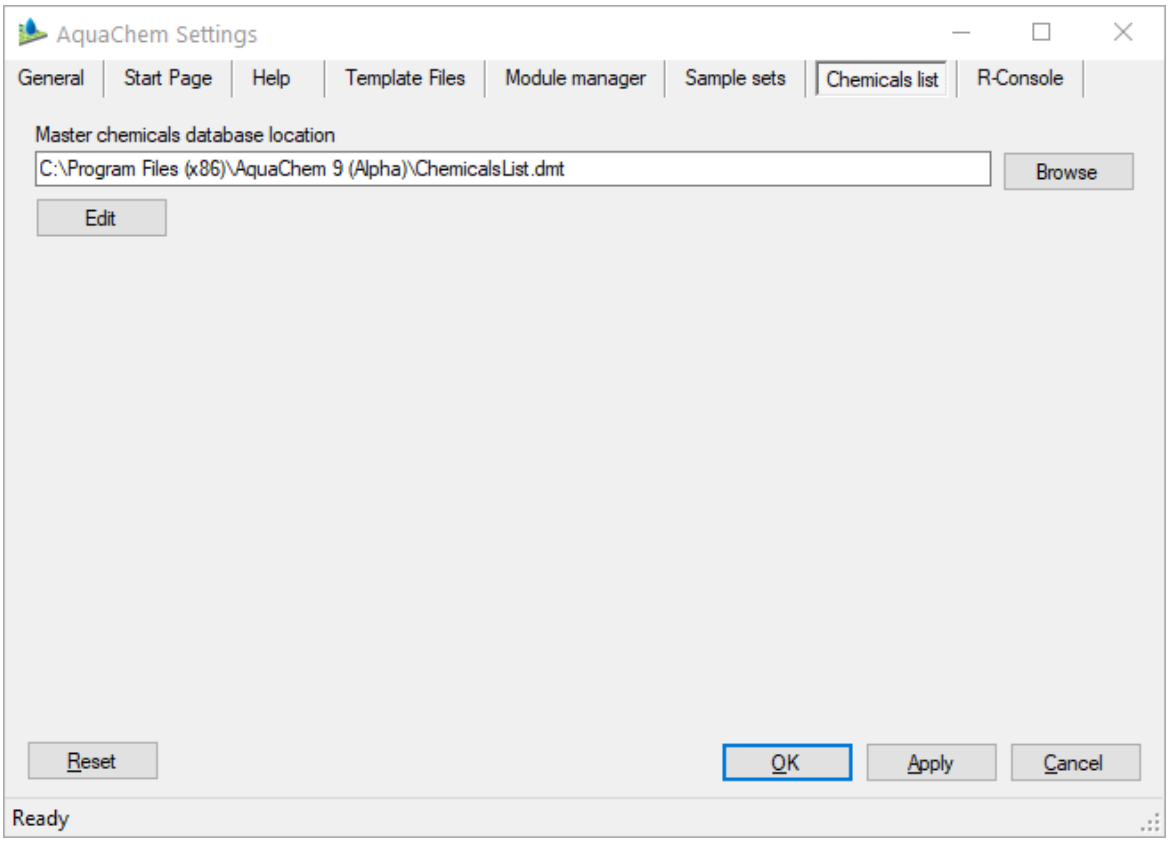
Here you can specify what happens when you activate station groups or sample sets:

Available Actions	When Activated: Station Group	Sample Group
Do Nothing	✓	✓
Show the Station List	✓	✗
Show the Sample List	✓	✓



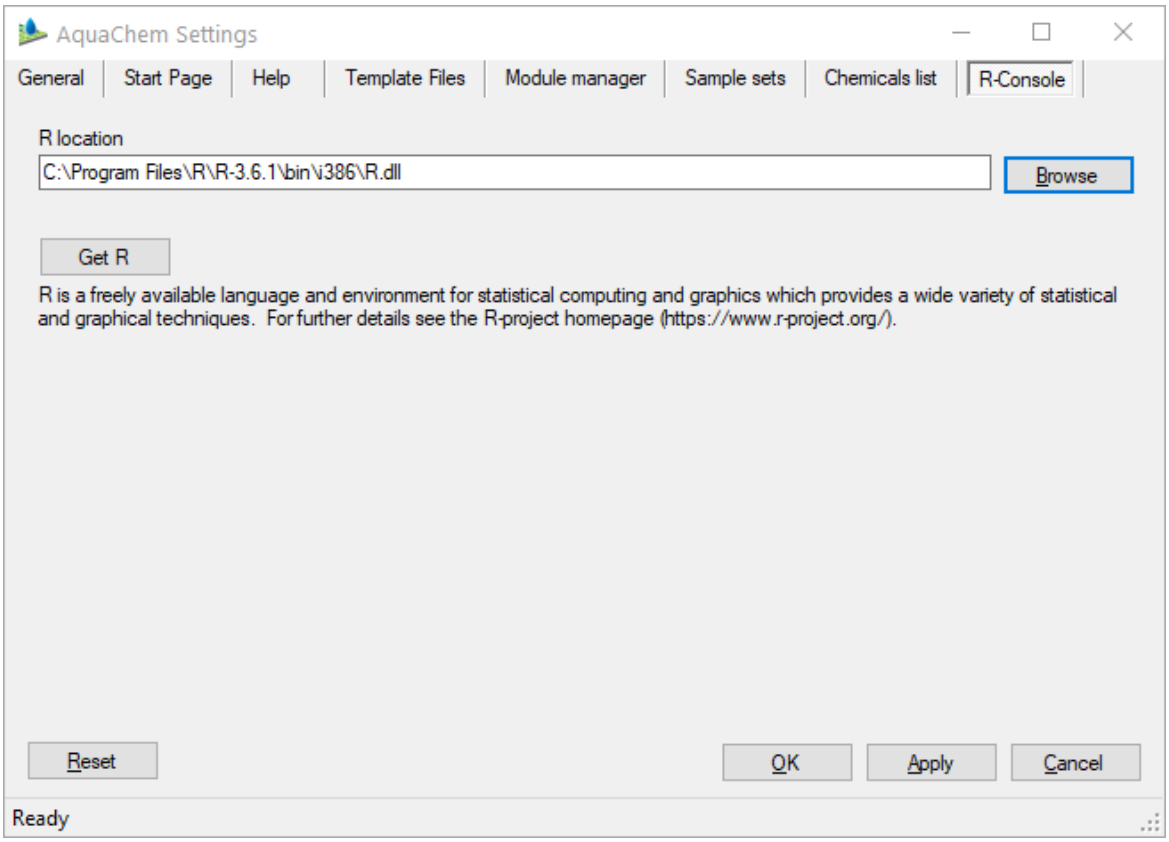
Chemicals list

Here you can specify the location of your Chemical List, which is a database of parameters and their properties. This is a common resource that is shared across all of your projects and can be managed centrally by your organization.



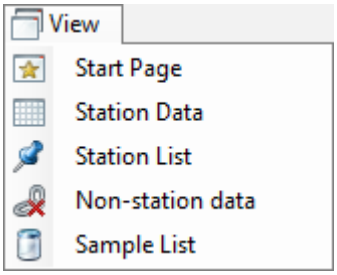
R-Console

Here you can specify where the R.DLL library is installed. The location where R.DLL is typically installed is shown below. Note, you will need to already have R locally installed in your environment following the installation instructions.



4.2 View

The View menu allows you to reopen any closed tabs:



Start Page

The Start Page Tab contains information about your version of AquaChem and available help and support resources.

 **Station Data**

The Station Data Tab provides an interface for working with data associated with the currently selected station group (e.g. samples).

 **Station List**

The Station List Tab provides an interface for working with the currently selected station group.

 **Non Station Data**

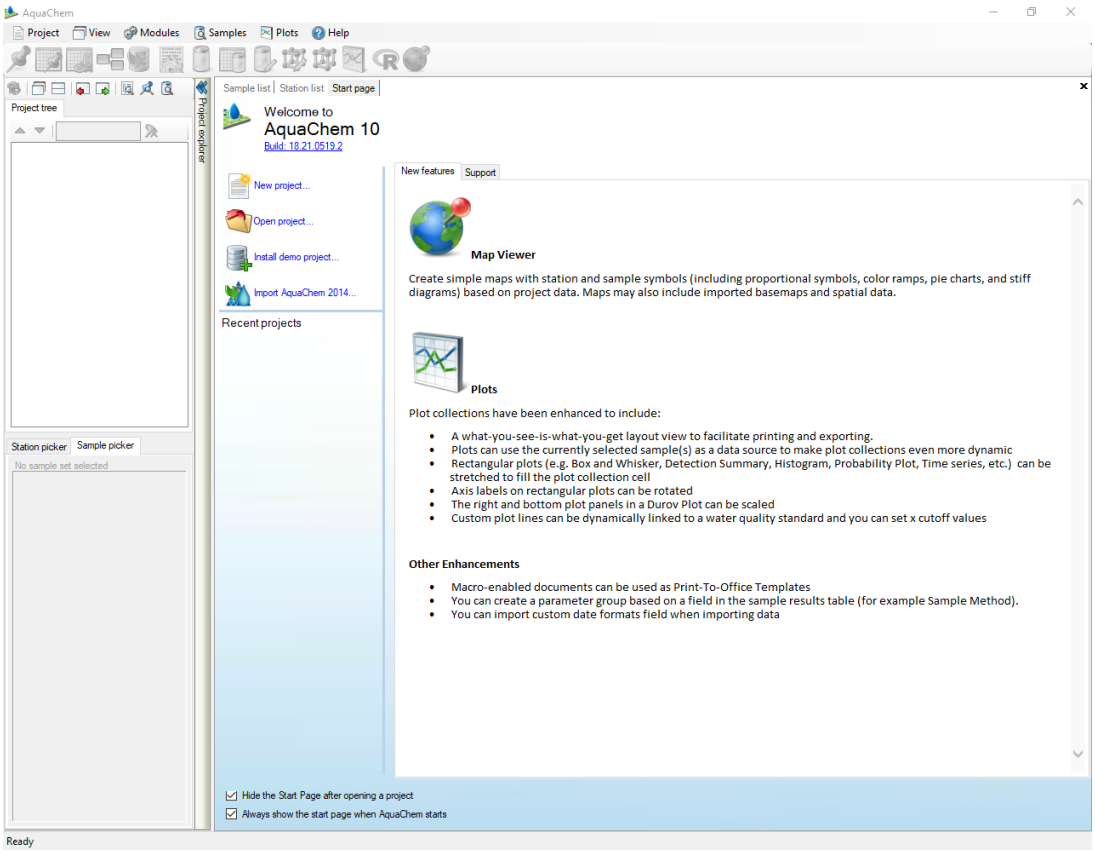
The Non Station Data Tab provides an interface for working with data that is not related directly to stations.

 **Sample List**

The Sample List provides an interface for working with the active sample group and related results.

4.2.1 Start Page Tab

When first launching AquaChem, you will find a Start Page to help you perform common tasks such as creating a new project or opening an existing project – even installing the Demo Project which is used in the Quick Start Tutorial.



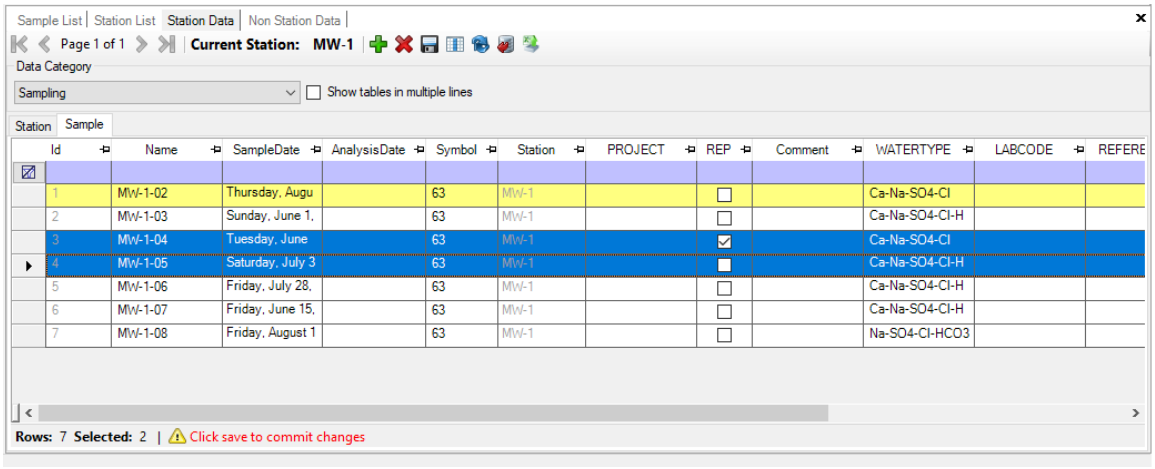
There is a lot of useful information on the Start Page such as:

- The **New Features** tab will describe each of the new features.
- The **Release Notes** tab will display our online Readme file. This contains detailed information about the new features, a list of features and bugs fixed from previous versions, as well as known issues and limitations of the current version.
- The **Support tab** provides additional sources of information to help you, including:
  - How to *contact our support team*. If you have a question or concern with the product, you can use this link to initiate an email to the support team and it will include all the System Information which can be very helpful for our support team to help resolve your concern.
  - If you are having difficulties explaining the concern try using the *Problem Step Recorder* – it does just what the name implies – it creates a recording of the steps you took (all the clicks) with screen captures to help make it clear what you were trying to do.
  - The AquaChem YouTube channel with videos of tutorials, recorded webinars, and more;

- The online Frequently Asked Questions (FAQs); and
- Available Training Options.

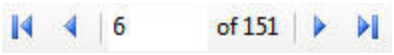
4.2.2 Station Data Tab

The Station Data tab provides a detailed view of the active Station's attributes as denoted in the Station Picker. The Station Data tab displays available information about the currently selected station based on the active Data Category. Detailed information about the active station can be viewed, added, edited or deleted through the Station Data tab.



Toolbar

The toolbar for the Station Data tab contains the following controls:



Navigates data pages; skipping to the first page (in the sort order), to the previous page, to the specified page, to the next page or to the last page.


Adds a new record.


Deletes the currently selected record(s) from the database.


Saves the changes you have made.


Allows you to select which columns you want to show or hide.

Refreshes the data in the current tab.

Exports the data from the current tab.

Exports the data from the current tab to an Excel template. (see below)

Working with data

The first line shown on the tables in the Station Data Tab contains field names/column headers; below this is the filter line, which is highlighted in light blue and denoted by the clear filter button () in the left-most column. The filter line can be used to restrict records to display based on the values in one or more field and is described in detail in the Data Filtering section.

You can select one or more records (that will turn bright blue) in the data table by clicking on the buttons on the left-hand side of the grid (using the <SHIFT> and <CRTL> keys for selecting multiple records). You can perform the following actions by right-clicking on the selected record(s) in the currently displayed table:

Hide/Show Columns: allows you to select which columns you want to show or hide

Show All Columns: unhides all hidden columns

Select All Rows: selects all records in the currently displayed page

Copy: copies the selected record(s) and the header row to the clipboard for use in other applications (e.g. Excel, notepad, etc.)

Add Record: appends a new record to the end of the current page

Save: saves any edited records to the database (note that records with unsaved edits are highlighted in yellow)

Delete Record: deletes the selected record(s) from the database

Export: Exports the table to a file format of your choice: Excel (.xls, .xlsx), Access (.mdb, .accdb), Text (.csv), HyperText (.htm), and portable document (.pdf)

Print to Office: Exports the data from the current tab to an Excel template (see below)

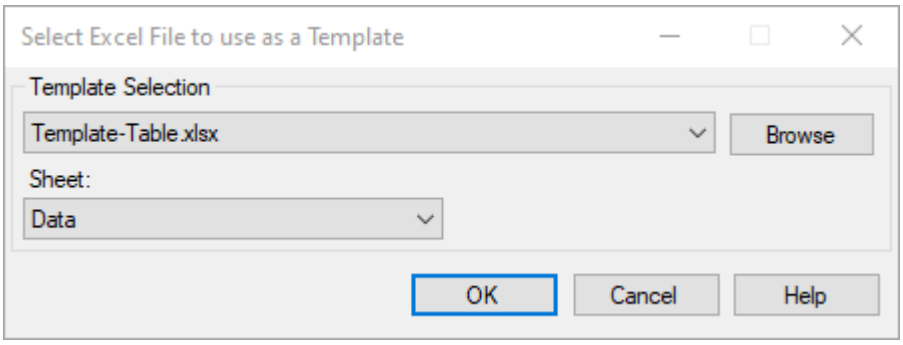
Refresh: Refreshes the data in the current tab from the project database

Resize Columns to Fit Grid: resizes columns to fit the table columns within the workspace

Values in fields may be modified for the actively selected record (denoted by a ), by clicking in the cell you wish to edit and entering the desired value. The Station Data tab may be used to quickly view or manage data for numerous samples or other station-based data.

Print to Excel Template

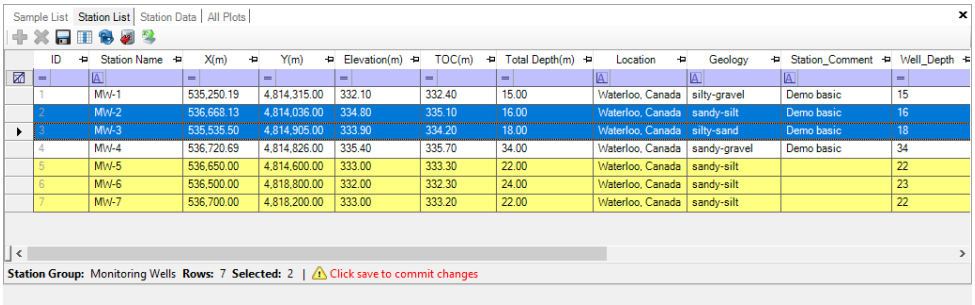
When printing your Station Data to an Excel template, you will be prompted to select a template. A template called "*Template - Table.xlsx*" is provided with AquaChem. You can modify this template by going to the folder where your templates have been stored (see AquaChem Settings for more details) and adjust it to suit your needs. Perhaps you may want to change the logo, add others etc. Templates stored in the Office/Excel Tables subfolder will be available in the drop down list under the Open Template option.



Once you have selected a template you can select the OK button and the Excel template will open with your data in it - ready for printing or further analysis!

4.2.3 Station List Tab

The Station List tab provides an overview of the available stations in the active station group as selected from the project tree and displays fields from the Station Table (the main table within the AquaChem database) for example: name, X-coordinate, Y-coordinate, Elevation etc. The Station List tab allows you to manage stations and their associated data.



Toolbar

The toolbar for the Station List tab contains the following controls:

 Adds a new record (only available if the All Stations station group is selected).

 Deletes the currently selected record(s) from the active station group. To delete a station from the project entirely you must activate the 'All Stations' group before deleting.

 Saves the changes you have made to the project database.

 Allows you to select which columns you want to show or hide.

 Refreshes the data in the current tab from the project database.

 Exports the data from the current tab.

 Prints the data from the current tab to an Excel template (see below).

Working with the Data

The first line shown on the tables in the Station List Tab contains field names/column headers; below this is the filter line, which is highlighted in light blue and denoted by the clear filter button () in the left-most column. The filter line can be used to restrict records to display based on the values in one or more field and is described in detail in the Data Filtering section.

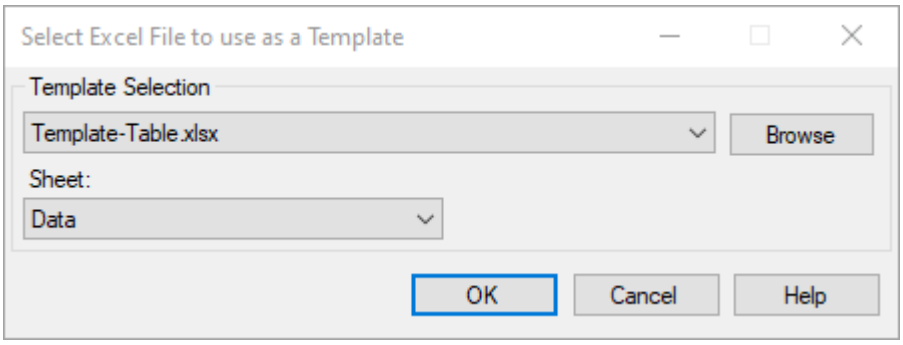
You can select one or more records (that will turn bright blue) in the data table by clicking on the buttons on the left-hand side of the grid (using the <SHIFT> and <CRTL> keys for selecting multiple records). You can perform the several actions by right-clicking on the selected record(s) in the currently displayed table, including showing/hiding fields and records, copy, paste, adding the selected station(s) to a new/existing station group, refreshing the data from the project database, and resizing the columns to fit the station list table within the current workspace.

Values in the data fields may be modified for a selected station (simply click in the cell you wish to edit); or a new station may be created here (selecting the  icon), and the values for these fields may be defined. The Station List tab may be used to quickly enter numerous stations, and define the basic attributes for each station.

Print to Excel Template

When printing the Station List table to an Excel template you will be prompted to select a template. A template called "*Template - Table.xlsx*" is provided with AquaChem. You can modify this template by going to the folder where your templates have been stored (see

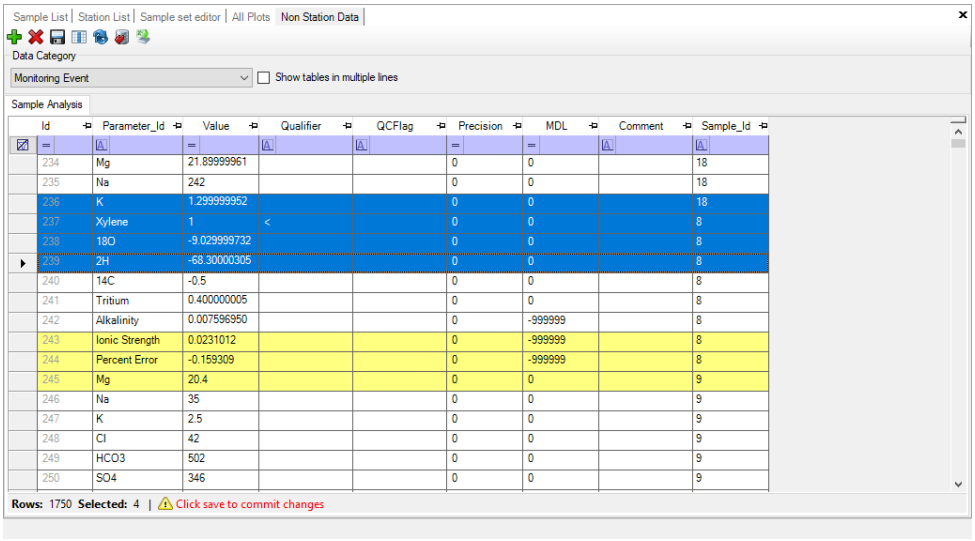
AquaChem Settings for more details) and adjust it to suit your needs. Perhaps you may want to change the logo, add titles for the project or client, etc. Templates stored in the Office/Excel Tables subfolder will be available in the drop down list under the Open Template option.



Once you have selected a template, you can select the OK button and the Excel template will open with your data in it - ready for printing or further analysis!

4.2.4 Non Station Data Tab

The Non Station Data tab provides you with the ability to view tables that are not directly associated with the Station Table (e.g. the Sample Analysis and Parameter tables). You can find out more information about how to add a Non Station Data table in your database in the Template Manager section. The Non Station Data tab displays available information based on the active Data Category. Information in the Non Station Data tab can be viewed, added, edited or deleted.



Toolbar

The toolbar for the Non Station Data tab contains the following controls:

 Adds a new record.

 Deletes the currently selected record(s).

 Saves the changes you have made.

 Selects which columns you want to show or hide.

 Refreshes the data in the current tab.

 Exports the data from the current tab.

 Prints the data from the current tab to an Excel template.

Working with the Data

The first line shown on the table in the Non Station Data tab contains field names/column headers; below this is the filter line, which is highlighted in light blue and denoted by the clear filter button () in the left-most column. The filter line can be used to restrict records to display based on the values in one or more field and is described in detail in the Data Filtering section.

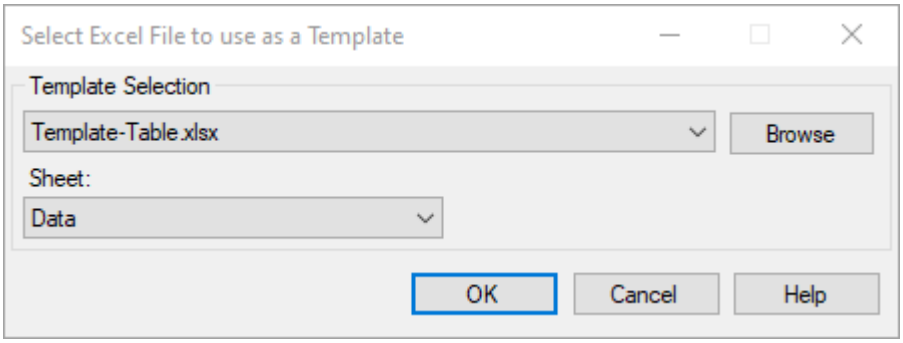
You can select one or more records (that will turn bright blue) in the data table by clicking on the buttons on the left-hand side of the grid (using the <SHIFT> and <CRTL> keys for selecting multiple records). You can perform the several actions by right-clicking on the selected record(s) in the currently displayed table, including showing/hiding fields and records, copy, paste, adding the selected station(s) to a new/existing station group, refreshing the data from the project database, and resizing the columns to fit the station list table within the current workspace.

Values in the data fields may be modified for a selected record (simply click in the cell you wish to edit); or a new record may be created here (selecting the  icon), and the values for these fields may be defined. The Non Station Data tab may be used to quickly enter or edit data for tables not directly associated with a station (i.e. a database table that does not a link to the station table as defined in the Template Manager).

Print to Excel Template

When printing a Non Station Data table to an Excel template, you will be prompted to select a template. A template called "*Template - Table.xlsx*" is provided with AquaChem. You can modify this template by going to the folder where your templates have been stored (see AquaChem Settings for more details) and adjust it to suit your needs. Perhaps you may want

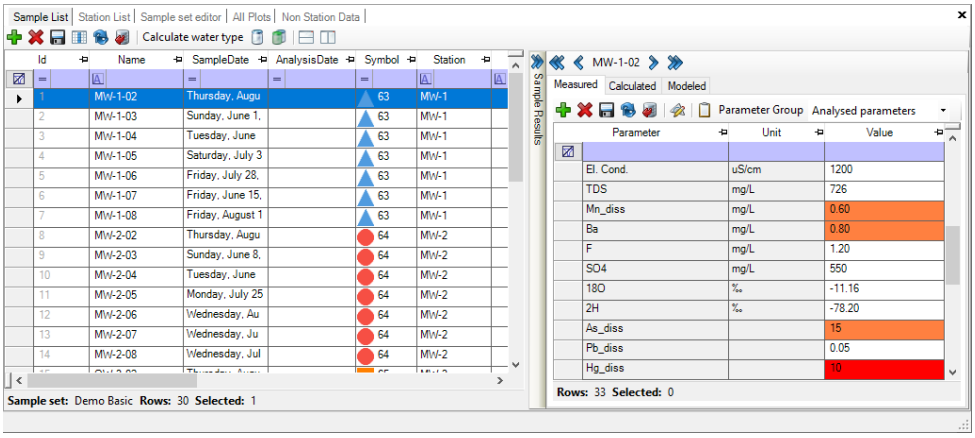
to change the logo, add titles for the project or client, etc. Templates stored in the Office/Excel Tables subfolder will be available in the drop down list under the Open Template option.



Once you have selected a template, you can select the OK button and the Excel template will open with your data in it - ready for printing or further analysis!

4.2.5 Sample List

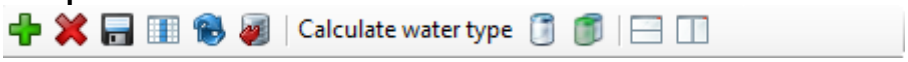
The Sample List tab provides an overview of the samples in the selected Sample Set or Station Group. This tab displays fields from the Sample table (left) and also displays results for the active sample, as denoted by the ▶ symbol in the sample table (right). Note that results with values that exceed an active Water Quality Standard will be color coded.



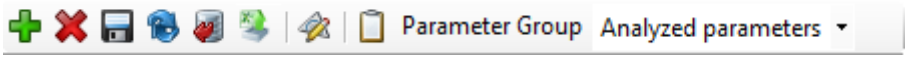
Toolbars

The Sample table and results viewer toolbars in the Sample List tab contain the following controls:

Sample Table Toolbar



Measured Sample Results Toolbar



Calculated Sample Results Toolbar

Modeled Sample Results Toolbar

 Adds a new record to the appropriate (i.e. sample or result) table.

 Deletes the currently selected record(s) from the project database.

 Saves the changes you have made to the project database.

 Allows you to select which columns you want to show or hide in the sample table.

 Refreshes the data from the project database.

 Exports the data from the applicable table.

 Calculates the water type for the selected record(s).

 Calculates the water type for all records in the sample list.

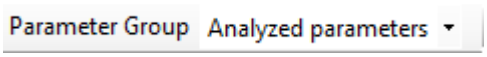
 Splits the sample table and results viewer horizontally.

 Splits the sample table and results viewer vertically.

 Exports the data from the applicable table to a selected Excel Template file.

 Provides the option to display concentration results using a single/consistent unit for all applicable parameters in the results viewer.

 Provides the option to display the active water quality standards.



Allows you to filter displayed results to the selected parameter group.

Writes the active calculated field (denoted by) to a selected numeric field in the Sample List.

Opens the calculation settings for the project.

Working with the Data

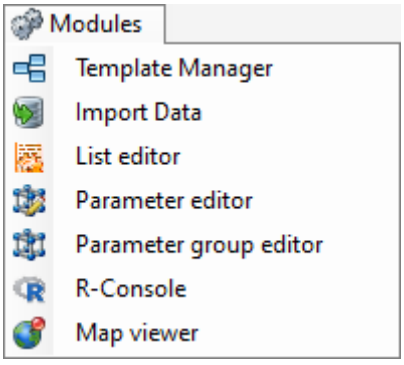
The first line shown on the sample table in the Sample List Tab contains field names/column headers; below this is the filter line, which is highlighted in light blue and denoted by the clear filter button ( ) in the left-most column. The filter line can be used to restrict records to display based on the values in one or more field and is described in detail in the Data Filtering section.

You can select one or more records (that will turn bright blue) in the data table by clicking on the buttons on the left-hand side of the grid (using the <SHIFT> and <CRTL> keys for selecting multiple records). You can perform the several actions by right-clicking on the selected record(s) in the currently displayed table, including showing/hiding fields and records, copy, paste, adding the selected station(s) to a new/existing station group, refreshing the data from the project database, and resizing the columns to fit the station list table within the current workspace.

Values in the data fields may be modified for a selected sample (simply click in the cell you wish to edit); or a new sample may be created here (selecting the icon), and the values for these fields may be defined. The Sample List tab may be used to quickly enter numerous samples and their results.

4.3 Modules

Available AquaChem modules can be found in this menu. Each module is summarized below and explained in further detail in following sections:



Template Manager

The Template Manager provides the tools to modify the AquaChem database structure, and define user-level views. The Template Manager captures the schema of the database and displays database and view settings. The following features are available:

- Adding and deleting tables/fields
- Altering the properties of each table and field defining primary keys, defining relationships between tables
- Grouping tables under logical data categories
- Defining visibility of tables and/or fields
- Defining user level table and/or field names, units, and data formats (where applicable)
- Save user templates as a new database schema structure
- Rename fields, add fields to data categories, and modify the field formats

For more details, please refer to the Template Manager section.

Import Data

AquaChem has several import options for you to import your data into the program. These include: Chemical, General, and Images. To find more information on all these options review the Importing Data section.

List Editor

The List Editor allows you to create, manage, and edit and lists for use in the Template Manager. Lists are used to define standard/accepted values for certain fields (e.g. a list for the "Watershed" field in the Station table may contain a list of all of the watersheds in your project area). The purpose of lists is generally to provide consistent and/or streamlined data entry.

Parameter Editor

The Parameter Editor module allows you to define and manage the parameters available in your project. Available functions include adding, removing, editing parameters and their attributes including names, descriptions, units, molecular formulas, and molecular weights.

Parameter Group Editor

Parameter Group Editor module allows you to define and manage groups of parameters that can be used to categorize, filter, and simplify management and analysis of your sample results data. Individual parameters may belong to more than one parameter group. For example, the parameter calcium may belong to one or more the following groups in a project: ions, cations, major ions, or EPA 200.8 (e.g the analytical method used to quantify the calcium concentration). Note that the groups Ions and Cation are automatically generated based on the valence attribute specified in the Parameter Editor.

R-Console

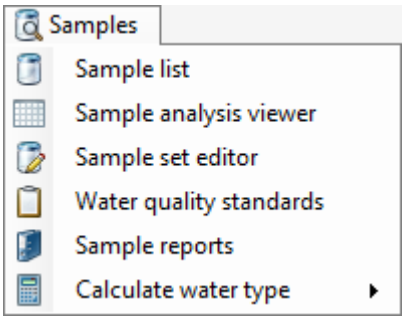
The R-Console module allows you to create, edit, run, and manage R scripts in your project. The R-Console includes an interface to build variables based on the data in your project.

Map Viewer

The Map Viewer module allows you to create, edit, and manage simple maps in your project. The Map Viewer allows you to add thematic plots of station and sample plots including categorized symbols, proportionally sized/colored symbols, Stiff diagrams, radial plots, and pie charts by location. Import and map supplemental spatial data on the map including shapefiles and basemap images.

4.4 Samples

Modules specifically related to Samples in AquaChem can be found in this menu. Each module is summarized below and explained in further detail in following sections:



 Sample List

The Sample List provides an interface for managing samples and results. The following features are available:

- Adding, deleting, and editing samples
- Adding, deleting, and editing results for the active sample
- Comparing results to active Water Quality Standards
- Creating static sample sets

For more details, please refer to the Sample List section.

 Sample Analysis Viewer

The Sample Analysis Viewer provides an interface for viewing and filtering analytical results for selected samples or for the active station or sample set. The following features are available:

- View sample results from a Sample Set, Station Group, a Selected Station or Selected Samples
- View and filter data based on one or more criteria
- Optionally view associated fields from the Station and/or Sample tables in the same record

For more details, please refer to the Sample Analysis Viewer section.

 Sample Set Editor

The Sample Set Editor provides the tools to create dynamic sample sets and station groups based on one or more user-defined conditions. The following features are available:

- Save, edit, load, and delete a sample set
- Create station groups based on the current sample set
- Define, edit, and delete sample set conditions that are based on the values of:
  - station parameters (e.g. station name)
  - sample parameters (e.g. analysis date)
  - sample results (e.g. concentration of a specified parameter)
  - sample results relative to water quality standards

For more details, please refer to the Sample Set Editor section.

 Water Quality Standards

The Water Quality Standards tab allows you to work with water quality standards in your project. The following features are available:

- Save, edit, and delete a water quality standard
- Import a Water Quality Standard from Excel or delimited text files
- Add, edit, delete water quality criteria for given parameters

For more details, please refer to the Water Quality Standards section.

 Sample Reports

The Sample Reports tab allows you to create custom tabulations of your samples and their results based on one or more criteria including: station, sample date ranges, parameters or groups, and/or exceedances of one or more active Water Quality Standards. The report can also produce general statistics for samples included in the report.

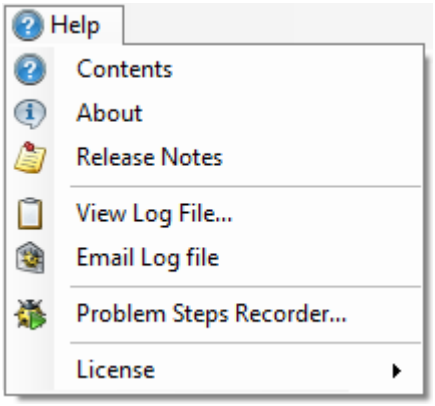
For more details, please refer to the Sample Report section.

 Calculate Water Type

The Calculate Water Type menu item allows you to determine the major ionic constituents in your sample(s) based on the results and specified parameters. For more details, please refer to the Calculate Water Type section.

4.5 Help

The Help menu contains options for learning more about AquaChem and facilitating support.



Contents

Displays either the online or in-program Help depending on the settings specified in the AquaChem Settings.

About

Displays the Info dialog. This contains the AquaChem version number, serial number, and information on how to contact Waterloo Hydrogeologic.

Release Notes

This option opens your default internet browser to display the online ReadMe file explaining the changes and additions to the program for the last several releases.

View Log File...

This opens up the AquaChem log file in the applicable text editor; usually in Notepad. This log file can be helpful for troubleshooting issues with the support team.

Email Log File

This opens a new email in your default mail client (usually Outlook) with the Log File attached, relevant system information, and addressed to our Technical Support department (support@waterloohydrogeologic.com). The log file can be helpful when trouble shooting issues with the support team.

Problem Steps Recorder

By selecting Help / Problem Steps Recorder you will initiate a Windows program you can use to record the steps you are taking within AquaChem that is causing difficulties. This can be helpful to send to Technical Support to better describe exactly the steps you are taking when you encounter a problem.

The program is very simple to use - simple select Start Record and then reproduce your steps within AquaChem. Once you have finished, click the Stop Record button and you will be prompted to save the recording as a .zip file that you can send to Technical Support.

License

Provides a link to our online help for Licensing AquaChem.

Chapter 5 Template Manager

The  Template Manager is one of the most powerful tools provided with AquaChem. It allows you to edit the structure and requirements of your database.

The Template Manager provides the tools to:

- Add or Delete tables and/or fields
- Alter the properties of tables and fields
- Define relationships between tables
- Group tables under logical data categories
- Save database templates for future projects
- Set visibility of tables and/or fields
- Define valid ranges or lists of values for fields
- Setting user level table and/or field names, display units (where applicable), and data formats (where applicable)

Understanding the Template Manager

AquaChem comes with a simplified version of our standard water quality database structure (in metric and imperial templates) that are currently in use around the world. When creating a new project, you have the option of selecting any of the provided database templates or simply selecting No Template and have only the table and fields required by AquaChem added to the project. This allows you to completely customize your project.

All database structure templates that come with AquaChem also come with their respective report templates. As such, if one of the existing database templates is selected during the project creation, these templates will be copied to your project by default. You can edit and customize them later or even remove them from your project if desired.

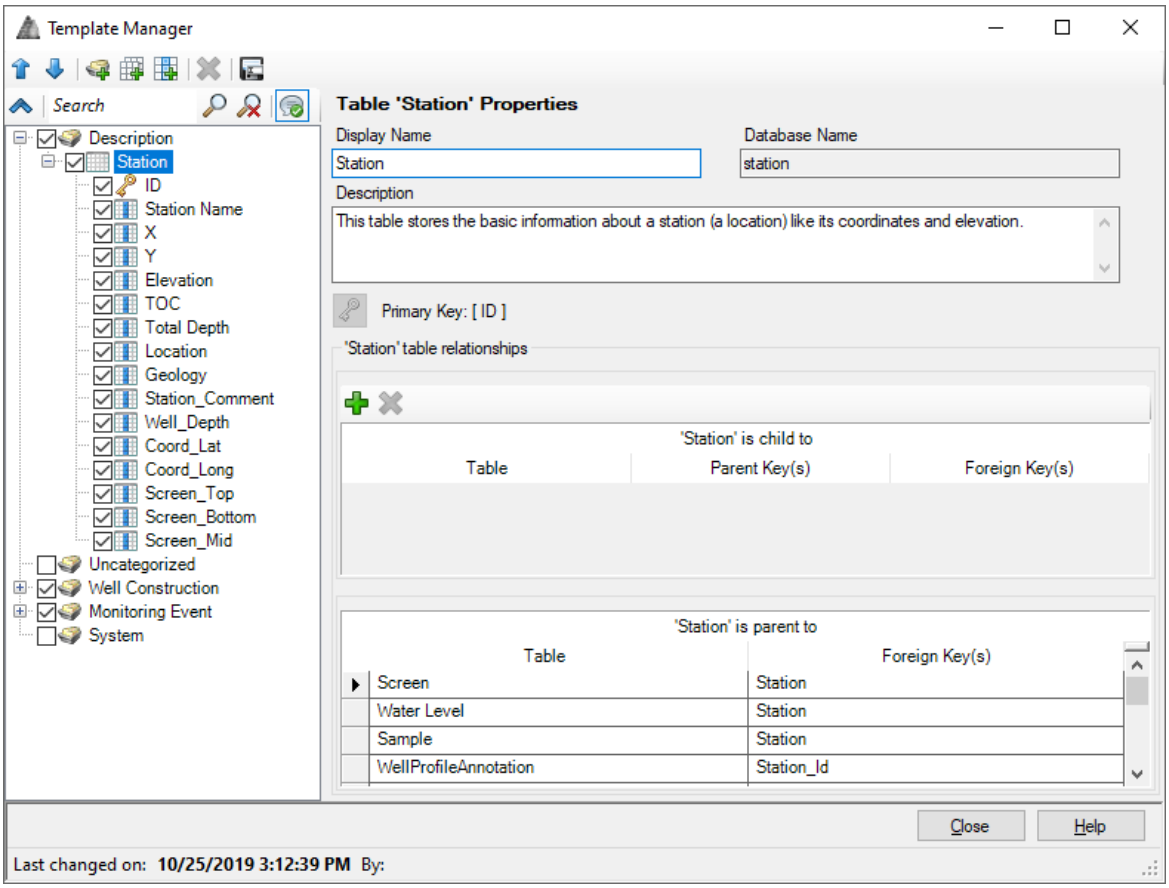
The Template Manager also allows you to modify the data views of the database. For example, you may only need to view tables that are related to geological investigation data. The Template Manager allows you to hide all unwanted tables and/or fields from applicable views and display only a smaller set of relevant tables and/or fields.

The Template Manager allows you to export the currently active database structure as a new database structure, for use in creating new similar projects.

You can launch the Template Manager from the main toolbar by selecting the  icon or by selecting **Modules** > **Template Manager** from the main menu.

5.1 Interface

On the left hand side of the Template Manager Window, you will find the tables and fields organized into categories. By selecting any item in the tree on the left hand side you will find all the properties of the item displayed to the right.



In the image above you can see the Station Table properties displayed. All the fields in this table are found by opening the Station table branch and clicking on the items that belong to it in the tree. Primary Key fields are indicated with a icon while all other fields use the icon.

Please Note: certain tables and fields are required by AquaChem - therefore you may not be able to change the Database Name of these (they will be grayed out). However, you can change the Display Name so that these tables and fields appear as you would like to see them in the main AquaChem interface.

You can adjust which tables and fields you see within the AquaChem interface by simply adjusting the visibility option (i.e. turn tables and fields on or off).

- ☐ Not visible in the main AquaChem interface
- ☑ Visible in the main AquaChem interface

To add more items to your database structure (you can add as many as you like) you need to use the following options in the tool bar:

 to add a new category
 to add a new table
 to add a new field

To adjust the order of items in your database structure you need to use the following options in the tool bar:

 moves the item (category, table or field) you currently have selected up
 moves the item (category, table or field) you currently have selected down

5.2 How to add Tables and Fields

Adding a Table to the Template

When you are ready to adjust the structure of your database and want to add a new table use the  icon.

You will find a dialog appears when you can specify the Table Name as well as the Category the table should go into.

Then you can add as many fields as need for your table by using the  icon.

Be sure to provide a name for each of your fields as well as indicate which field you would like to assign as the primary key for the table.

 **Please Note:** if you do not assign a primary key field to a table, AquaChem will add a field named *tablename_ID* and set it to the primary key, as well as making it an auto-increment field.

 **Please Note:** the auto-increment option is only available at the time of table creation (or field creation). You cannot assign this option to a field after the field has been created. Therefore, it is important for you to consider your table properties carefully before beginning to make new tables.

Take note to select the appropriate Data Type for each of your fields and specify whether or not Nulls are allowed in that field.

If you wish to set a field to be an auto-increment field its data type MUST be integer.

If you set a field to be double (think of this as a measured number) then you should also set a Unit Category and a Unit.

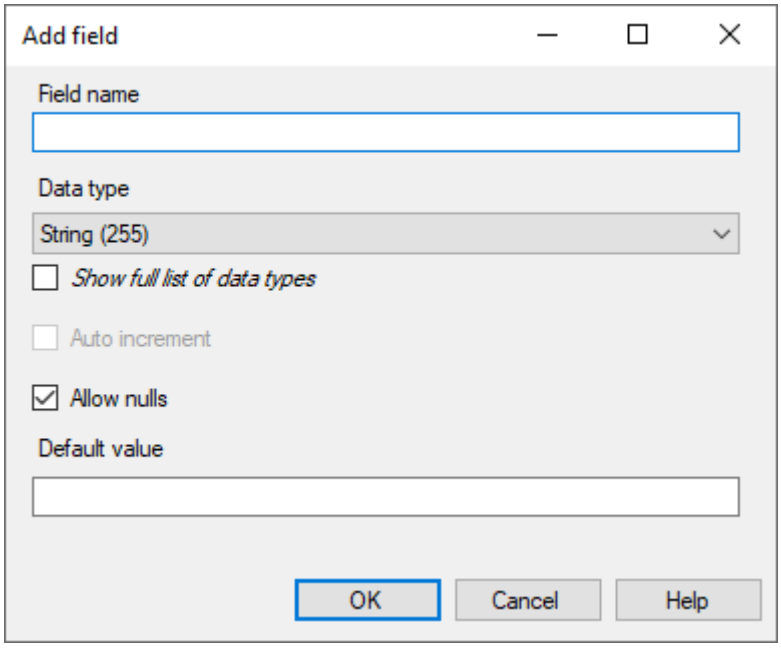
By default the table will be automatically linked to the Station table. However, you now have the option to remove this link (uncheck the Automatic link to station table option at lower left). We refer to these tables as Non Station Data tables.

Please Note: to enter data to a Non Station table manually there is a tab called Non Station Data Tab that allows for this. You can also import data to a Non Station table using the General Import options within the Data Transfer System described in the Importing Data - General section.

When you select the OK button the table will be created and you will find it in the database tree within the Template Manager.

Adding a Field to a Table

If you decide you need additional fields in the table simply select the icon and the Add Field dialog will appear.

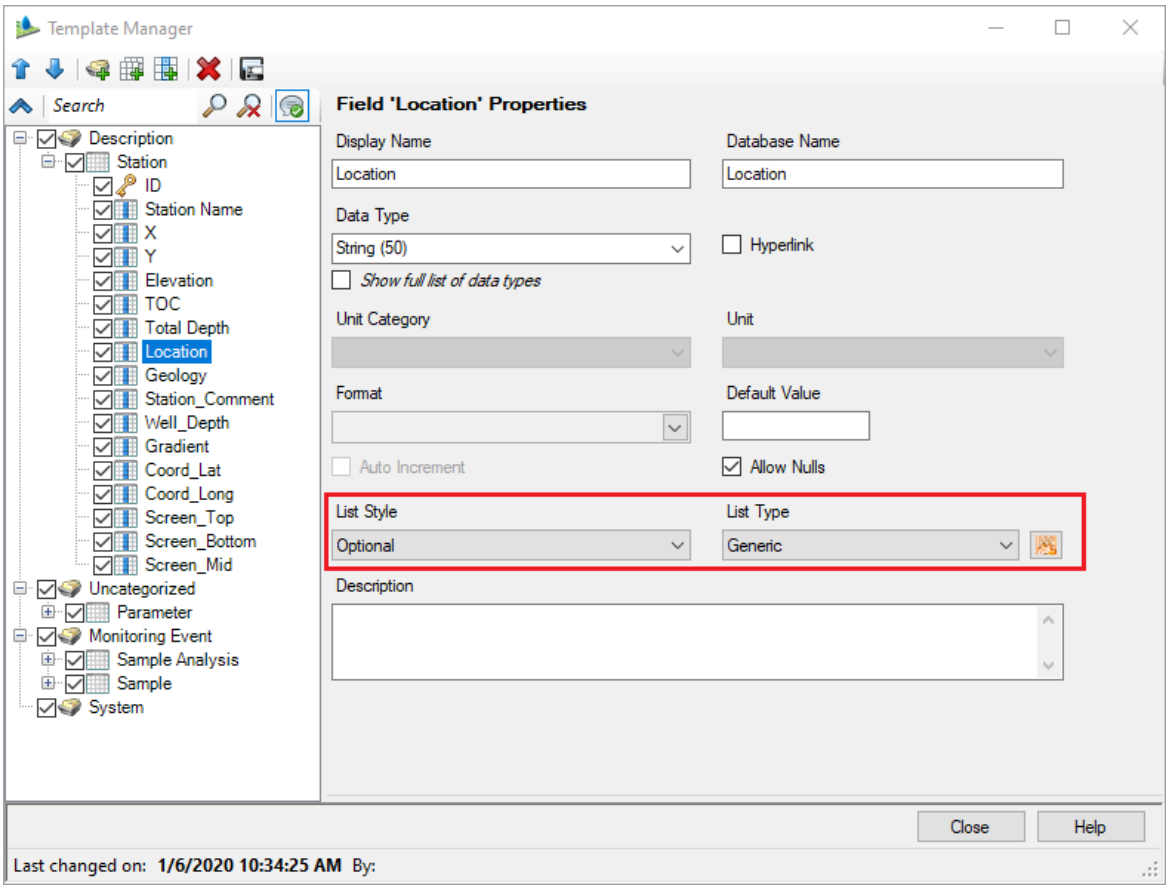


Simply provide a name for the field and select the appropriate Data Type from the drop down list. Select the OK button and the new field will be added to your table.

5.3 How to set a Field to use a List

Would you like to establish a set of valid values allowed to be entered for a field? You can do this by setting a field to use a List and then create the list within the List Editor.

When you select a field in the Template Manager you will find the option to set a List Style as well as a List Type.



You will find three options in the List Style drop down:

- **None**: there will be no list available for this field
- **Optional**: there will be a list available for this field, however you can still enter values other than item in the specified list
- **Required**: you can only enter items from the list for this field (no other values will be allowed)

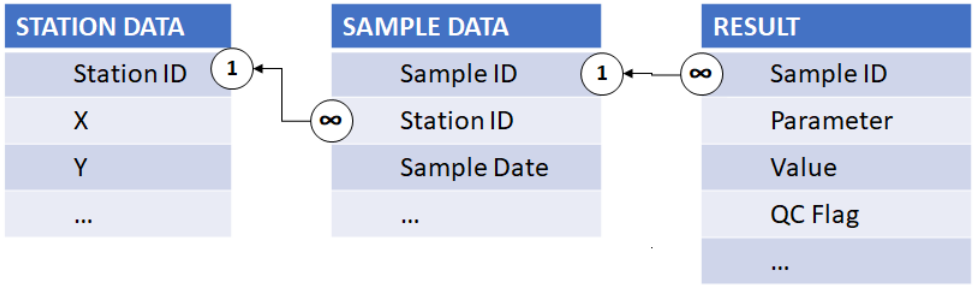
You will notice that you have one option in the List Type drop down:

- **Generic**: you will need to create a list in the List Editor (you will notice the icon appears so you can launch this module and make your list right from here). Note that a second option is available in AquaChem, which links to a custom material specification module for managing lists of soils/geologic formations.

5.4 How to Adjust Table Relationships

Tables within a database template in AquaChem can be connected to one another through a Parent-Child relationship: One table can be referred to as the Parent table and it is related to a Child table by a Foreign key.

Two of the most important examples of this in AquaChem are the defined relationships between the Station Data and the Sample Data tables and between the Sample Data and the Result Tables.



Parent Table		Child Table	
Table Name	**Primary Key Field**	**Table Name**	**Foreign Key Field**
Station Data	Station ID	Sample Data	Station ID
Sample Data	Sample ID	Result	Sample ID

In the example above, the Sample Data table, which contains information about each sample (e.g. Sample Collection Date) can also be linked to (and therefore be associated with) with the location where it was collected via the Station Data table, which contains information about the Station and its location. The way this link is established is by a foreign key. Station ID is the Primary Key in the Station Data (Parent) table and it is the Foreign Key in the Sample Data (Child) table. Similarly the Sample ID is the Primary Key in the Sample Data and is linked to information in the Result table via the Sample ID field which is the Foreign key. As indicated in the figure above, the Primary key must contain unique values (e.g. different stations cannot share the same ID), while the Foreign Key can, and often does, contain repeated values (e.g. many samples can be collected at the same station).

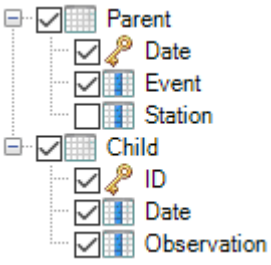
If you are adding new tables to your database you might also want to establish relationships between your new tables.

Here is an example of how you can establish a relationship between 2 tables:

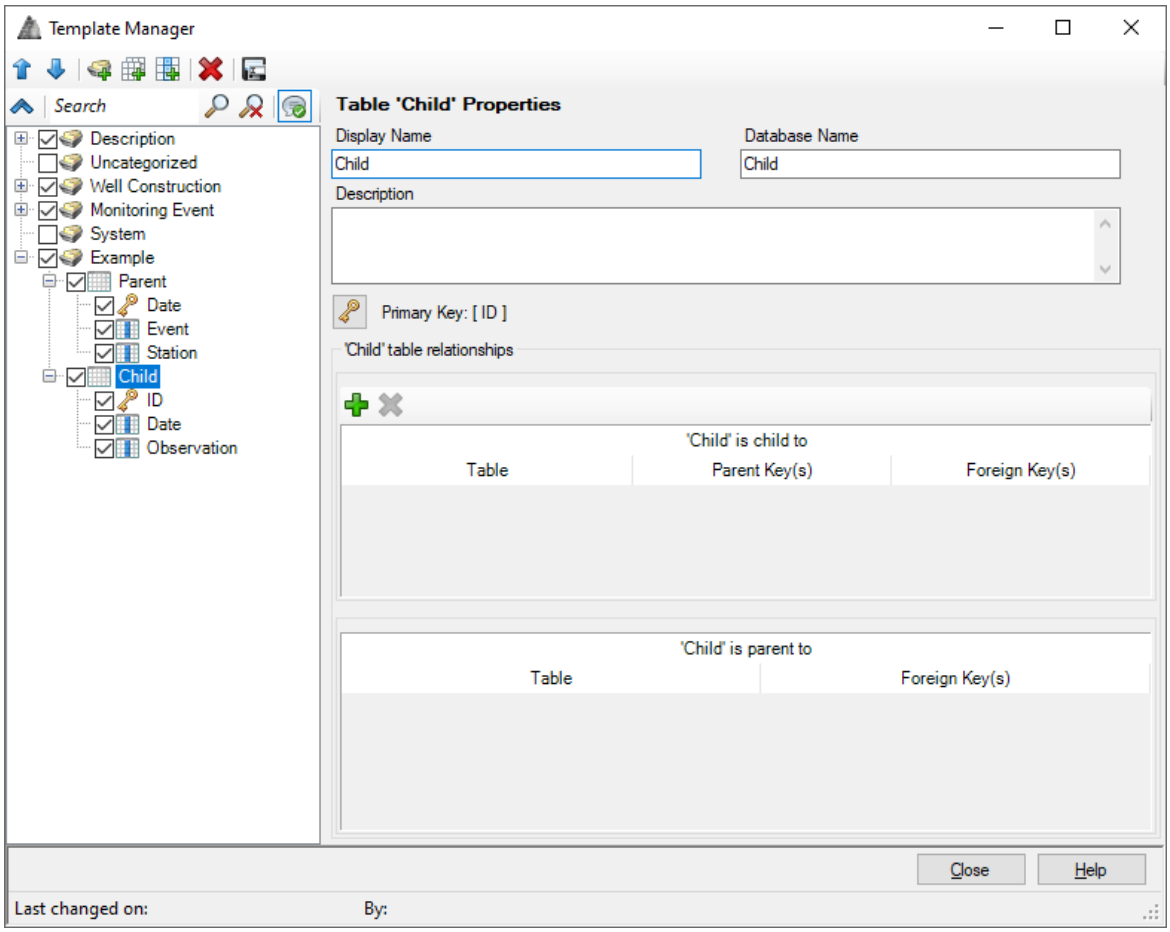
- For example, if you have created two new tables in your database - one called Parent and the other called Child

- The Parent table has a date field as the primary key as well as a field to enter the name of an event for your project. And the Child table has an auto-increment ID field as the primary key, as well as a date field (which we will use to establish the relationship back to the Parent Table) as well as a field to record an observation.

- Here is how these 2 tables would look in the Template Manager:

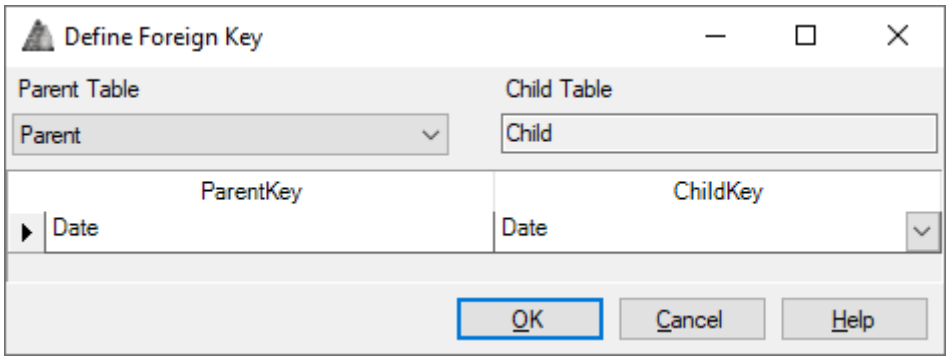


- Next, we can select the Child table to find the settings for this table which includes an option to set the relationships for the table:



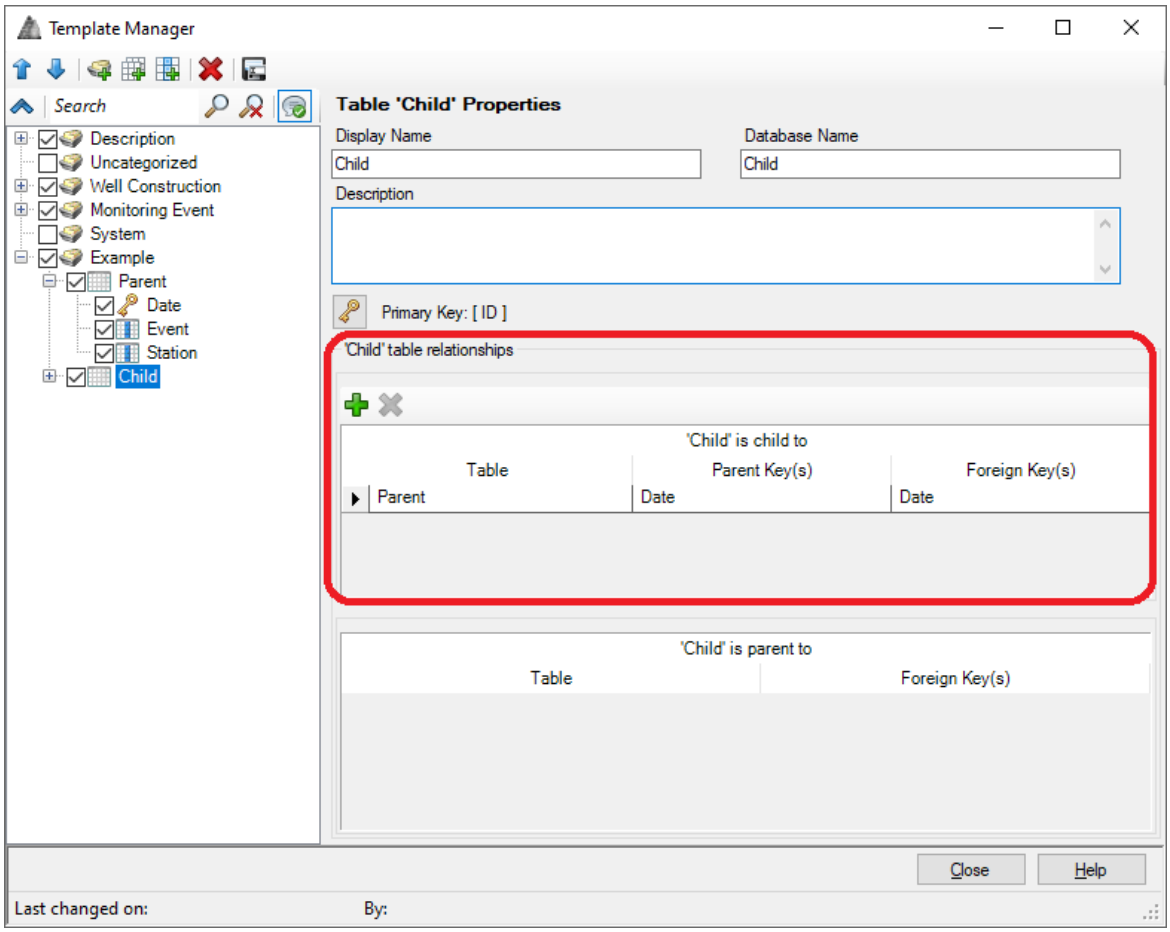
- Select the  to add a new relationship to this child table and the Define Foreign Key dialog will appear. From the drop down list select the parent table (in this example it is

called Parent). Then select the "Date" field as the ParentKey and the "Date" field as the ChildKey:



Please Note: it is common practice (although not required) to use the same name for the field in both the Parent table and the Child table; however, the fields ***must*** have the same data type.

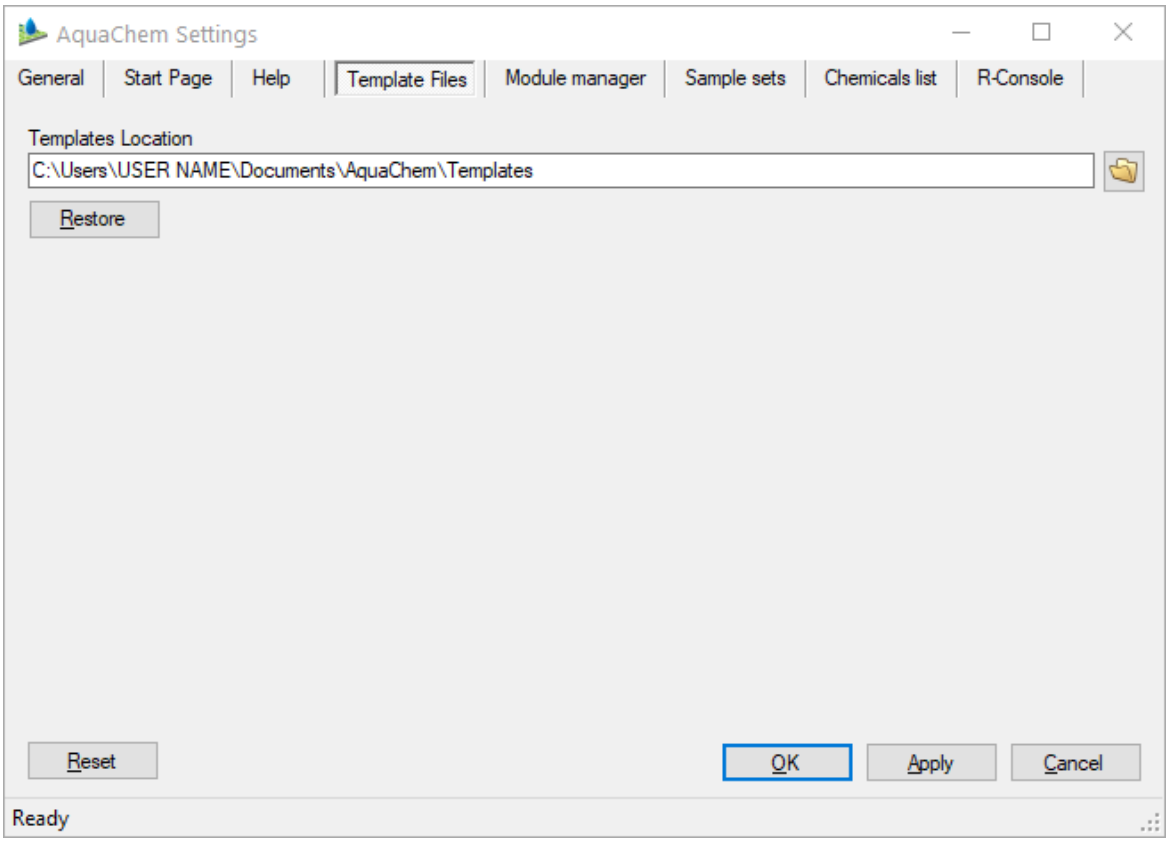
When you select the OK button and review the Child table you will see that the relationship has been established.



5.5 Managing Database Templates

If you have made many changes to the database structure as well as perhaps set up List Editor lists on fields in your database and think you might want to re-use the structure for another project you should export your project settings as a template by selecting the icon in the Template Manager.

This will save a *.hgat file where all your templates are saved as specified in your AquaChem Settings. You can find out where your templates are saved by selecting **Project** > **AquaChem Settings** from the main menu.

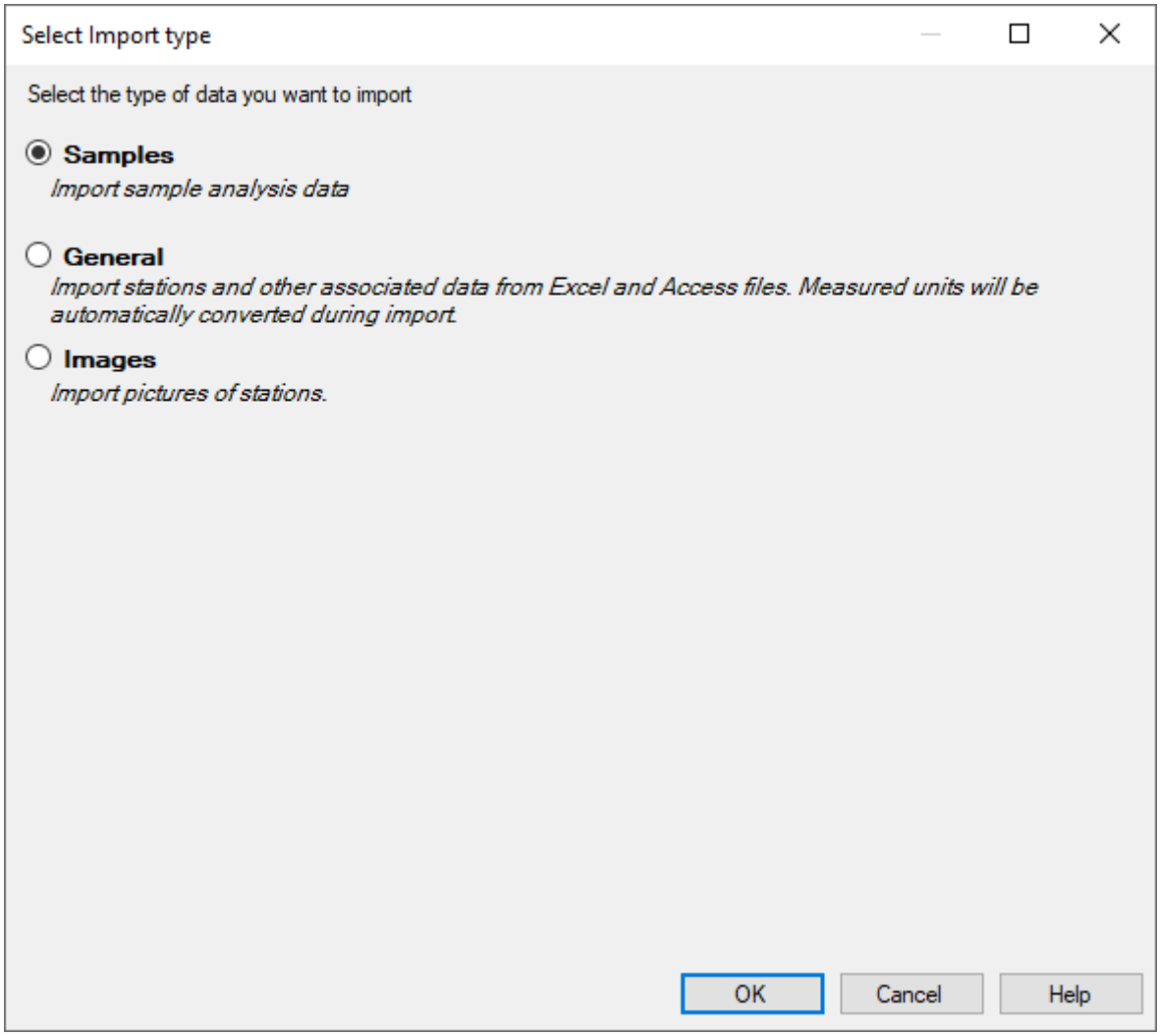


This way when you go to create a new project, you will now have the option to select your own database template (instead of just the standard ones provided with AquaChem).

Chapter 6 Import Data

The Import Data module is a flexible tool used for importing data into an AquaChem project. When starting a new project, it will likely be necessary to enter data from other sources into the AquaChem database. While you can enter data manually on the Station List Tab, Sample List tab, Station Data Tab, and/or Non Station Data Tab, it is often far more efficient to import your data.

You can launch the Import Data module by selecting Modules / Import or by selecting the  Import Data icon from the toolbar. The module will launch and give you several options for importing depending on what kind of data you wish to import.



You need to select the option you want and then select the Next button to launch the appropriate module to import your data:

- The Samples option is available if you are importing chemical results (usually received from a lab) and you need to separate out text qualifiers (i.e. the < sign) from your result value.
- The General option should be used when you are importing general tabular data.
- The Images option is available to import pictures of stations.

Please Note: When formatting your Excel source file for importing using the Samples or General import options, it is important to organize your station names so they will be recognized by the import routine. If left unspecified, Excel will assume the data type format based on the first 8 rows of each column; therefore, if you have some station names that are completely numeric at the top of the file to be imported, the import options may have difficulty recognizing them as names (Data Type String). To avoid this, you will need to ensure that you manually assign the data type within Excel as Text. To do this:

- right-click on the cells (or their column) and select Format Cells...
- Selecting the Text option in the Number tab dialog that appears.

You will notice that your numeric station names are now left justified in the Excel column. Similarly, if you have completely numeric Sample ID's you will need to do the same for this column. In fact any field in the AquaChem database that is set to have a data type "String" you will need to do this in order to be able to import completely numeric values.

6.1 Samples

The Samples method for importing is specifically designed to facilitate importing external data sources of sample and related sample result data into the data structure of AquaChem for sample and result data. The Samples import process consists of seven steps:

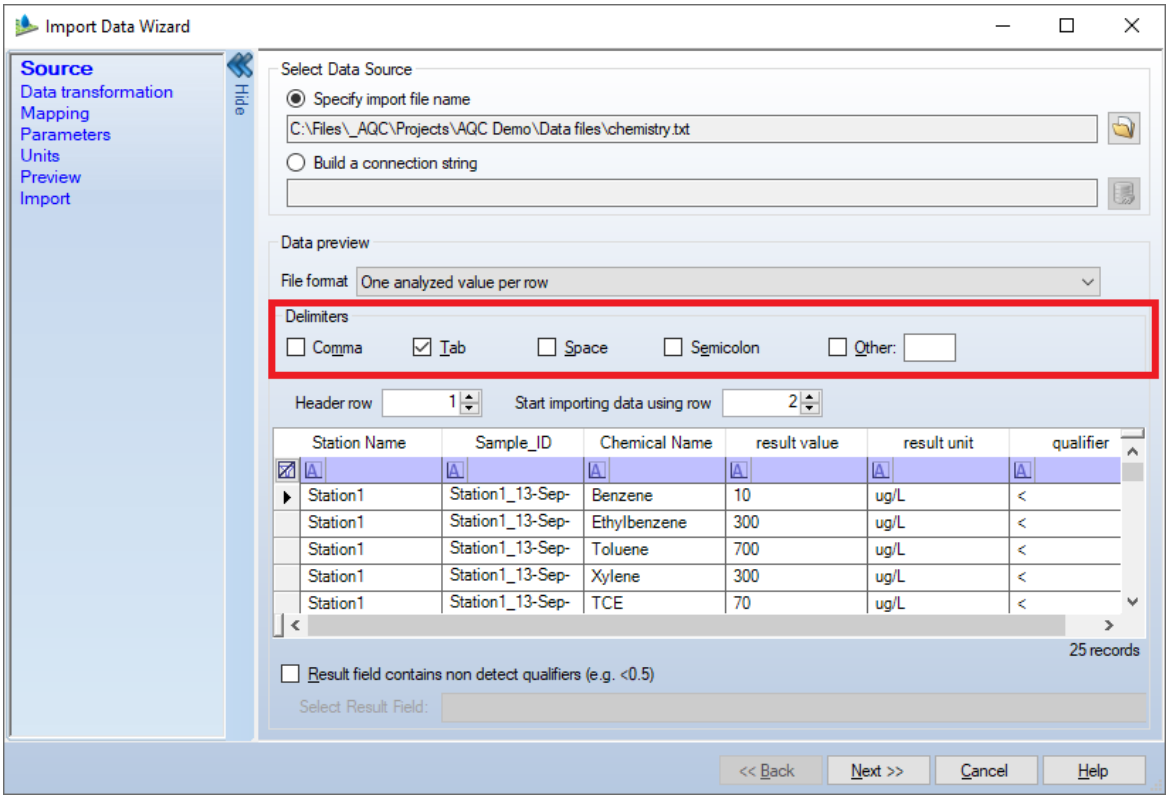
- Source
- Data Transformation
- Mapping
- Parameters
- Units
- Preview
- Import

Each of these steps is described in the sections below.

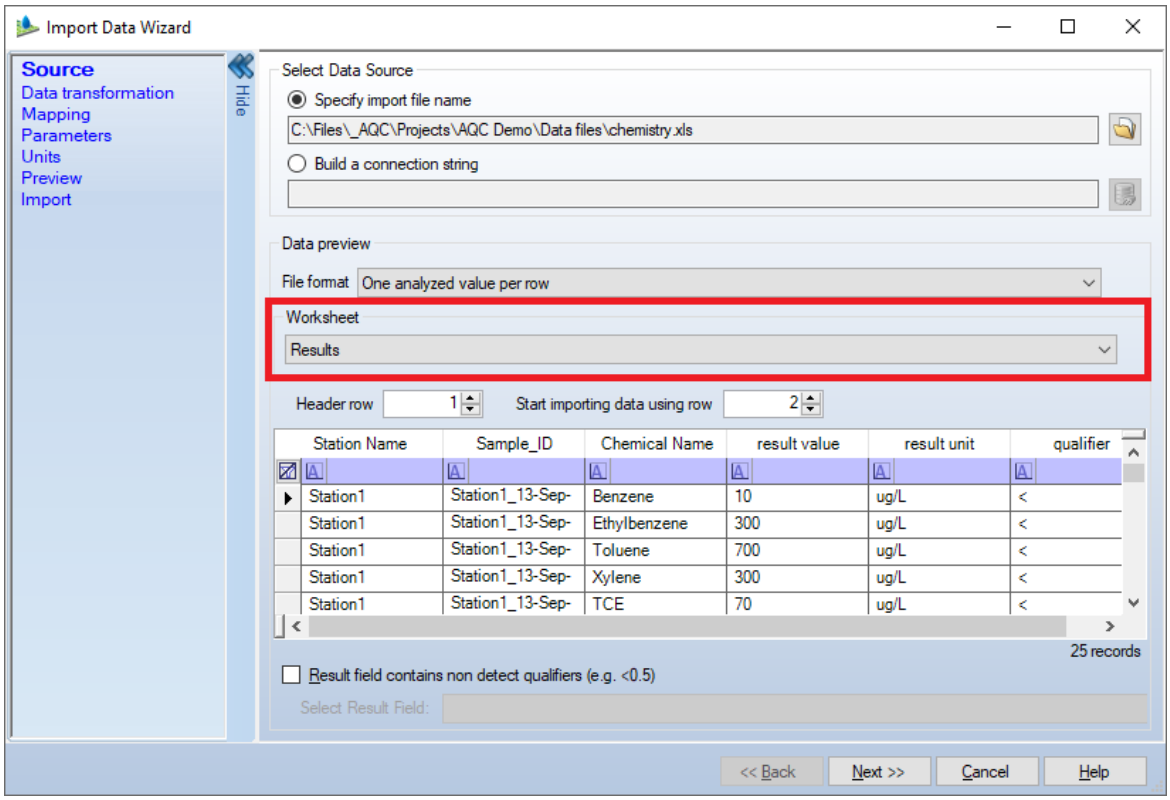
Step 1: Source Selection

The first step in the general import process begins with selecting the file you wish to import and supports the following file formats:

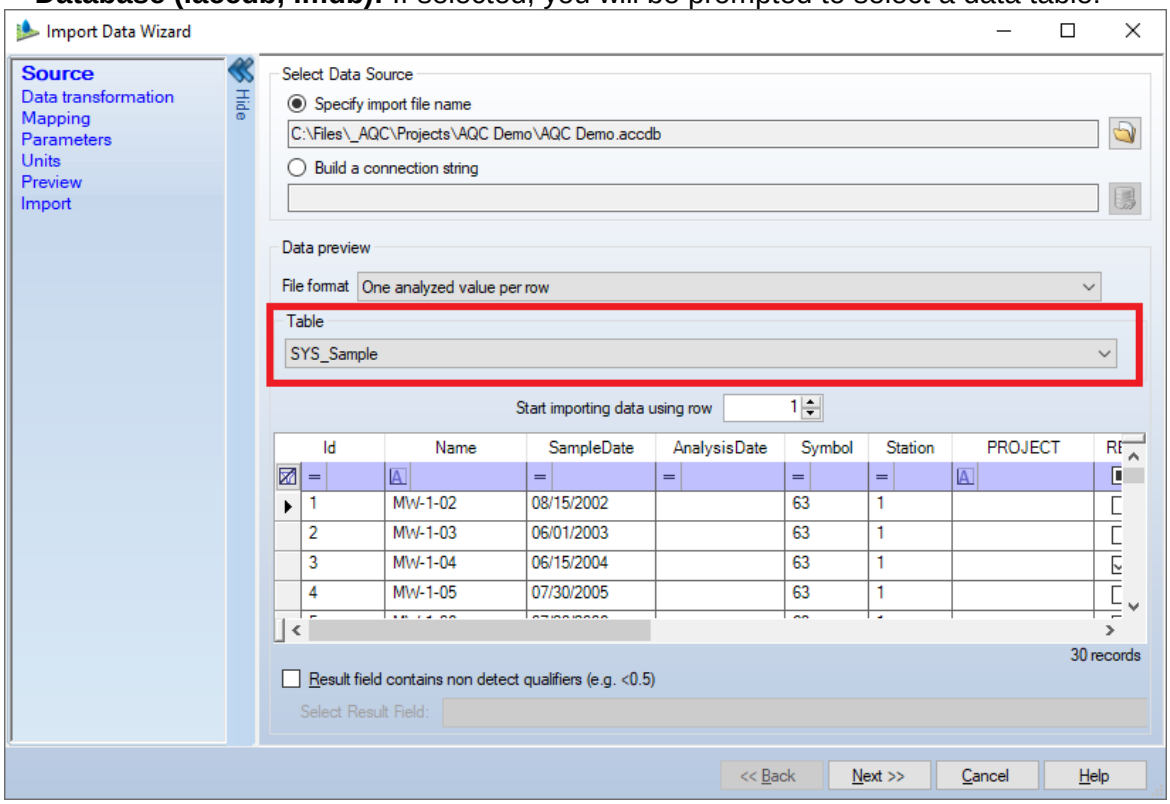
- **Delimited Text (.txt, .csv):** If selected, you will be prompted to select one or more delimiters:



- **Spreadsheet (.xlsx, .xlsx):** If selected, you will be prompted to select a worksheet or named range:



- **Database (.accdb, .mdb):** If selected, you will be prompted to select a data table:



File Formats

As part of the Samples import process, you may select one of two file formats:

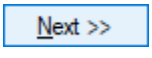
- **One analyzed value per row:** data are organized in a formal data table with a unique sample parameter value in each row/record in the source file:

Station Name	Sample_ID	Chemical Name	result value	result unit	qualifier
Station1	Station1_13-Sep-14	Benzene	10	ug/L	<
Station1	Station1_13-Sep-14	Ethylbenzene	300	ug/L	<
Station1	Station1_13-Sep-14	Toluene	700	ug/L	<
Station1	Station1_13-Sep-14	Xylene	300	ug/L	<
Station1	Station1_13-Sep-14	TCE	70	ug/L	<
Station2	Station2_13-Sep-14	Benzene	25	ug/L	
Station2	Station2_13-Sep-14	Ethylbenzene	598	ug/L	
Station2	Station2_13-Sep-14	Toluene	724	ug/L	
Station2	Station2_13-Sep-14	Xylene	451	ug/L	
Station2	Station2_13-Sep-14	TCE	77	ug/L	
Station3	Station3_13-Sep-14	Benzene	31	ug/L	
Station3	Station3_13-Sep-14	Ethylbenzene	1100	ug/L	
Station3	Station3_13-Sep-14	Toluene	1200	ug/L	
Station3	Station3_13-Sep-14	Xylene	625	ug/L	
Station3	Station3_13-Sep-14	TCE	125	ug/L	

- **Values in rows or columns:** data are organized in a pivoted table format with multiple parameter values for the same sample in each row/record in the source file:

Station	Sample	Units	Ca	Mg	Na	K	Cl	SO4	CO3	HCO3
MW-5	MW-5-1	meq/L	0.045	0.0025	0.0025	0.0025	0.005	0.0025	0	0.09
MW-5	MW-5-2	meq/L	0.0025	0.045	0.0025	0.0025	0.005	0.0025	0	0.09
MW-5	MW-5-3	meq/L	0.0025	0.0025	0.0875	0.0025	0.005	0.0025	0	0.09
MW-5	MW-5-4	meq/L	0.045	0.0025	0.0025	0.0025	0.005	0.045	0	0.005
MW-5	MW-5-5	meq/L	0.0025	0.045	0.0025	0.0025	0.005	0.045	0	0.005
MW-5	MW-5-6	meq/L	0.0025	0.0025	0.0875	0.0025	0.005	0.045	0	0.005
MW-5	MW-5-7	meq/L	0.045	0.0025	0.0025	0.0025	0.09	0.0025	0	0.005
MW-5	MW-5-8	meq/L	0.0025	0.045	0.0025	0.0025	0.09	0.0025	0	0.005
MW-5	MW-5-9	meq/L	0.0025	0.0025	0.0875	0.0025	0.09	0.0025	0	0.005
MW-6	MW-6-1	meq/L	0.04	0.005	0.005	0.005	0.01	0.005	0	0.08
MW-6	MW-6-2	meq/L	0.005	0.04	0.005	0.005	0.01	0.005	0	0.08
MW-6	MW-6-3	meq/L	0.005	0.005	0.075	0.005	0.01	0.005	0	0.08

Below the source-specific controls, you may select a starting data row and, in the case of text or spreadsheet files, a header row. A preview of the data is provided in the lower portion of the Source import step. Here you may preview the data and rename field headers if desired. There is also an option to select a result value field and parse it if it contains non-detect qualifiers.

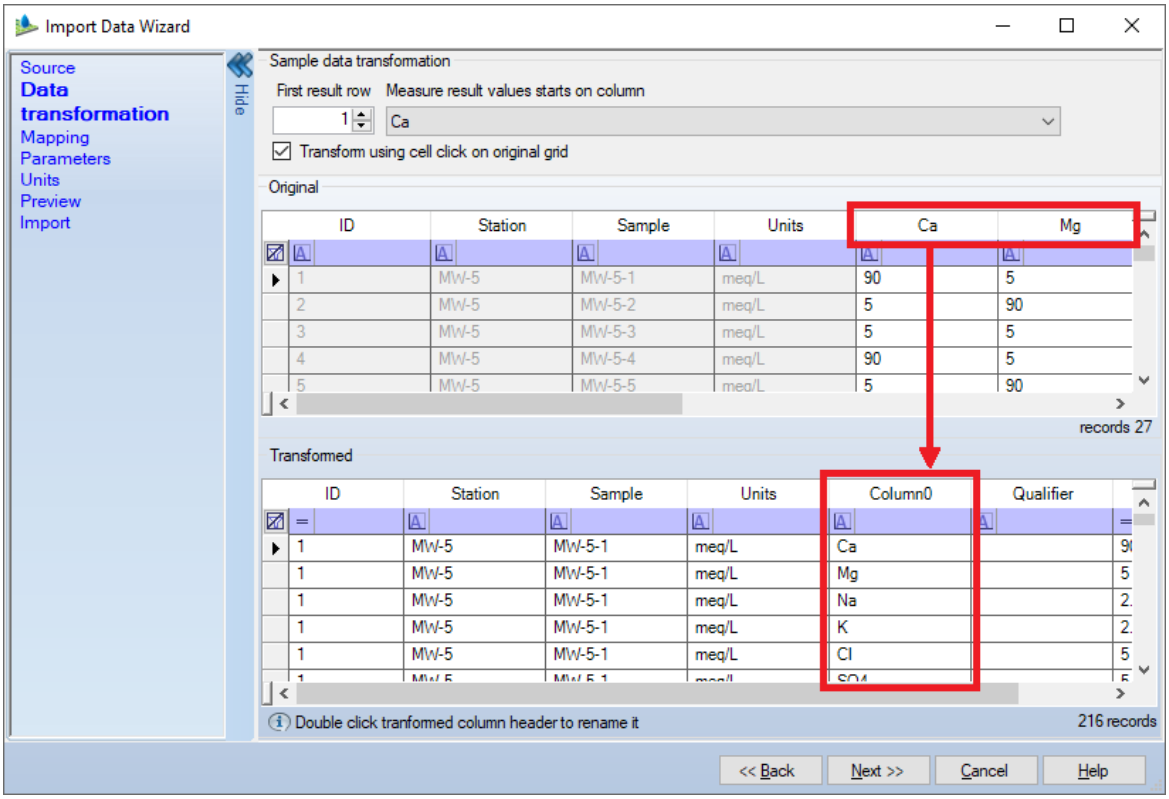
Once you have selected a data file and corresponding source options, select 

to proceed with the import. If the "values in rows or columns" option is selected, you will be

guided through some additional steps to transform the data at Step 2; otherwise, you can skip a step and proceed to the Step 3 (Mapping).

Step 2: Data Transformation

The step allows you to convert the samples as rows or columns file format into the one analyzed value per row format. To perform the transformation, select the anchor cell to pivot the data around either by using the row and column options, or by clicking in the corresponding cell in the Original data pane.

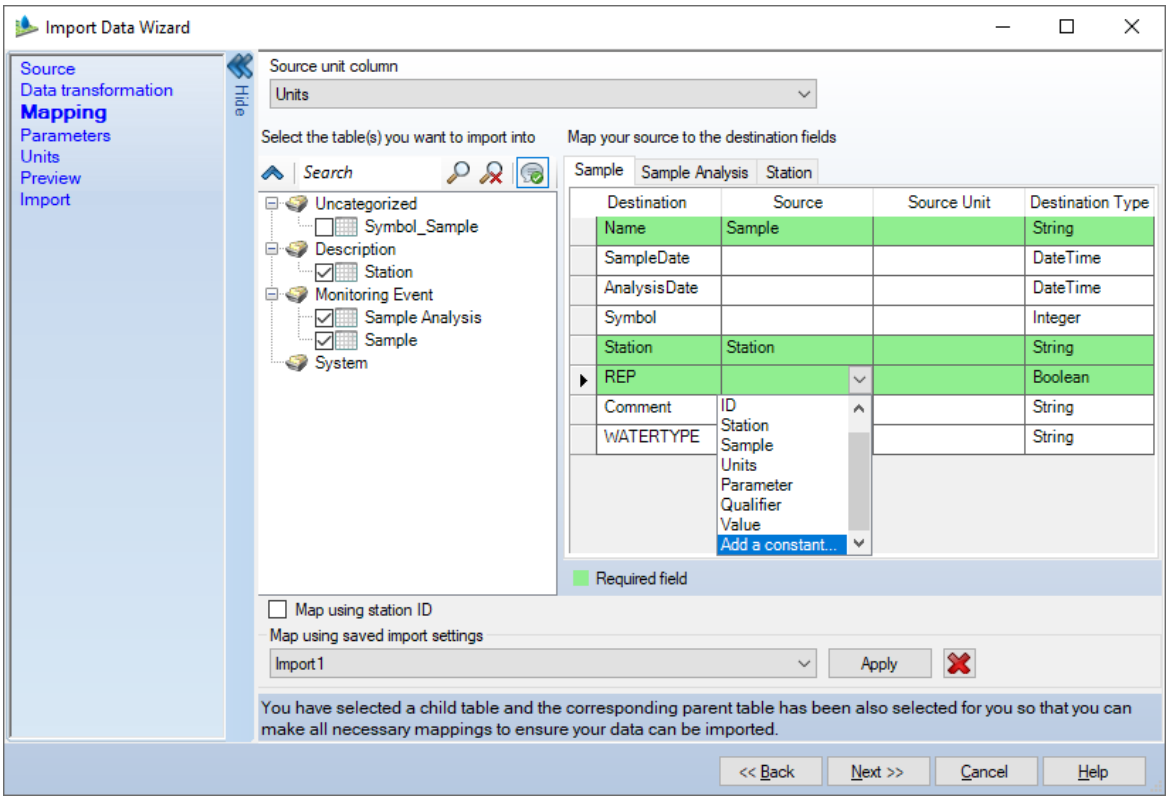


Once you have selected the anchor cell, the Transformed data pane will be populated with the transformed data. Note that one or more new column(s) will be added to the field corresponding to the column header row(s). This includes parameter names and may include parameter measurement units. The column header(s) will be automatically assigned a sequential name starting with "Column0". You may rename the column header by double-clicking a header to facilitate the Mapping step. Value and qualifier fields will also be added with transformed data.

Step 3: Field Mapping

At the Mapping step, the Sample and Sample Analysis tables will be automatically selected. You may select additional destination tables and corresponding data fields into which you

wish to import the source data. The destination tables are selected using the categorized data table tree. For example, you may wish to select the Station table to import station data while importing samples:



Once the destination tables have been selected, as shown above, a tab will be added for each table. The currently selected tab will information about importing the data for the destination table in the following four columns:

- **Destination:** The data fields in the destination table.
- **Source:** corresponding fields from the source data file.
- **Source Unit:** measurement unit from the source data file.
- **Destination Type:** the data type of the destination field.

Required fields will be highlighted green. In the case of the Samples table, the Sample name and Station Name field are always required. You may toggle the requirement of fields using the Template Manager. Boolean fields (e.g. the REP field in the example above) are also required.

As part of the Mapping step, you must select data fields from the source data file that was selected during the Source step in the Source column. If the headers in the source file match the name of the destination field in the AquaChem database - they will map automatically. If the headers do not match, you may click in the unmapped Source column and a dropdown will appear allowing you to select a source field, as shown for the REP field above. Included in the dropdown is the option to add a constant value rather than a field. In the case above, we will select "Add a constant..." and enter a value of FALSE.

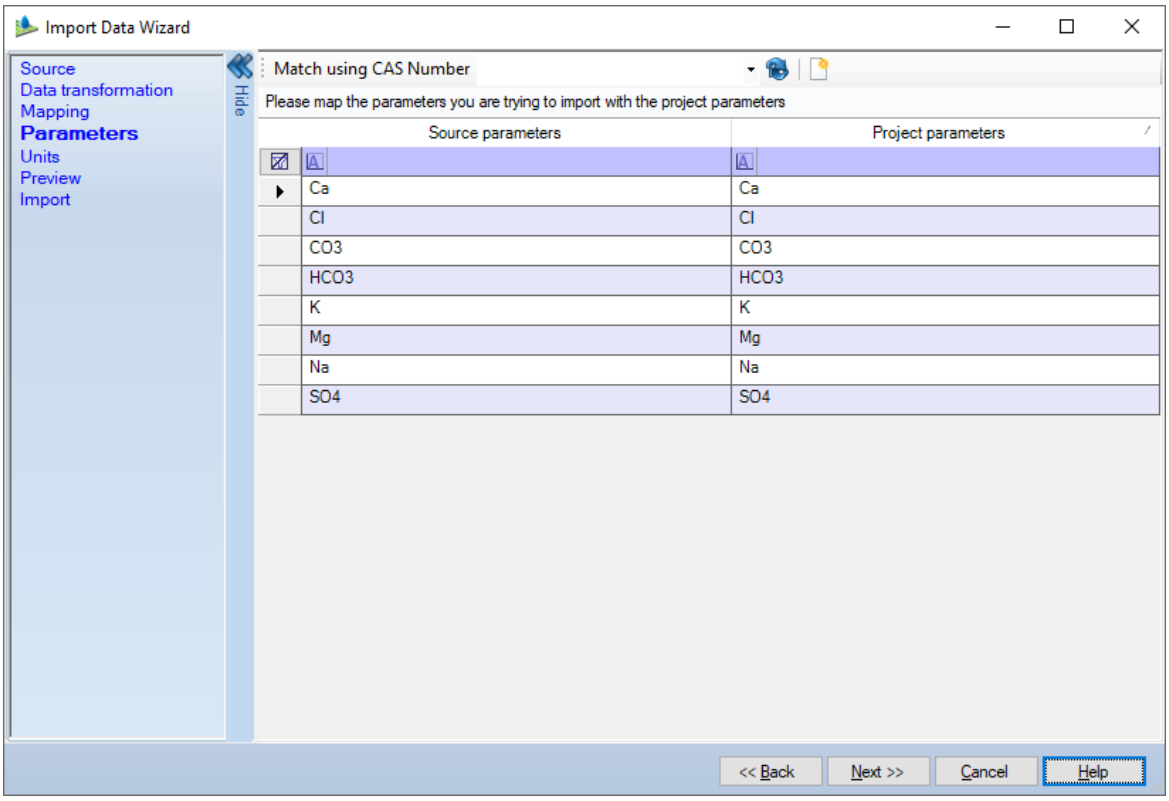
You must select a Unit field associated with the Sample Results table (e.g. the units apply to the value and method detection limit fields) as part of the Import process using the source unit dropdown at the top of the form. For all other destination fields that are numeric, you must select a measurement unit for the source data in the "Source Unit" column; available source units will be of the same unit category as units of the Destination field, which are displayed in brackets in the Destination column. If the selected source units do not match the destination units, then the values will be converted into the destination units. If the units match, then the values will be imported without conversion.

If you have previously imported data using the same source formats (i.e. same tables, fields, and units) and have saved the import data mappings at the Import step, you may select the settings from the "Map using saved import settings" dropdown and click the Apply button to recall and use these previous mappings.

Select the Next >> button to proceed to the next step - Parameters.

Step 4: Map Parameters

At this step, you will map parameters from the source data to the destination data. Source parameters matching exactly with parameters already present in your AquaChem project will be mapped automatically:



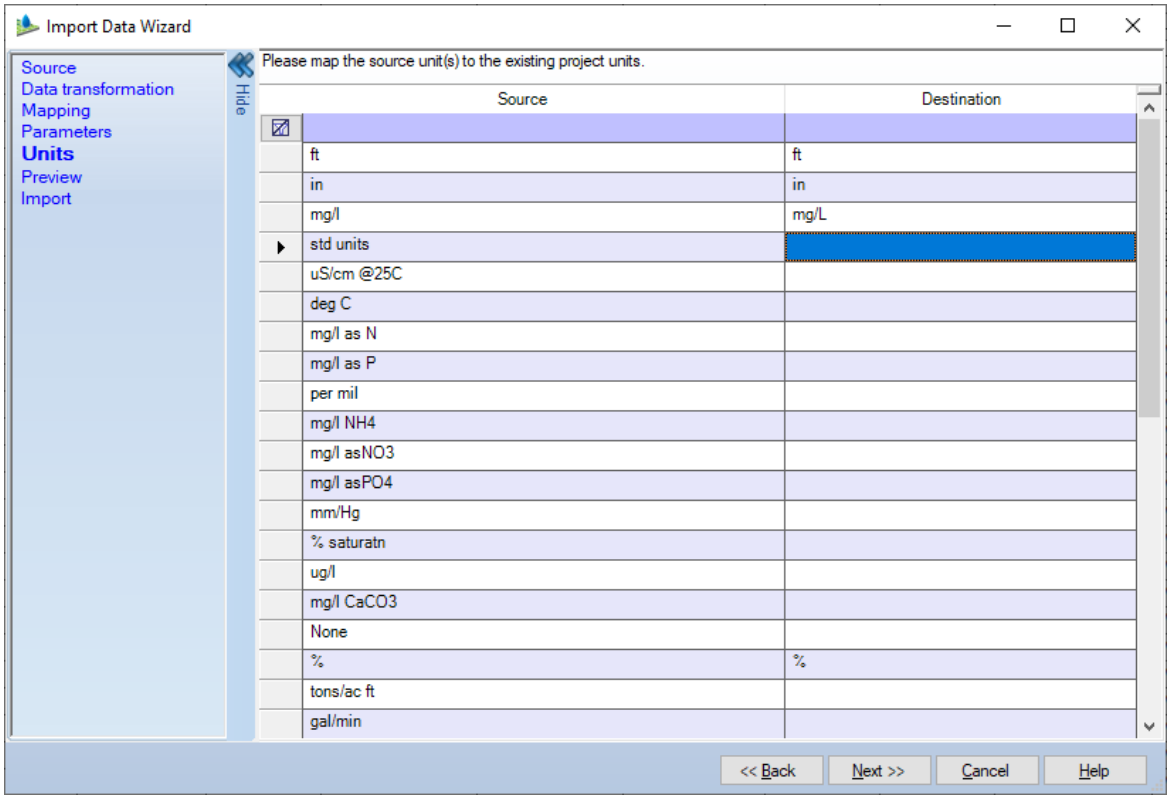
For unmapped parameters, there are three options to complete the parameter mapping:

- **Manual:** click in the Project Parameters column of an unmapped parameter and use the Parameter Picker to select an existing parameter or create a new parameter.
- **CAS Number**: if your project and import source parameters both include Chemical Abstract Service (CAS) Number, you can map the parameters using matched values. Simply select a CAS number field from the source data and click the refresh button ( ).
- **Create Stubs:** select this option to create new parameters with minimal information using the source parameter name. You can complete the parameter information at a later time using the Parameter Editor.

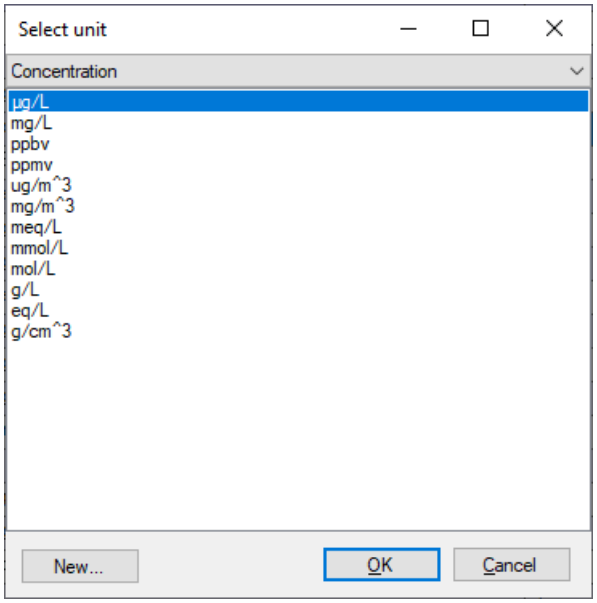
Once all the source parameters have been mapped select the Next >> button to proceed to the next step - Units.

Step 5: Select Units

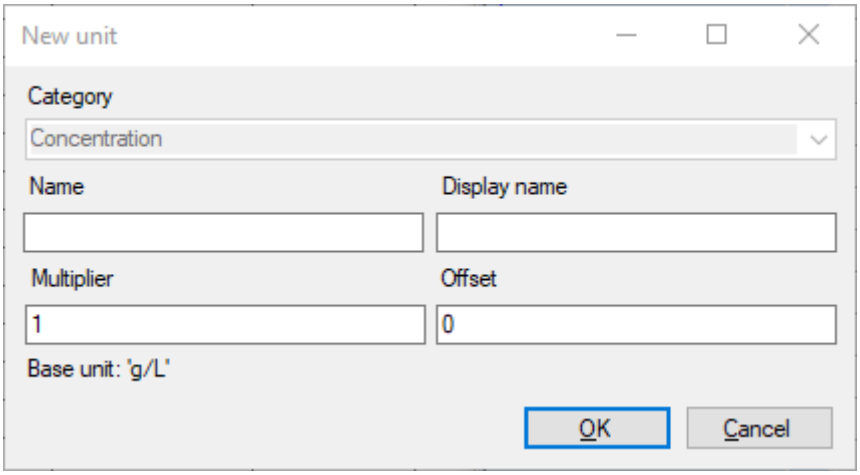
At this step, you will map measurement units from the import data source to the project units. Source units matching exactly with units already present in your AquaChem project will be mapped automatically:



Unmapped units must be selected using the unit picker. Units are grouped into categories, which can be selected using the dropdown at the top of the picker:



If the source unit is not present in the unit picker, you may click the New... button to add a new measurement unit for the selected category:



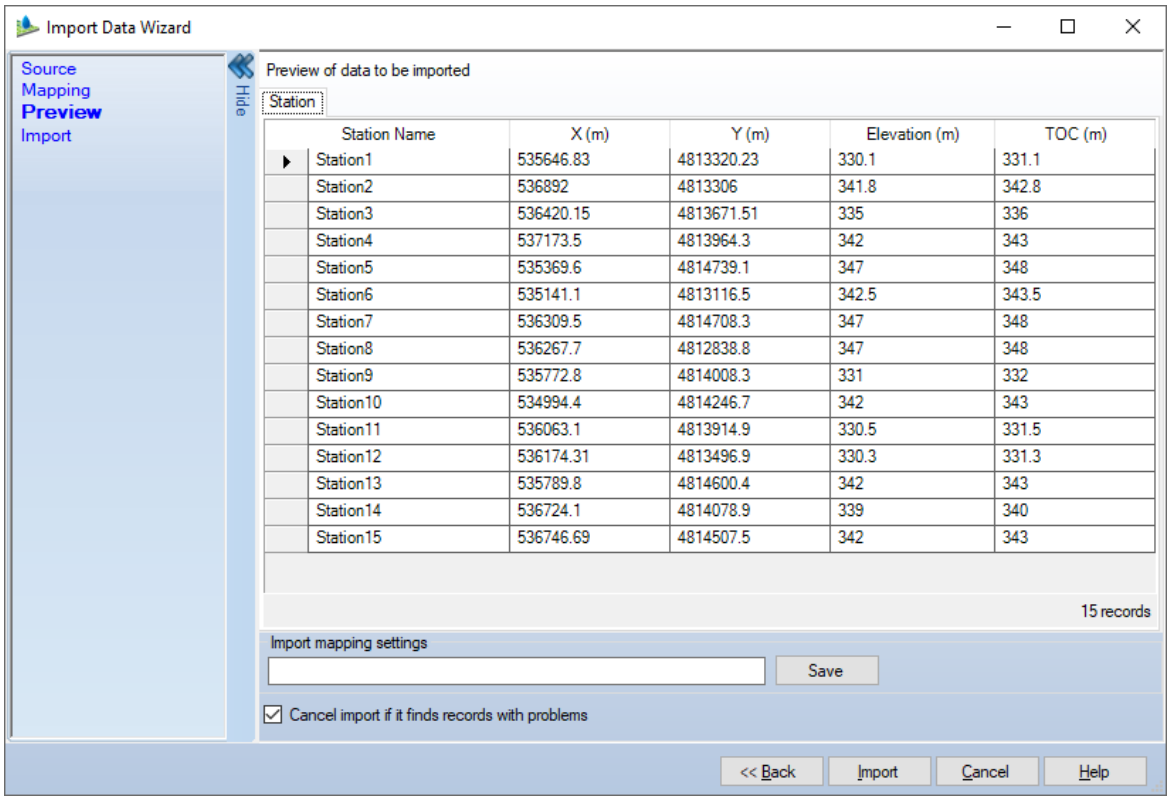
The new unit must include a Name, a display name for use in labels, and a multiplier and offset relative to the listed base unit. For example if the new unit is mg/L and the base unit is g/L, then the multiplier would be 0.001.

Select the Next >> button to proceed to the next step - Preview.

Step 6: Preview the Import

At this step, you may preview the data to be imported. You also have the options to:

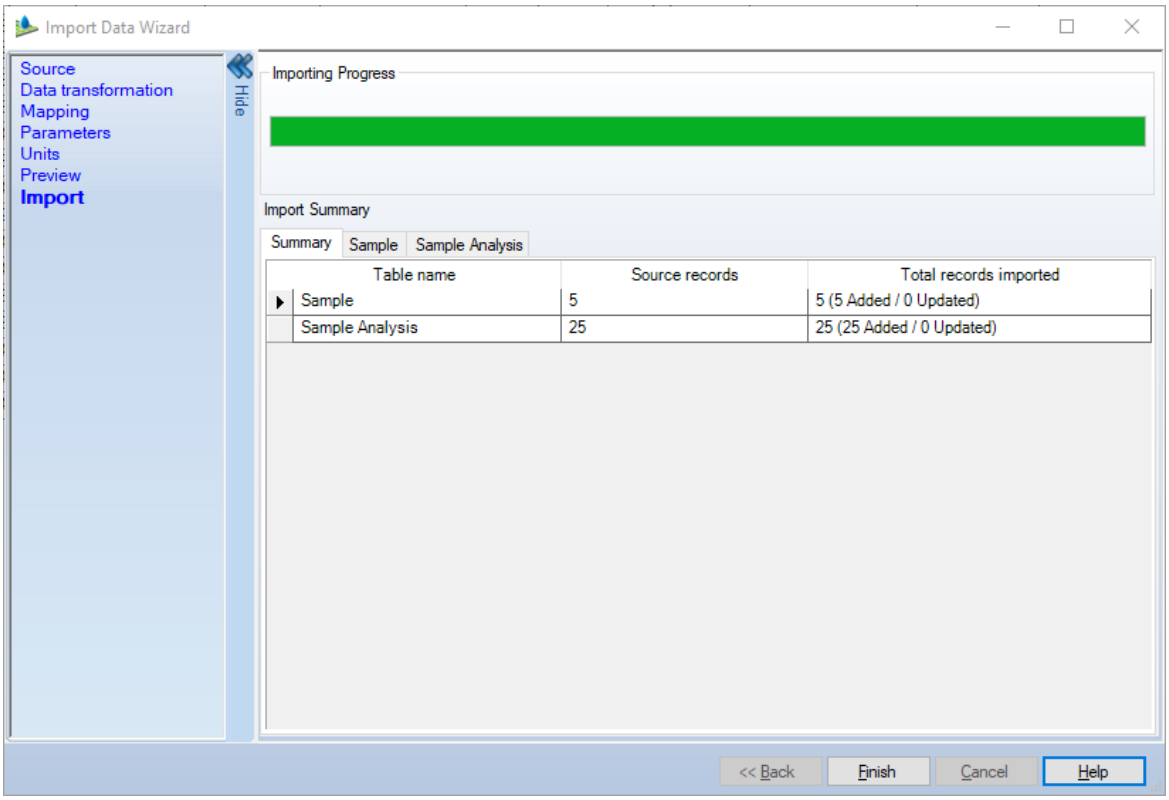
- save the import settings
- cancel the import if it finds records with problems



Select the Next >> button to proceed to the next step - Import.

Step 7: Data Import

Once this step is reached, you can watch the progress of your import. When it is completed, it will summarize how many records were in the source file and how many were imported to each table in the database.



If problems with the import data were detected during the import process, errors and/or warning will be displayed along with available options to fix them. Example issues may include:

- source data type that does not match the destination data type,
- duplicate records within the source data, and
- duplicate records between the source and destination data.

If you are satisfied with the import summary, select the Finish button to finalize the import and close the wizard. Your data will be available for review in the Destination table. Alternatively, you may return to a previous step using the << Back button or abandon the import process by using the Cancel button.

6.2 General

The General import option imports information from a tabular input source directly into one or more tables. The General import process consists of four steps:

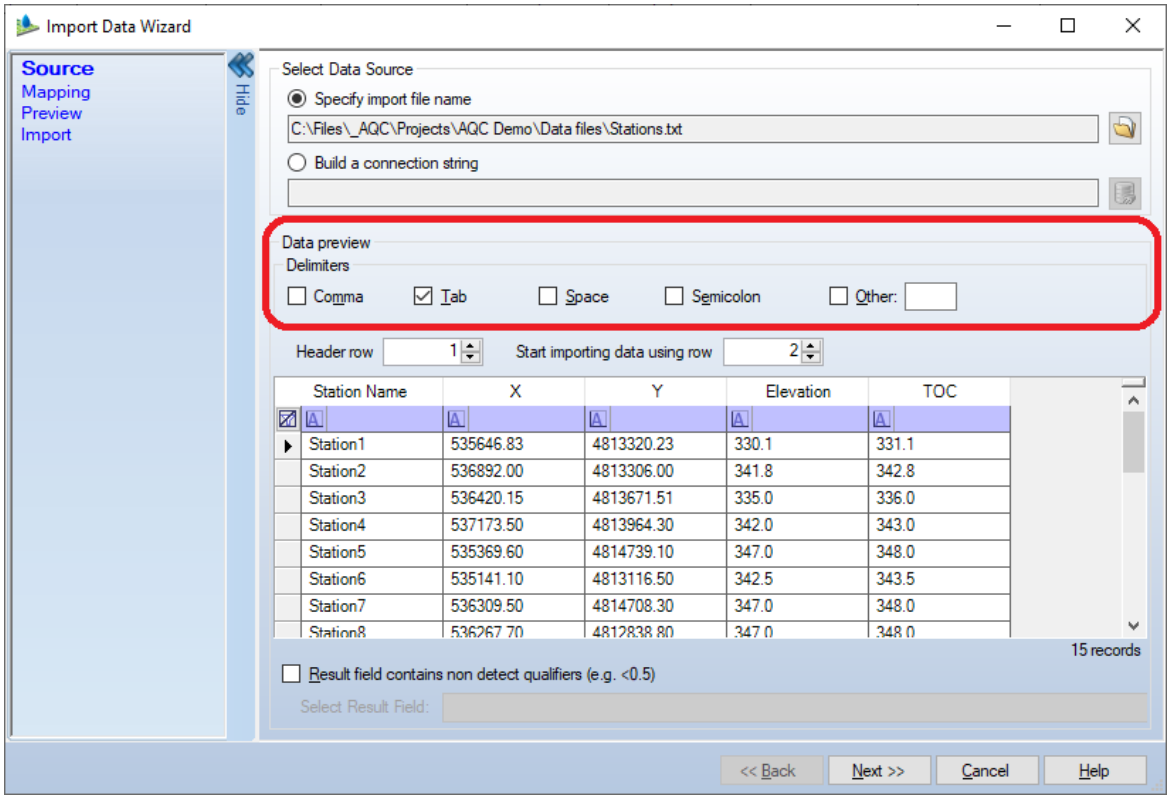
- Source
- Mapping
- Preview
- Import

Each of these steps is described in the sections below.

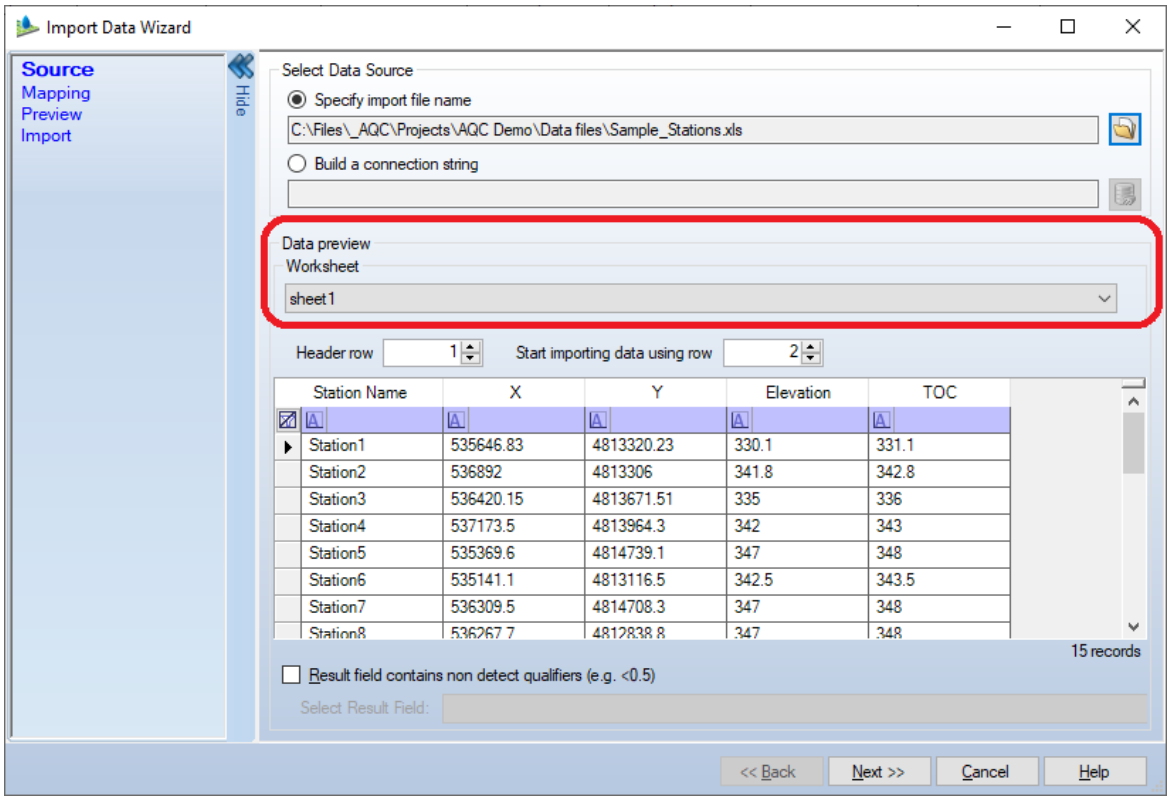
Step 1: Source Selection

The first step in the general import process begins with selecting the file you wish to import and supports the following file formats:

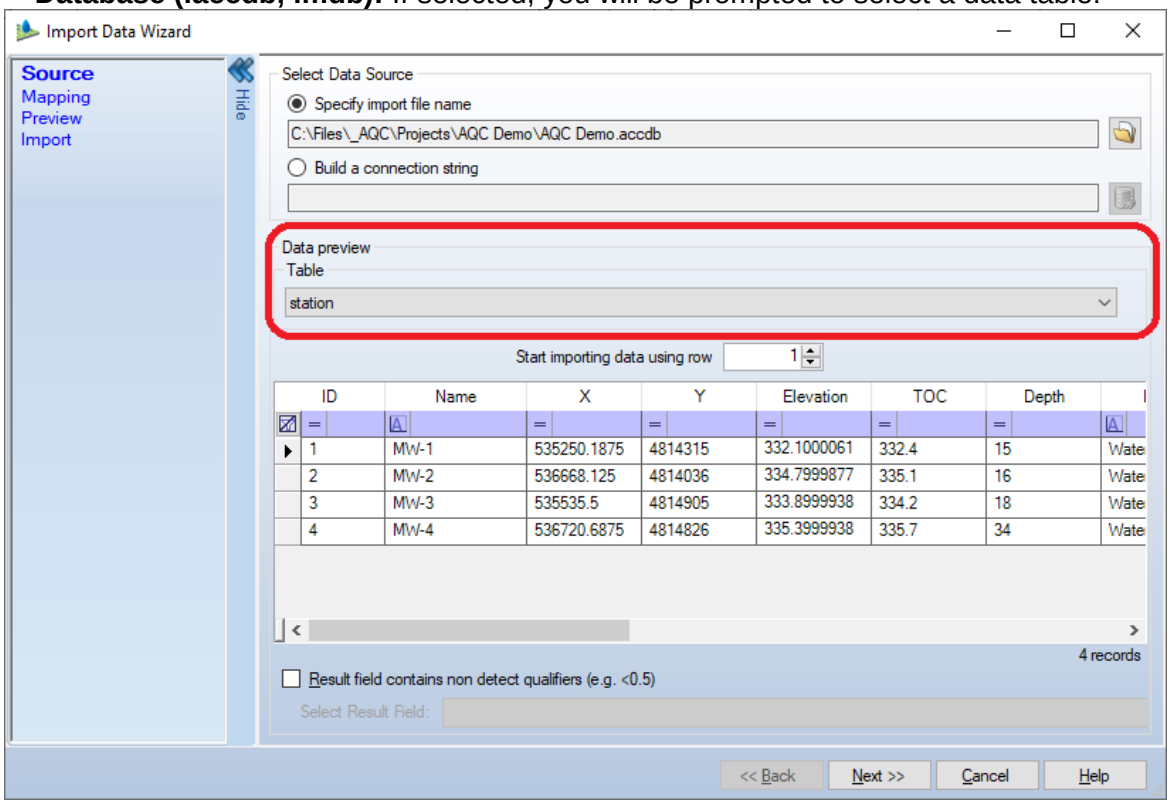
- **Delimited Text (.txt, .csv):** If selected, you will be prompted to select one or more delimiters:



- **Spreadsheet (.xlsx, .xlsx):** If selected, you will be prompted to select a worksheet or named range:



- **Database (.accdb, .mdb):** If selected, you will be prompted to select a data table:

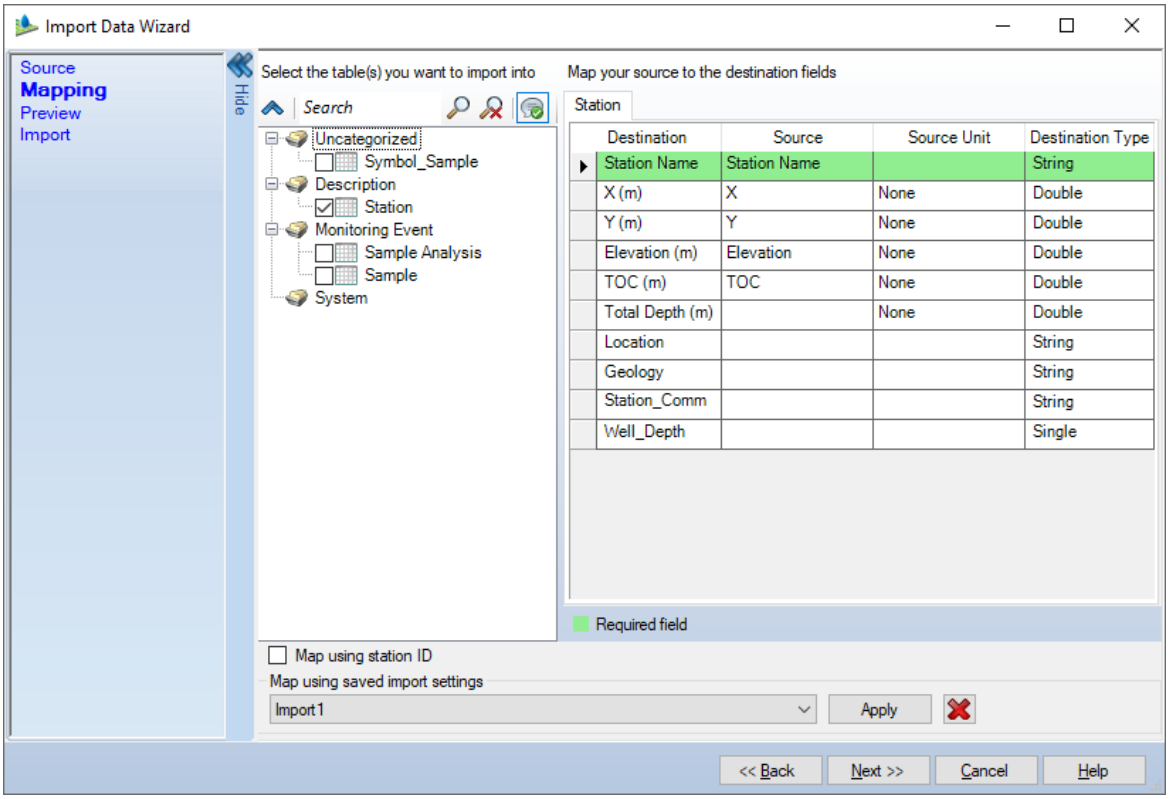


Below the source-specific controls, you may select a starting data row and in the case of text or spreadsheet files, a header row. A preview of the data is provided in the lower portion of the Source import step. Here you may preview the data and rename field headers, if desired. There is also an option to select a result value field and parse it if it contains non-detect qualifiers.

Once you have selected a data file and corresponding source options, select Next >> to proceed to the Mapping step.

Step 2: Field Mapping

At the Mapping step, you select the destination table and corresponding data fields into which you wish to import the source data. The destination table is selected using the categorized data table tree. In this example, we have selected the Station table in the Description category:

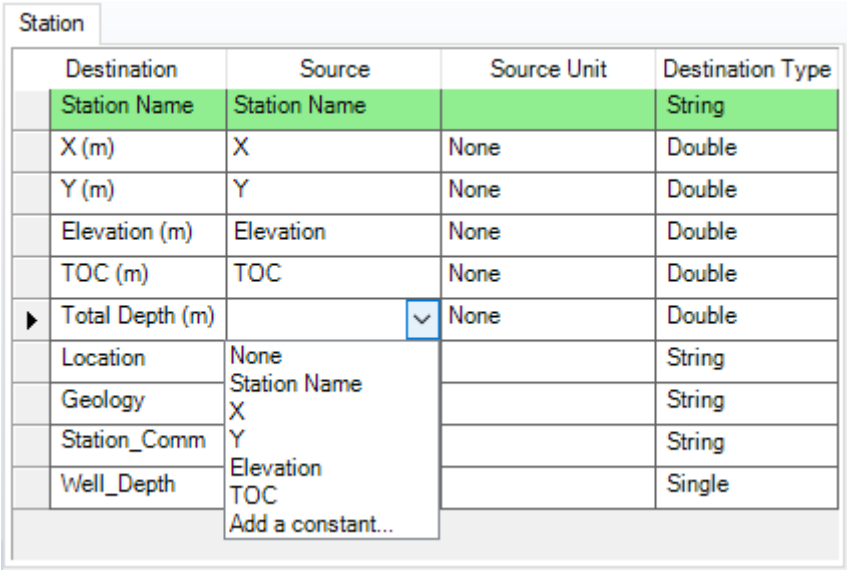


Once the destination table has been selected, as shown above, a table will be shown with the following four columns:

- **Destination:** the data fields in the destination table.
- **Source:** corresponding fields from the source data file.
- **Source Unit:** measurement unit from the source data file.
- **Destination Type:** the data type of the destination field.

Required fields will be highlighted green. In the case of the Station table, the Station Name field is always required. You may toggle the requirement of fields using the Template Manager.

As part of the Mapping step, you must select data fields from the source data file that was selected at the previous Source step in the Source column. If the headers in the source file match the name of the destination field in the AquaChem database - they will map automatically. If the headers do not match, you may click in the unmapped Source column and a dropdown will appear allowing you to select a source field, as shown for the Total Depth field below:



Note that included in the dropdown is the option to add a constant value rather than a field.

For destination fields that are numeric, you may select a measurement unit for the source data in the "Source Unit" column, Available source units will be of the same unit category as units of the Destination field, which are displayed in brackets in the Destination column. If the selected source units do not match the destination units, then the values will be converted into the destination units. Note that if the units match or if no units are selected (e.g. None), then the values will be imported without conversion.

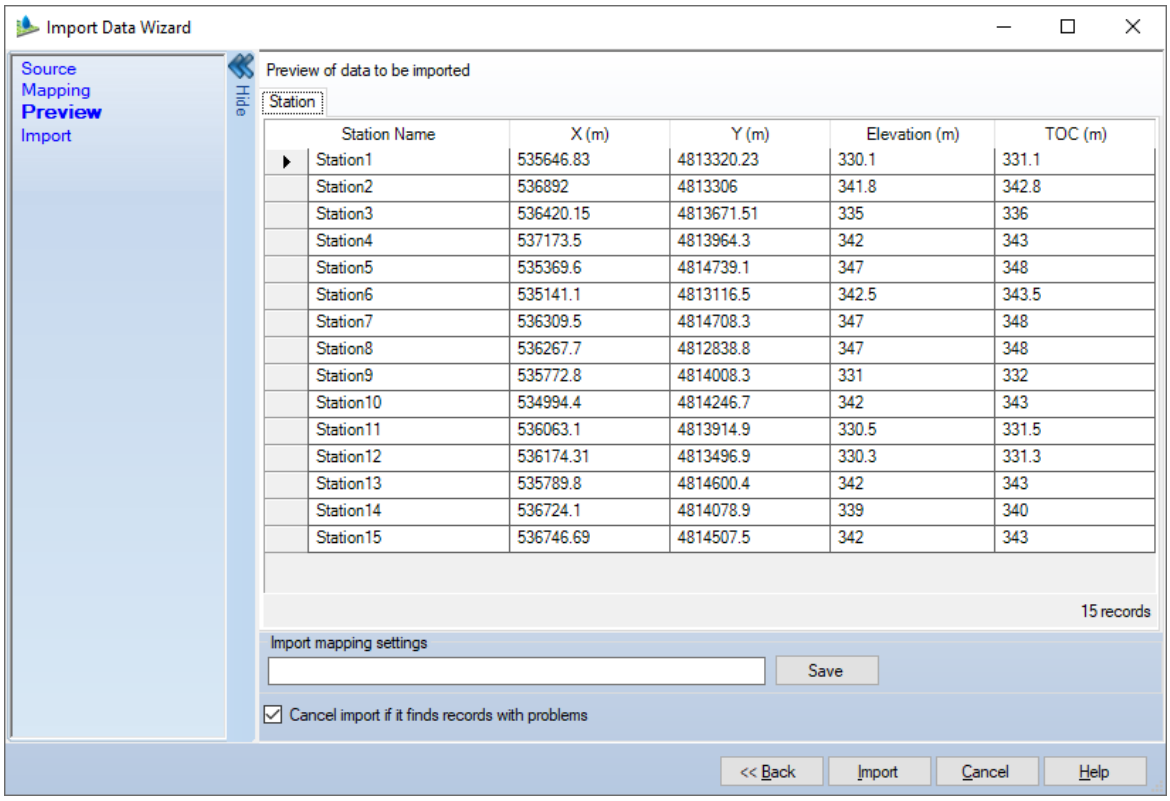
If you have previously imported data using the same source formats (i.e. same fields and units) and have saved the import data mappings at the Import step, you may select the settings from the "Map using saved import settings" dropdown and click the Apply button to recall and use these previous mappings.

Select the Next >> button to proceed to the next step - Preview.

Step 3: Preview the Data

At this step, you may preview the data to be imported. You also have the options to:

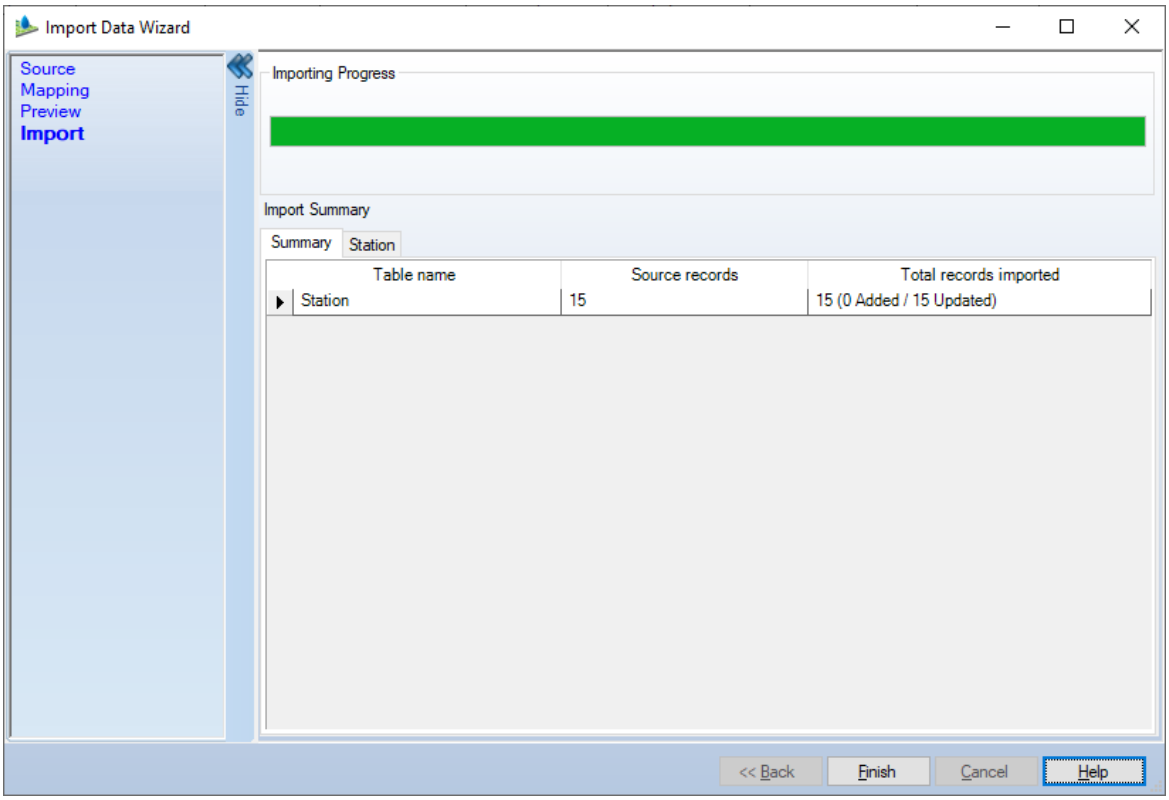
- save the import settings
- cancel the import if it finds records with problems



Select the Next >> button to proceed to the next step - Import.

Step 4: Data Import

Once this step is reached you can watch the progress of your import. When it is completed it will summarize how many records were in the source file and how many were imported.



If problems with the import data were detected during the import process errors and/or warning will be displayed along with available options to fix them. Example issues may include:

- source data that does not match the destination data type,
- duplicate records within the source data, and
- duplicate records between the source and destination data.

If you are satisfied with the import summary, select the Finish button to finalize the import and close the wizard. Your data will be available in the Destination table. Alternatively, you may return to a previous step using the << Back button or abandon the import process by using the Cancel button.

6.3 Images

This option allows for importing images into a specified image field related to a given station and is a two-step process:

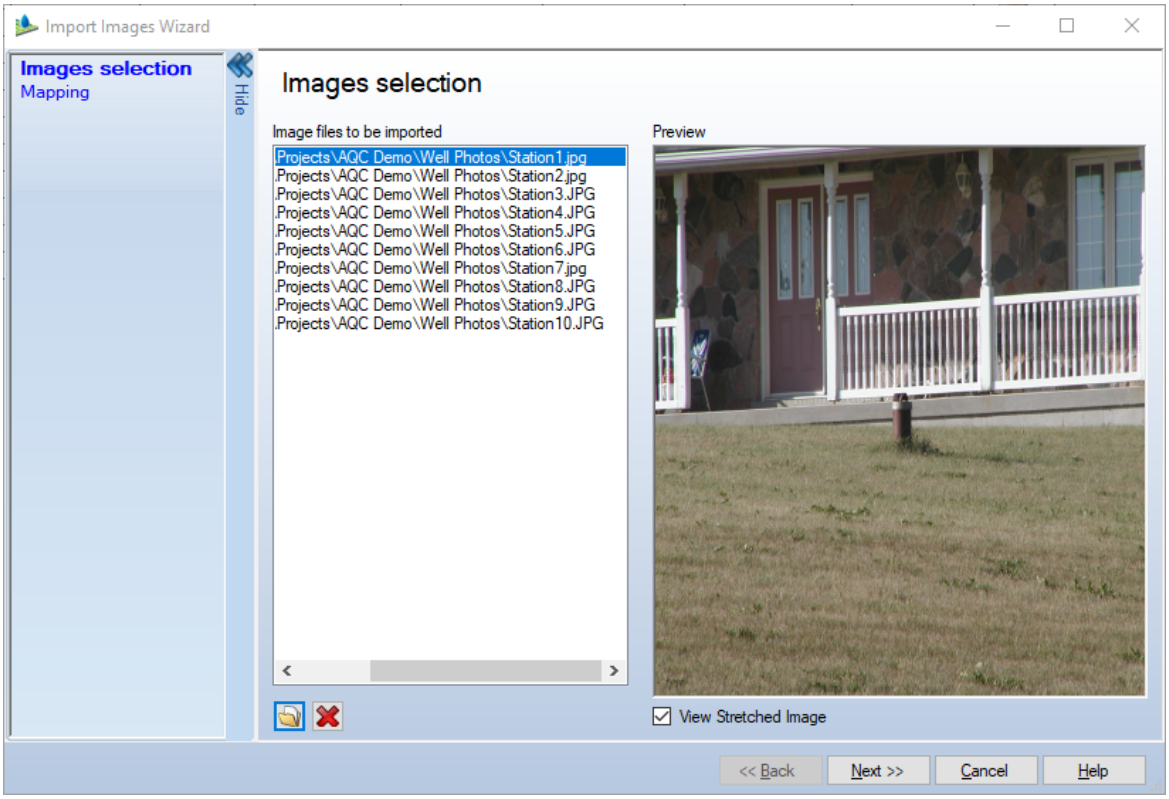
- Image Selection
- Mapping

Step 1: Image Selection

The first step in the general import process begins with selecting the files you wish to import and supports the following file formats:

- Bitmaps (.bmp)
- Enhanced Metafiles (.emf, .wmf)
- Icons (.ico)
- JPG (.jpg, .jpeg)
- PNG (.png)

To add images to be imported, select the load button. To remove images, select the remove button. The image selection step also includes an optional built-in preview pane:



Once you have selected the images to be imported, select Next >> to proceed to the Mapping step.

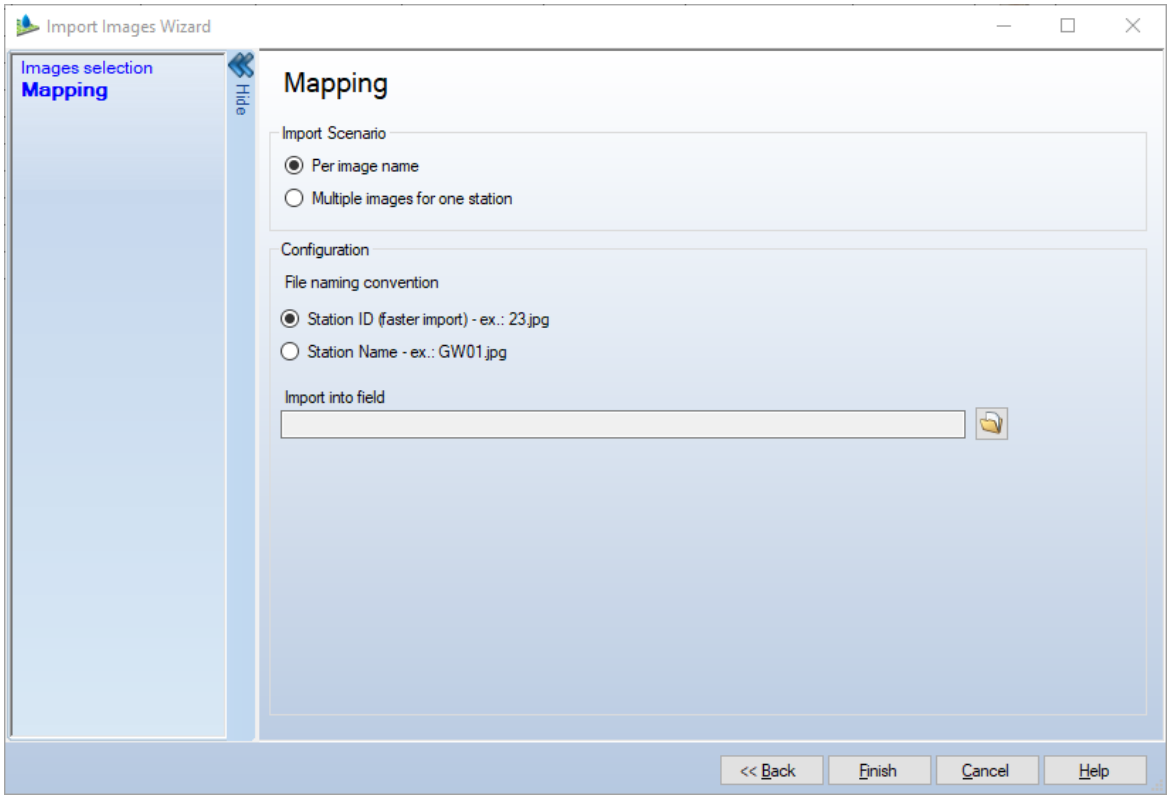
Step 2: Field Mapping

At the Mapping step, you must first select one of two import scenarios:

- by image name
- multiple images for one station

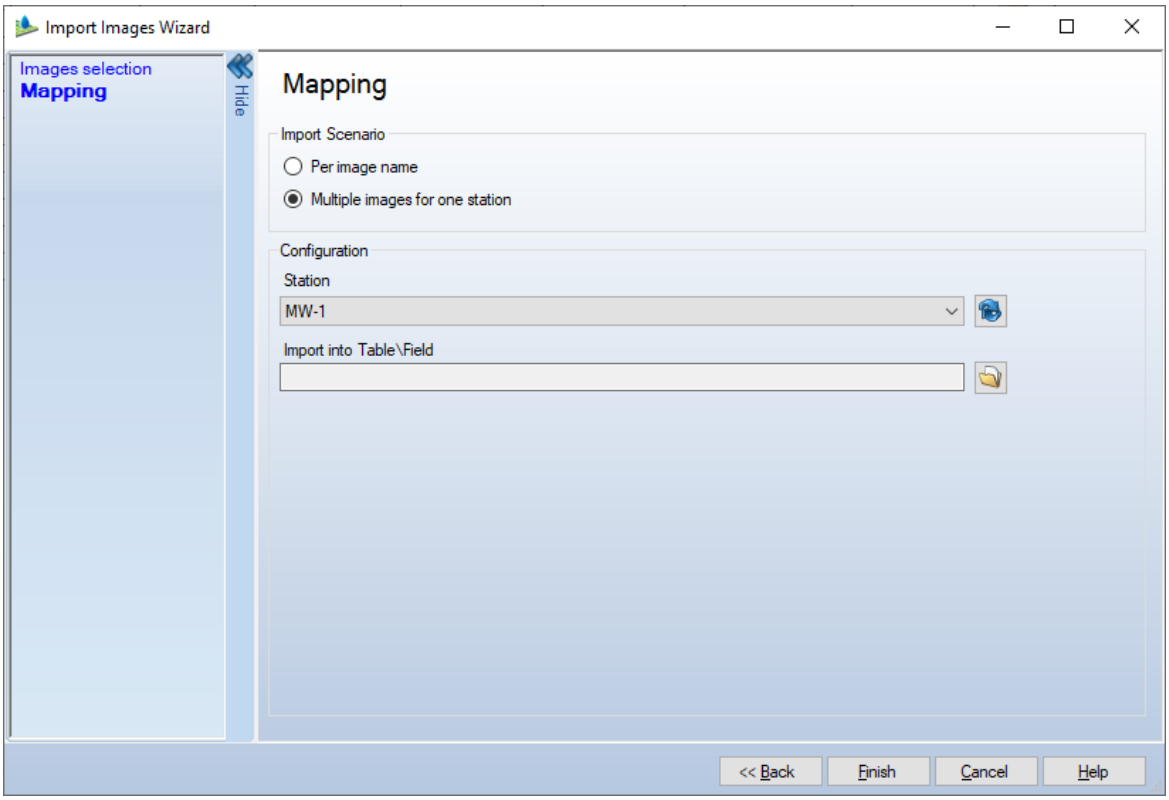
Import Images by name

This import scenario requires that the file name of each image matches either the corresponding **Station ID** or **Station Name** and images will be imported directly into the specified field in the Station table.



Multiple Images for one station

This import scenario allows you to import multiple image files into any table or field that is linked to the Station table; however, the images will be imported for a single (specified) station:



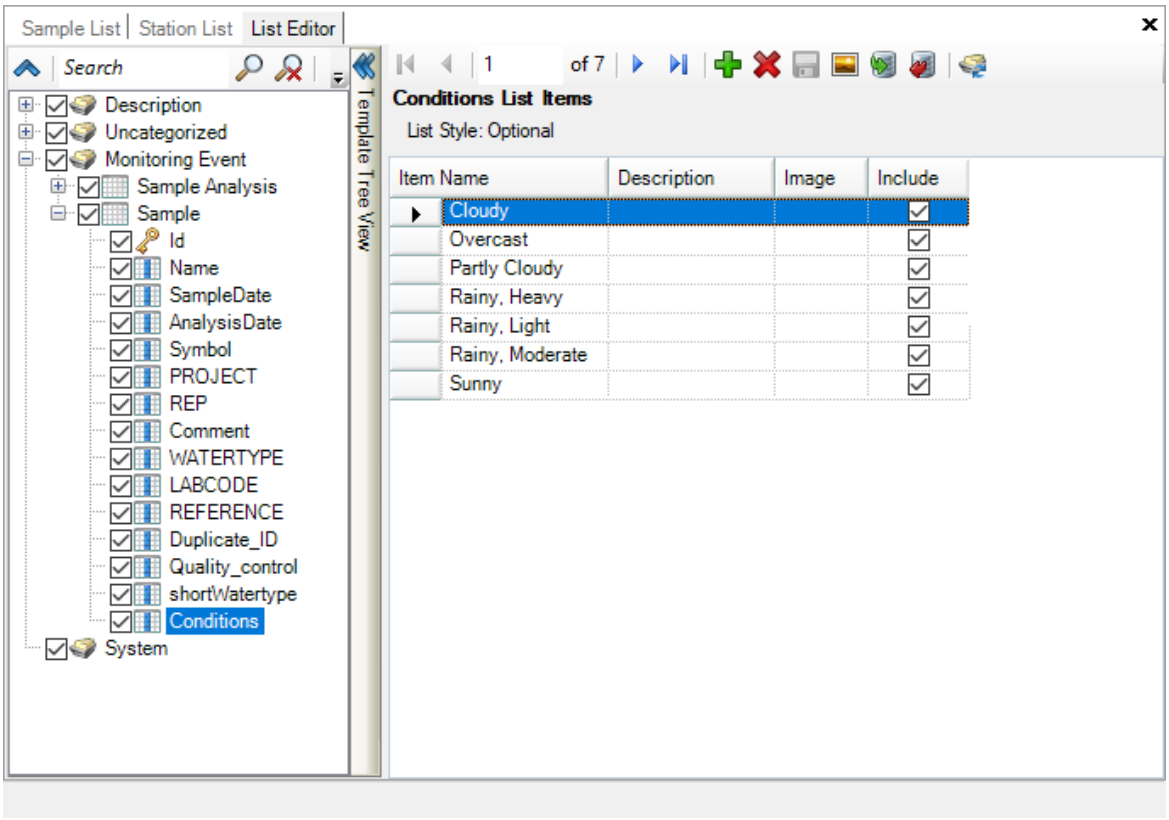
Once you have selected the import scenario and mapped the images to a destination data field, select Finish to import the images.

Chapter 7 List Editor

The List Editor provides the ability to create and customize lists for any field - allowing for efficient and consistent data entry. A field that is set to use an optional or required list in the Template Manager module becomes a drop down list within the interface (i.e. in the Sample List, Station List, Station Data tab, and Non Station Data tab).

You can open the List Editor from the Modules menu or click on the button in the main toolbar.

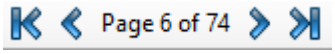
The List Editor will appear as a tab in the main AquaChem view, as shown in the following screenshot. Note that the List Editor can be dragged out of the main AquaChem view and dragged to a secondary monitor if you wish.



On the left side of the tab you will find the database structure tree (similar to what you find in the Template Manager or Query Builder).

Select the field you wish to edit a list for by highlighting it in the tree. Note that in order to work with a List, the field must be set to use an optional or required list in the Template Manager module.

On the right side of the tab you can generate and manage your list by using any of the following buttons:

Use the  buttons to navigate through the individual entries for a list.

Use the  button to add a new entry to the list.

Use the  button to delete the selected entry from the list.

Use the  button to save the list.

Use the  button to import images file (.jpg, .bmp, and .png) to be entries in the list.

Use the  button to import names for your entries in the list.

Use the  button to export the list.

Use the  button to add unique values from the field to the list.

Please Note: When importing a file to create your list ensure that you have the same format for your source file as what appears in the List Editor. That means there are 4 columns with the following headers: Item Name, Include, Description, and Image. The minimum that needs to be populated is the Item name.

Please Note: If you want to re-use this list in a new project, you must save the database template. Then create a new project with this new database template, and the list will be available. For details on saving database templates, see the Managing Database Templates section.

Chapter 8 Map Viewer Module

In AquaChem, you can use the **Map Viewer** Module to easily map location-based representations of your project data and add external data layers to enrich your map.

To Open the Map Viewer Module:

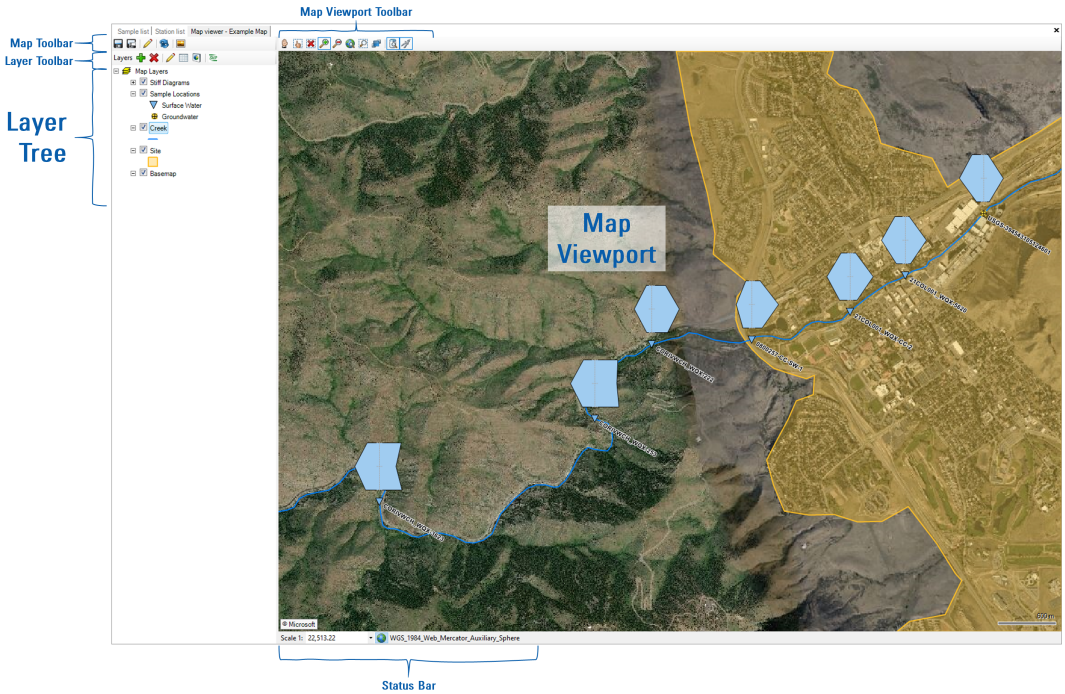
- Click the Map Viewer [ ] button on the main toolbar
  or
- Select **Modules > Map Viewer** from the Main Menu

Layout

The layout of the Map Viewer is divided into two separate panes and their related controls:

1. The **Layer Tree** lists map layers that have been added to the map and includes the layer toolbar.
2. The **Map Viewport** displays visible map layers that are rendered in the (bottom to top) order in the Layer Tree and includes the Map Viewport Toolbar and Status Bar

The Map Viewer also includes the Map toolbar which controls the map view itself.



Map Toolbar

The Map Toolbar provides controls for managing the map:

 **Save**: saves changes to the current Map View in the Project Tree.

 **Save as...**: saves a copy of the current Map View with a new name in the Project Tree.

 **Rename map**: renames the current Map View.

 **Refresh layer data**: refreshes layers and associated data in the current Map View.

 **Export Map**...: exports the current map to an image or PowerPoint template.

Map Layers and the Layer Tree

The layer tree organizes map data layers that have been added to the map. A data layer is a specific dataset that contains geographic information in either vector or image/raster format. Layers will be rendered in the map in the order in which they the layer tree. The layer at the bottom of the tree will be rendered first and therefore will be shown as beneath overlapping layers that are higher in the tree. In addition to layer order, the layer tree provides controls on how each map layer will be rendered, including a ☑ checkbox that toggles each layers's visibility and a toolbar for additional controls.

Vector Datasets

Vector datasets represent discrete locations as one or more points, polylines, or polygons. Each point, polyline, or polygon is composed of spatial information (i.e the set of vertices that define the point, polyline, or polygon) and associated attributes (i.e. information about the point, polyline, or polygon). There are two types of supported vector datasets in AquaChem 10.0:

- **Project data-driven datasets** are vector datasets that are based on a sample set or station group and are dynamically generated by AquaChem based on the project database

- **Shapefiles** are an open source vector-based Geographic Information Systems (GIS) data format developed by ESRI (1998) that includes a set of points, polylines, *or* polygons. Shapefiles consist of a set of files with the same file name — four of these are required for use in the Map Viewer Module: .shp (spatial data), .shx (spatial index), .dbf (attribute data), and .prj (coordinate reference definition). Shapefiles can be imported from external sources in AquaChem.

Image Datasets

Aerial photographs and basemaps are commonly stored as images.

- **Image formats** are a grid based data covering a defined rectangular area. AquaChem 10.0 supports common image types with an associated world file.

  Please Note: the projection of the image *must* match that of the map. On-the-fly Image reprojection is not currently supported in AquaChem 10.0.

Layer Toolbar

The Layer Toolbar provides controls for managing and configuring map layers:

Add layer: opens the Add map layer window

Delete layer: removes the layer selected in the Map Tree

Labels: opens the Feature Labeler window

Attributes: opens the Data settings window

Chart Setup: opens the Charts and Symbols window (only applies to project data-driven layers)

Export to shapefile: Exports the selected layer to a shapefile (does not apply to raster/image layers)

Map Viewport

The map viewport is where map layers are displayed and provides controls to interact with the map layers.

Map Viewport Toolbar

The Map Viewport Toolbar provides controls to manipulate the viewport and interact with visible layers:

Pan Tool: allows you to pan around the map view. When this tool is active (framed in a solid blue line), you can:

- click and drag the mouse pointer on the map to pan around
- use the mouse wheel up/down to zoom in/out, respectively

 **Selection Tool**: allows you to select one or more features from the active layer. When this tool is active (framed in a solid blue line), you can:

- click on a feature in the active layer to select it
- click, drag, and release to select features in the active layer within the resulting rectangle

- press and hold the <shift> key while performing the above actions to add to the existing selection or
- press and hold the <control> key while performing the above actions to flip the selection

- click on the map where no features in the active layer exist to deselect all features in the active layer

 **Deselect All**: deselects all features in the mapview

 **Zoom in:** allows you to zoom in on the map. When this tool is active (framed in a solid blue line), you can:

- click on the map to zoom in by an approximate factor of 2
- click, drag, and release to zoom in to the resulting rectangle

 **Zoom out:** allows you to zoom out on the map. When this tool is active (framed in a solid blue line), you can:

- click on the map to zoom out by an approximate factor of 2
- click, drag, and release to zoom out based on the scale of the resulting rectangle to the current viewport

 **Zoom to full extent**: zooms the map viewport to the full extent of all layers in the layer tree.

 **Zoom to selection**: zooms the map viewport to the extent of the selected feature(s) in the active layer.

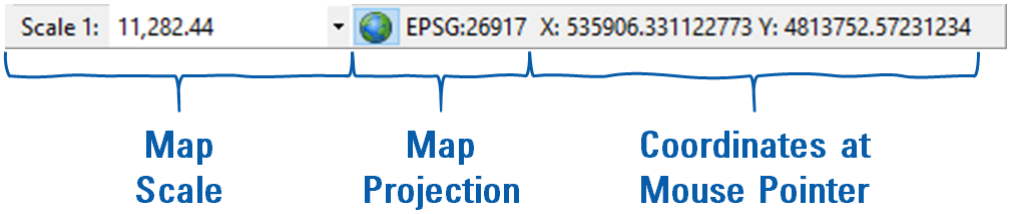
 **Zoom to Layer**: zooms the map viewport to the extent of the active layer.

 **Sync selected samples**: toggles whether the map selection is synchronized with sample selections in the rest of AquaChem (e.g. Sample Picker, Sample List, Plot Collection(s), etc.)

 **Show scale**: toggles the scale bar on the map. If turned on, a scale bar will be shown in the lower right hand corner of the map. The length of the scale bar (in terms of both the map and screen space) will automatically adjust based on the scale of the map on the screen to the nearest single digit value.

Status Bar

The Status bar provides additional controls for the map viewport



Map Scale: displays the current map scale and allows you to set the map scale to one of several common scales

Map Projection: displays the current map projection and allows you to set the map projection.

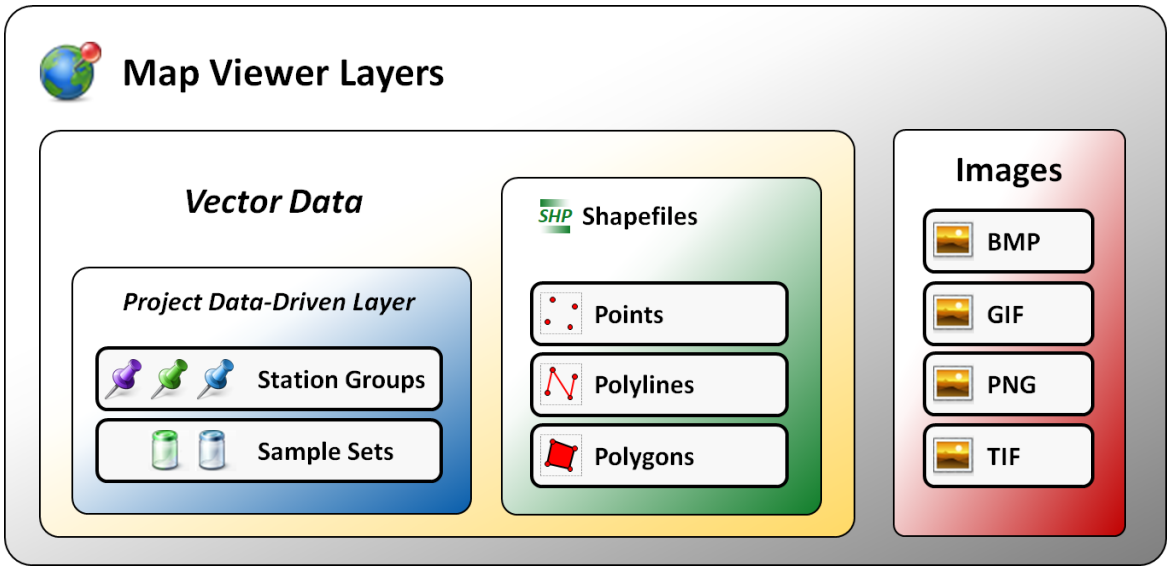
Coordinates: displays the map coordinates for the location of the mouse pointer on the map if it is located within the viewport

8.1 Add Map Layer

This section describes the layer types that are supported in the Map Viewer and how to add them.

Supported layer types

The following types of layers are supported file types are supported in the Map Viewer maps:



AquaChem Data (Project Data-Driven Layers

Station Groups from the project tree as defined in the station list (static groups) or sample set editor (dynamic groups)

Sample Sets from the project tree as defined in the sample list (static sets) or sample set editor (dynamic sets)

External Data Layer Types

Shapefiles are an open source vector-based Geographic Information Systems (GIS) data format developed by ESRI (1998) that includes a set of points, polylines, *or* polygons. Shapefiles consist of a set of files with the same file name — four of these are required for use in the Map Viewer Module: .shp (spatial data), .shx (spatial index), .dbf (attribute data), and .prj (coordinate reference definition). Shapefiles can be imported from external sources in AquaChem.

Images are a grid based data covering a defined rectangular area. AquaChem 10.0 supports common image types with an associated world file.

Please Note: the projection of the image ***must*** match that of the map. On-the-fly Image reprojection is not currently supported in AquaChem 10.0.

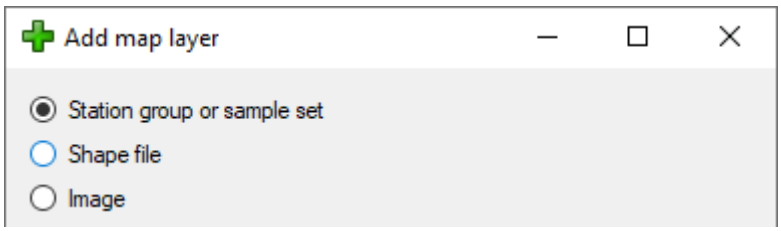
Adding a map layer

You can add a layer to the map by:

- Clicking the **Add layer** button [] in the map layers toolbar to open the Add map layer dialog
- Dragging-and dropping a station group or sample set onto the Layer Tree or Map Viewport
- Dragging-and-dropping a supported external file type (shapefile or image) from a Windows Explorer window onto the Layer Tree or Map Viewport

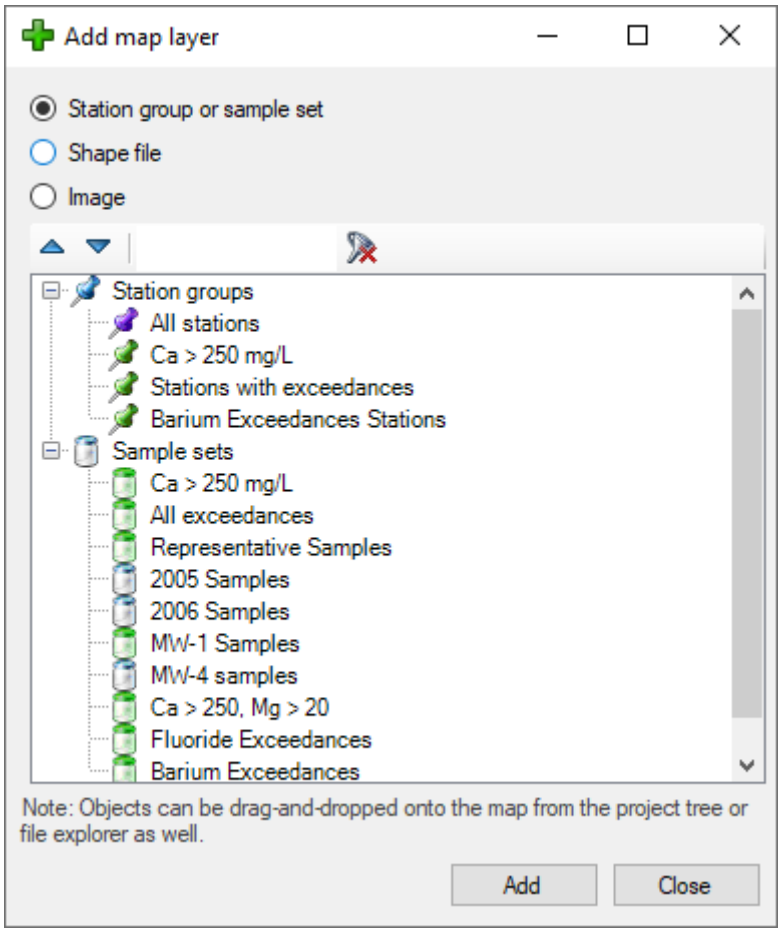
Add Map Layer Window

The Add Map Layer window includes a radio button selection for the type of layer to add:



Add Station Group/Sample Set

Selecting the station group or sample set option shows a searchable subset of the project tree that includes the station groups and sample sets:



Clicking the Add button adds the selected station group or sample set to the layer tree and map viewport.

Add Shapefile

Selecting the Shapefile and clicking the Add button opens the windows explorer and allows you to navigate to and select a shapefile to be added to the layer tree and map viewport.

Add Image

Selecting the Image and clicking the Add button opens the windows explorer and allows you to navigate to and select an inmage to be added to the layer tree and map viewport.

8.1.1 Image World File Format

World files are companion files to geospatial images that contain spatial reference information to locate the image within its projection.

Please Note: the projection of the image *must* match that of the map in AquaChem 10.0; on-the-fly Image reprojection is not currently supported.

Filename

In order to work with its associated image file, the worldfile must be located in the same folder as the image and have the same filename. The file extention must be as follows:

Image File Type/Extension	Associated World File Extention
.BMP	.BPW
.GIF	.GFW
.JPG	.JPW
.PNG	.PGW
.TIF	.TFW

Contents

An ASCII world File consists of an ASCII text file with six items, each on a separate line:

Line	Symbol	Description
1	Δx	pixel size in the x-direction in map units (typically meters or feet)
2	θ_y	rotation/skew about y-axis
3	θ_x	rotation/skew about x-axis
4	Δy	pixel size in the y-direction in map units (typically meters or feet). The value is typically negative to indicate that the first

		pixel of the image/raster is located at the top/North
5	x_0	x-coordinate of the center of the first (typically leftmost/East) pixel
6	y_0	y-coordinate of the center of the first (typically topmost/North) pixel

Example

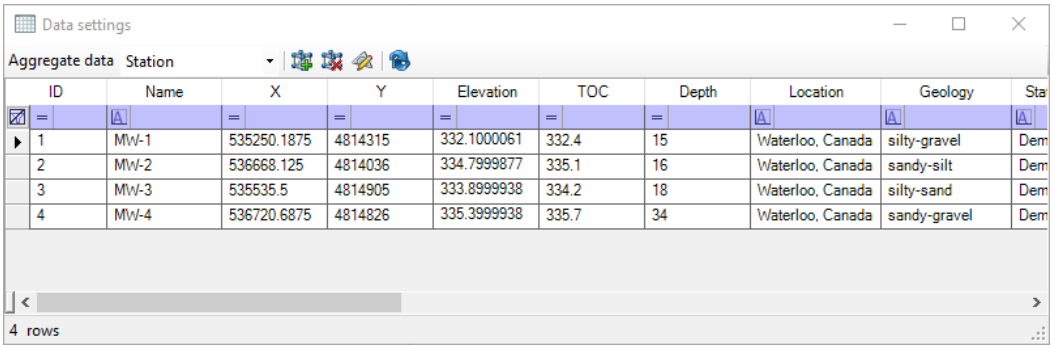
The image used in the Creating Maps called Basemap.tif has an associated world file (Basemap.tfw) with the following contents based on the UTM Zone 17N, NAD1983, projection in meters (EPSG 26917):

```
2.0000000000
0.0000000000
0.0000000000
-2.0000000000
532001.0000000000
4816499.0000000000
```

8.2 Map Data Settings

The Data Settings window in the Map Viewer Module allows you to review the attributes of vector data layers that have been added to the map, including station groups, sample sets, and imported shapefiles. The Data Settings window also allows you to control the scope of project data-driven layers (i.e. station groups and sample sets) as described below in the aggregating data section.

The Data Settings window can be accessed for the selected layer by clicking the Attributes button in the Layer Tree toolbar.



ID	Name	X	Y	Elevation	TOC	Depth	Location	Geology	Sta
1	MW-1	535250.1875	4814315	332.1000061	332.4	15	Waterloo, Canada	silty-gravel	Dem
2	MW-2	536668.125	4814036	334.7999877	335.1	16	Waterloo, Canada	sandy-silt	Dem
3	MW-3	535535.5	4814905	333.8999938	334.2	18	Waterloo, Canada	silty-sand	Dem
4	MW-4	536720.6875	4814826	335.3999938	335.7	34	Waterloo, Canada	sandy-gravel	Dem

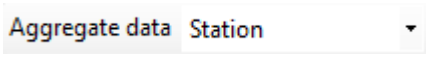
4 rows

The Data Settings window has two components:

- **Toolbar**: allows you to modify the attribute table of the selected map layer and is only available if the selected map layer is a station group or sample set.
- **Data view:** allows you to review the attribute data and includes the standard data filters available in AquaChem so that you can quickly find data of interest.

Toolbar

The Data settings toolbar (only available if the selected layer is a station group or sample set) provides controls for altering the scope and structure of the attribute table:



Aggregate data: allows you to change the scope of the data set and aggregate the data.

Select Parameter: lists and allows you to select the relevant parameter if the Minimum or Maximum aggregate data option is selected and is not shown otherwise.


Add Parameter: allows you to add one or more parameters as an attribute field.


Remove Parameters: allows you to remove one or more added parameters from the attribute table

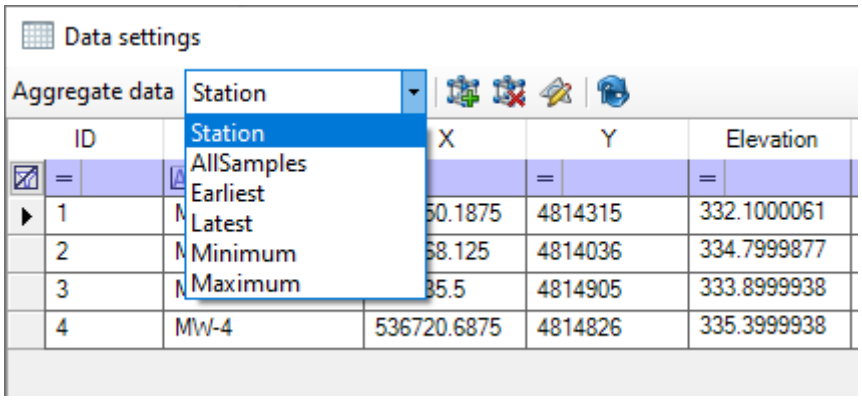

Change units: allows you to change the measurement units of an added parameter in the attribute table (e.g. from mg/L to meq/L)


Refresh data: refreshes the data in the attribute table and map.

Calculated parameters cannot be added to the attribute table; however, you can save values from a calculated field into the sample table using the save values  button in the Sample Results toolbar of the Sample List view and subsequently add the resulting sample parameter to the attribute table.

Aggregating Data

The Aggregate data dropdown in the Data Settings window allows you to change the data scope of the active sample set or station group and aggregate sample data based on the selected criteria. The following options are available:



- **Station**: one record will be displayed per station that is part of the selected station group or sample set. The attribute table will include a sequential record ID, the X- and Y-coordinates of the station, the station parameters (i.e. data fields from the station list), and any parameters that have been added using the toolbar. This is the default data aggregation setting for added station groups.

- **AllSamples**: one record will be displayed per sample that belongs to the selected station group or sample set. The attribute table will include a sequential record ID, the X- and Y-coordinates of the station, the sample parameters (i.e. data fields from the sample list), and any parameters that have been added using the toolbar. This is the default data aggregation setting for added sample sets.

  Stations in the selected sample set/station group that have multiple samples for a given station will result in multiple records in the attribute table and overlapping symbols on the map. For improved map performance and visual clarity, it may be useful to use one of the remaining four options which are guaranteed to produce one sample record per station.

- **Earliest**: one record will be displayed for the first sample collected at each station that belongs to the selected station group or sample set - The earliest sample is defined as the sample with the oldest sample date value in the station list. The attribute table will include a sequential record ID, the X- and Y-coordinates of the station, the sample parameters (i.e. data fields from the sample list), and any parameters that have been added using the toolbar.

- **Latest**: one record will be displayed for the most recent sample collected at each station that belongs to the selected station group or sample set - The latest sample is defined as the sample with the newest sample date value in the station list. The attribute table will include a sequential record ID, the X- and Y-coordinates of the station, the sample parameters (i.e. data fields from the sample list), and any parameters that have been added using the toolbar.

- **Minimum**: one record will be displayed for the sample collected at each station that belongs to the selected station group or sample set with the lowest measured value of the selected parameter. If more than one sample is returned per location because multiple samples have the same lowest value for the same parameter, then the first such record encountered will be returned. The attribute table will include a sequential record ID, the X- and Y-coordinates of the station, the sample parameters (i.e. data

fields from the sample list), and any parameters that have been added using the toolbar. If it is not already included, the minimum parameter will be added to the attribute table.

- **Maximum**: one record will be displayed for the sample collected at each station that belongs to the selected station group or sample set with the highest measured value of the selected parameter. If more than one sample is returned per location because multiple samples have the same highest value for the same parameter, then the first such record encountered will be returned. The attribute table will include a sequential record ID, the X- and Y-coordinates of the station, the sample parameters (i.e. data fields from the sample list), and any parameters that have been added using the toolbar. If it is not already included, the maximum parameter will be added to the attribute table.

Please Note: you must click the refresh [] button to apply any changes to the aggregate data options.

8.3 Charts and Symbols

The Charts and Symbols window in the Map Viewer Module allows you to define the symbology of station groups and sample sets that have been added to the map.

The Charts and Symbols window can be accessed for the selected layer by clicking the Chart Setup button in the Layer Tree toolbar.

Symbology Options

The Charts and Symbols Data Settings allows you to define the symbology for the selected station group or sample set using one of the following options:

Symbols

- **Simple Symbol**: symbols will be placed at the station coordinates. The symbols may be uniform or ramped based on a selected numeric parameter field.
- **Sample Symbol**: symbols based on the symbols defined in the symbol editor and shown in the sample list will be placed at the station coordinates.

Charts

- **Pie Chart**: one pie chart will be plotted on the map at the station coordinates per record in the attribute table.

-  **Radial Chart**: one radial chart will be plotted on the map at the station coordinates per record in the attribute table.

-  **Stiff Diagram**: one radial chart will be plotted on the map at the station coordinates per record in the attribute table.

For each of these options one symbol or chart will be placed on the map per record in the attribute table based on the aggregate data option in the Data Settings for that layer. This may result in overlapping symbols, particularly if the ***Station*** or ***AllSamples*** options are selected.

By default, the chart-based symbols will be formatted using the default settings for the respective chart type. Some formatting options (such as source parameters and colors) are provided in the settings described below and other settings (e.g. axis ranges) must be set by updating the default plot settings before setting the plot type to the desired chart type.

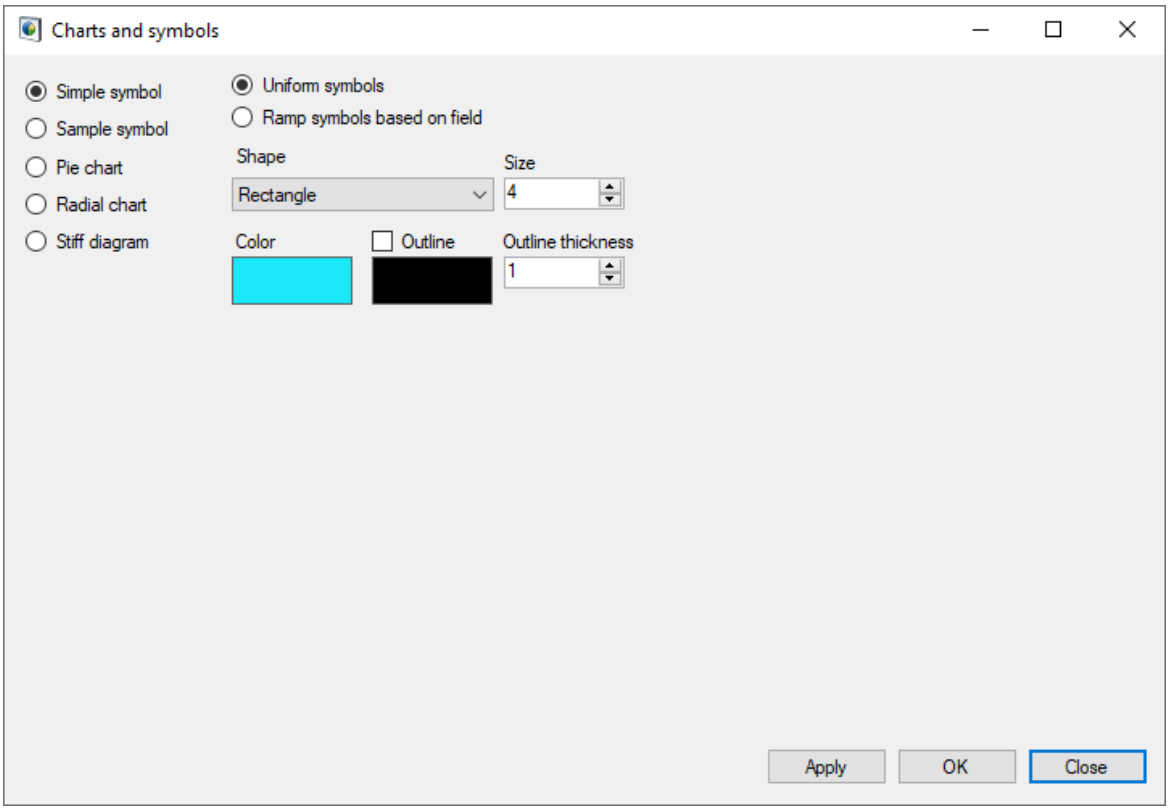
Simple Symbol

The simple symbol option allows to place uniform symbols or ramped symbols for each record in the layer attributes:

Uniform Symbols

The simple (uniform) symbols option allows you to specify the settings for a symbol that will be used to represent all records uniformly:

- **Shape**: choose from: diamond, ellipse (circle), hexagon, rectangle (square), pentagon, star, or triangle
- **Size:** set the size of the symbol
- **Color**: set the fill color of the symbol
- **Outline**: toggle the visibility of the symbol outline
- **Outline Color**: set the color of the symbol outline
- **Outline thickness**: set the thickness of the outline



Ramped Symbols

The simple (ramped) symbols option allows you to define a specified number of symbols that will be ramped/graduated by either size and/or color based on the value of a given parameter for each record:

- **Field:** allows you to specify a numeric parameter in the attribute table that will be used to ramp/graduate the symbols
- **Add Parameter**: opens the data settings window so that you can add a parameter if it is missing from the list

- **Ramp color checkbox**: allows you to specify if the symbols will be ramped/graduated by color
- **Ramp size checkbox**: allows you to specify if the symbols will be ramped/graduated by size

- **Shape**: choose from: diamond, ellipse (circle), hexagon, rectangle (square), pentagon, star, or triangle

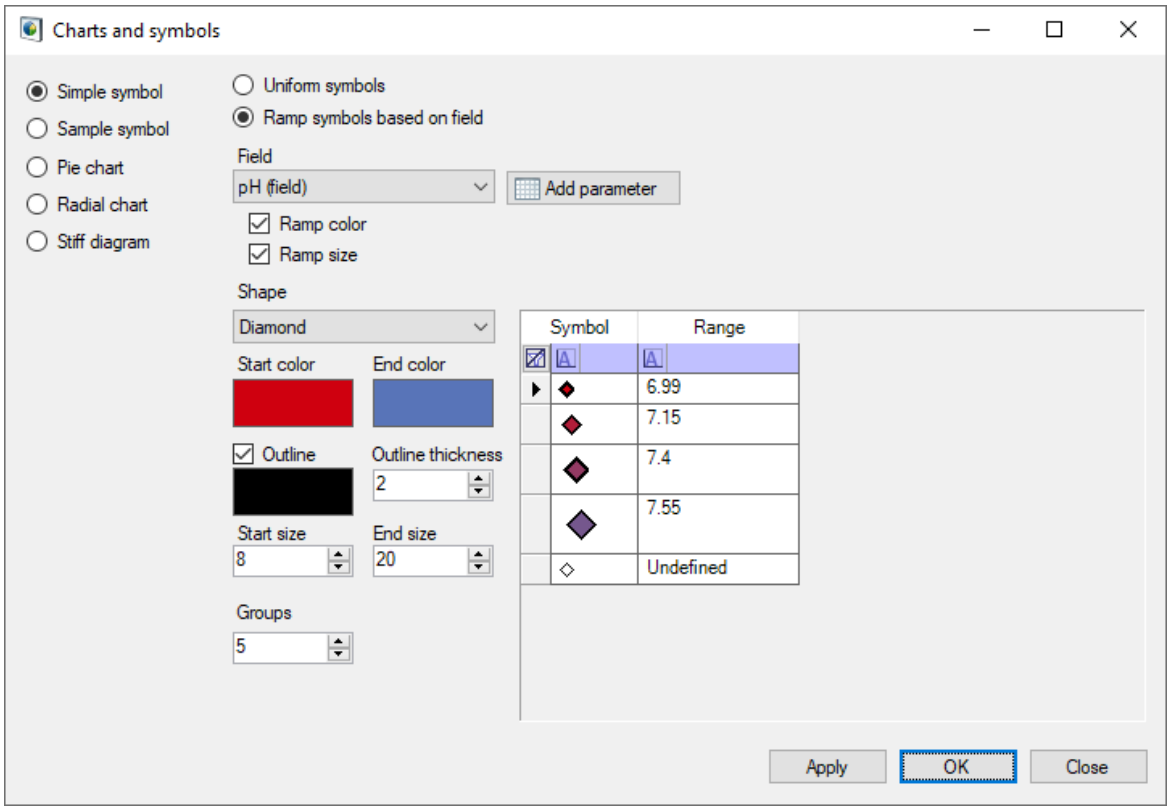
- **Start Color**: set the fill color of the symbol (with the lowest value if ramp color is off)
- **End Color**: set the fill color of the symbol with the highest value (shown if ramp color on)

- **Outline**: toggle the visibility of the symbol outline
- **Outline Color**: set the color of the symbol outline

- **Outline thickness**: set the thickness of the outline

- **Start Color**: set the fill color of the symbol (with the lowest value if ramp size is off)
- **End Color**: set the fill color of the symbol with the highest value (available if ramp size on)

- **Groups:** specify the number of graduated symbols to use. Note that one of the groups will always be the "Undefined" category in case one of the records includes a null value (e.g. no measurement) as shown below. The minimum number of groups is 2: which would include records with a numeric value and those without. The maximum number of groups is 20.



The ramp symbols option also includes a preview window allows you to review and edit the range of values for each symbol.

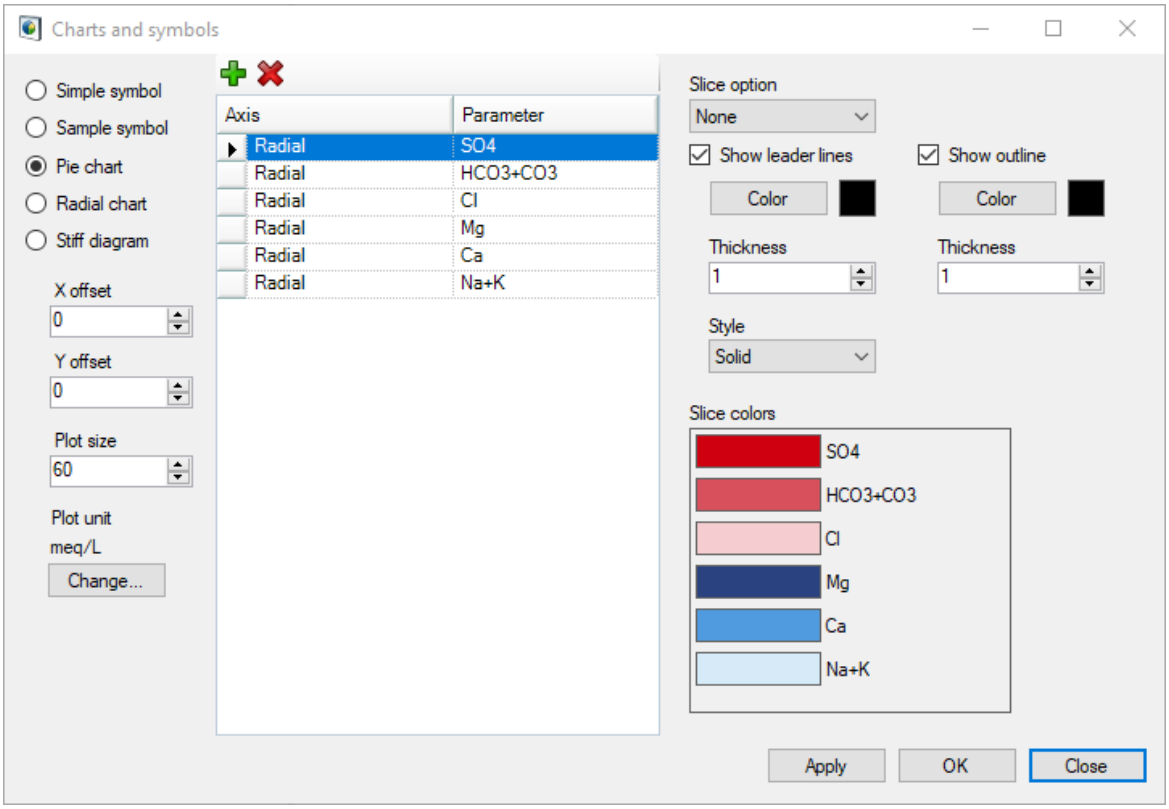
Sample Symbol

The simple (ramped) symbols option allows you to plot the defined in the symbol editor and shown in the sample list on the map. No special controls are provided for this option.

Pie Chart

The Pie Chart symbol option allows you to place one pie chart for each record in the layer attributes on the map:

- **Add Parameter**: adds a parameter to the pie chart using the parameter picker
- **Remove Parameter**: removes the selected parameter(s) from the list of parameters
- **Outline Color**: sets the color for the outline of the pie wedges
- **Outline Thickness**: sets the line thickness for the outline of the pie wedges
- **Slice Colors**: sets the colors of the individual parameters



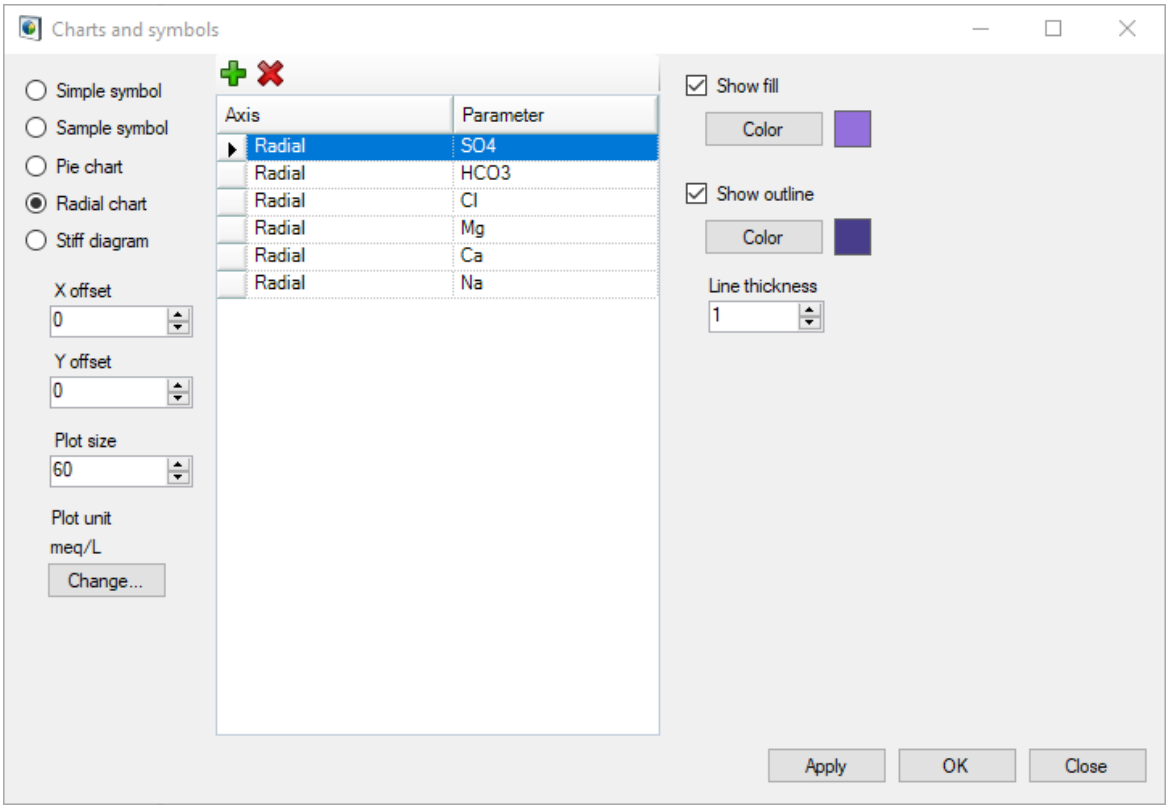
The left pane also includes plot option settings for the placement and sizing of the pie charts.

Radial Chart

The Radial Chart symbol option allows you to place one radial chart for each record in the layer attributes on the map:

- **Add Parameter**: adds a parameter to the radial chart using the parameter picker
- **Remove Parameter**: removes the selected parameter(s) from the list of parameters

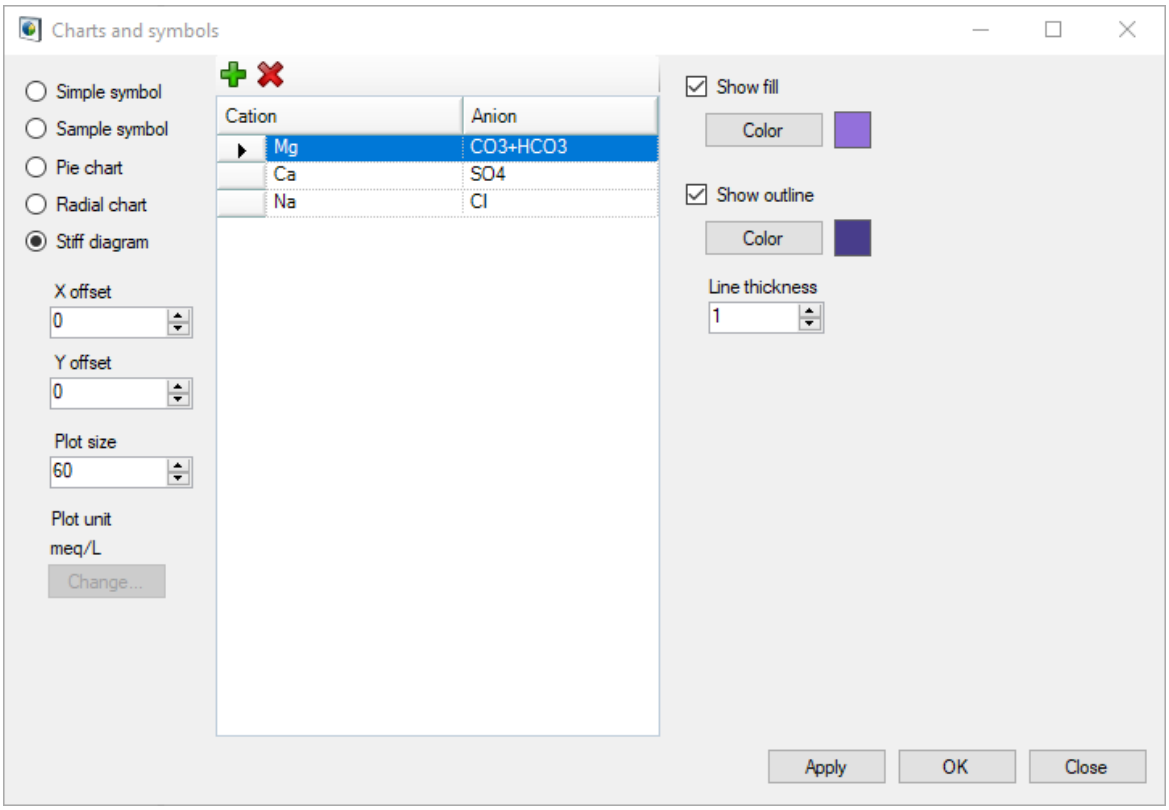
- **Show Fill**: toggles whether the radial plots will be filled
- **Fill Color**: sets the fill color for the radial plot
- **Show Outline**: toggles whether the radial plots will have an outline
- **Outline Color**: sets the color for the outline of the radial plot
- **Line Thickness**: sets the line thickness for the outline of the radial plot



Stiff Diagram

The Stiff diagram symbol option allows you to place one Stiff diagram for each record in the layer attributes on the map:

- **Add Parameter**: adds a parameter to the radial chart using the parameter picker (note that there must be an equal number of cations and anions
- **Remove Parameter**: removes the selected cation/anion pair(s) from the list of parameters
- **Show Fill**: toggles whether the Stiff diagrams will be filled
- **Fill Color**: sets the fill color for the Stiff diagram
- **Show Outline**: toggles whether the Stiff diagrams will have an outline
- **Outline Color**: sets the color for the outline of the Stiff diagrams
- **Line Thickness**: sets the line thickness for the outline of the Stiff diagrams



Plot Options

Layers with plot-based symbols (i.e. pie, radial, or Stiff) have additional settings for placing and sizing the plots:

- **X-Offset**: offset in the x-direction. A positive value will move the plots east relative to the station, while a negative value will move the plots west
- **Y-Offset**: offset in the y-direction. A positive value will move the plots north relative to the station, while a negative value will move the plots south
- **Plot Size**: set the size of the plot
- **Plot units**: select the measurement unit for the plot, where applicable.

By default, plots are centered on the station location. In some cases, it may be useful shift the plot away from the station so that other information can be mapped at the station. Please see the Creating Maps section of the tutorial for an example.

8.4 Feature Labeler

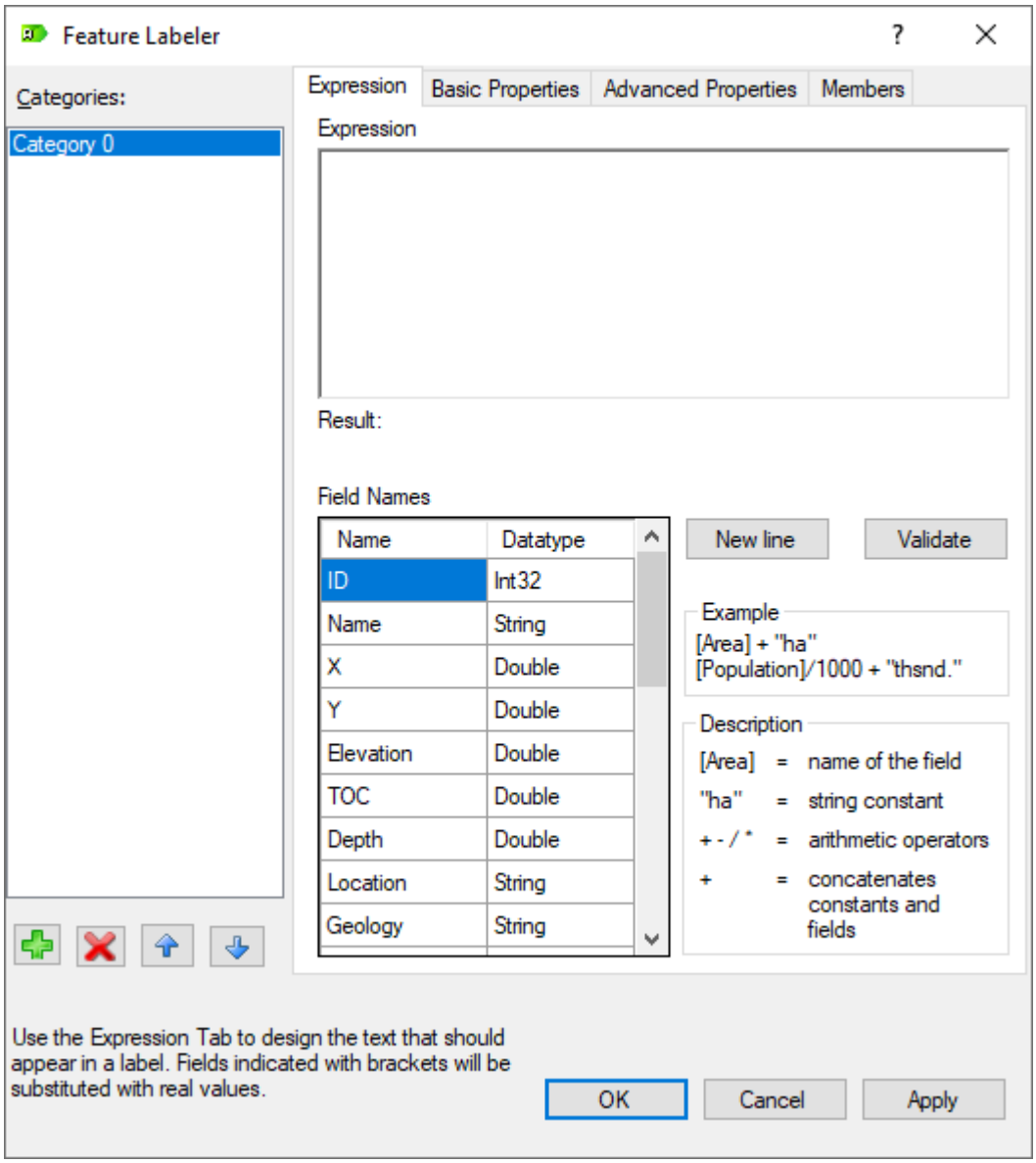
You can add and configure labels to a vector map layer by:

- Right-clicking on the map layer and selecting Labeling > Label Setup
- Clicking the **Labels** button [] in the map layers toolbar

Label Categories

The left pane of the Feature Labeler includes a list of label categories. A label category is a distinct set of labels for the map layer that can have its own label expression, basic/advanced style settings, and member definition.IN this way you can define customized labels for the map layer, for example differing label styles and values based on whether a sample exceeds a water quality standard.

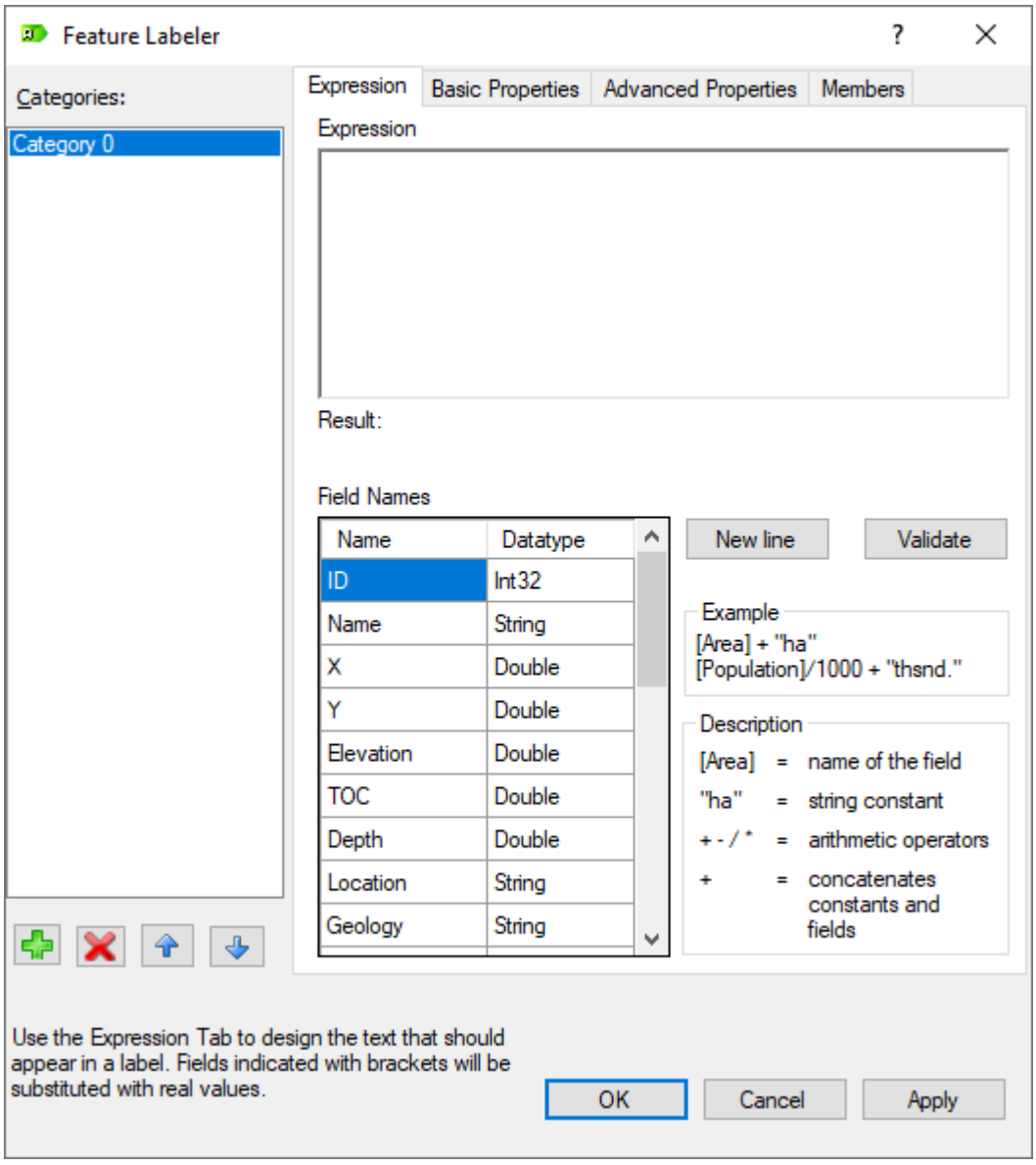
You can  add or  remove a label category. Label categories can be reordered by selecting a layer and using the  and  buttons.



Expression

The Expression tab provides an interface that helps you define the label values for the current label category.

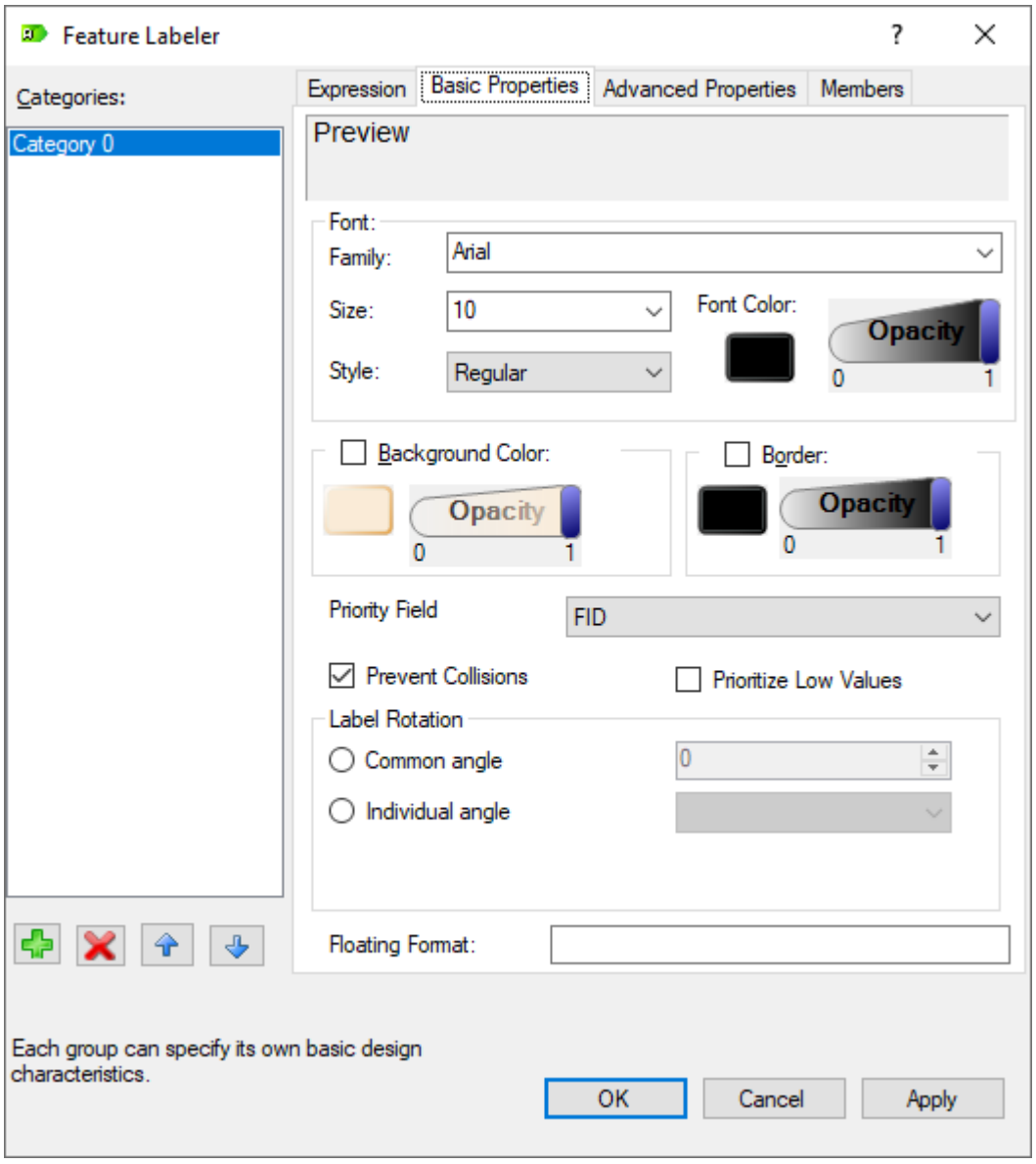
- **Expression**: the input form to define the label based on field attributes
- **Field Names**: provides a list of fields in the attribute table. Clicking a field name will select it. Double-clicking a field name will add it to the statement input.
- **New Line button**: adds a line break to the label expression
- **Validate button**: allows you to test the input statement and will return an example the statement is valid and an error if not.



Please Note: field names that include a space are not supported by the labeling engine and will - you will need to change the alias of the field name in the Template Manager.

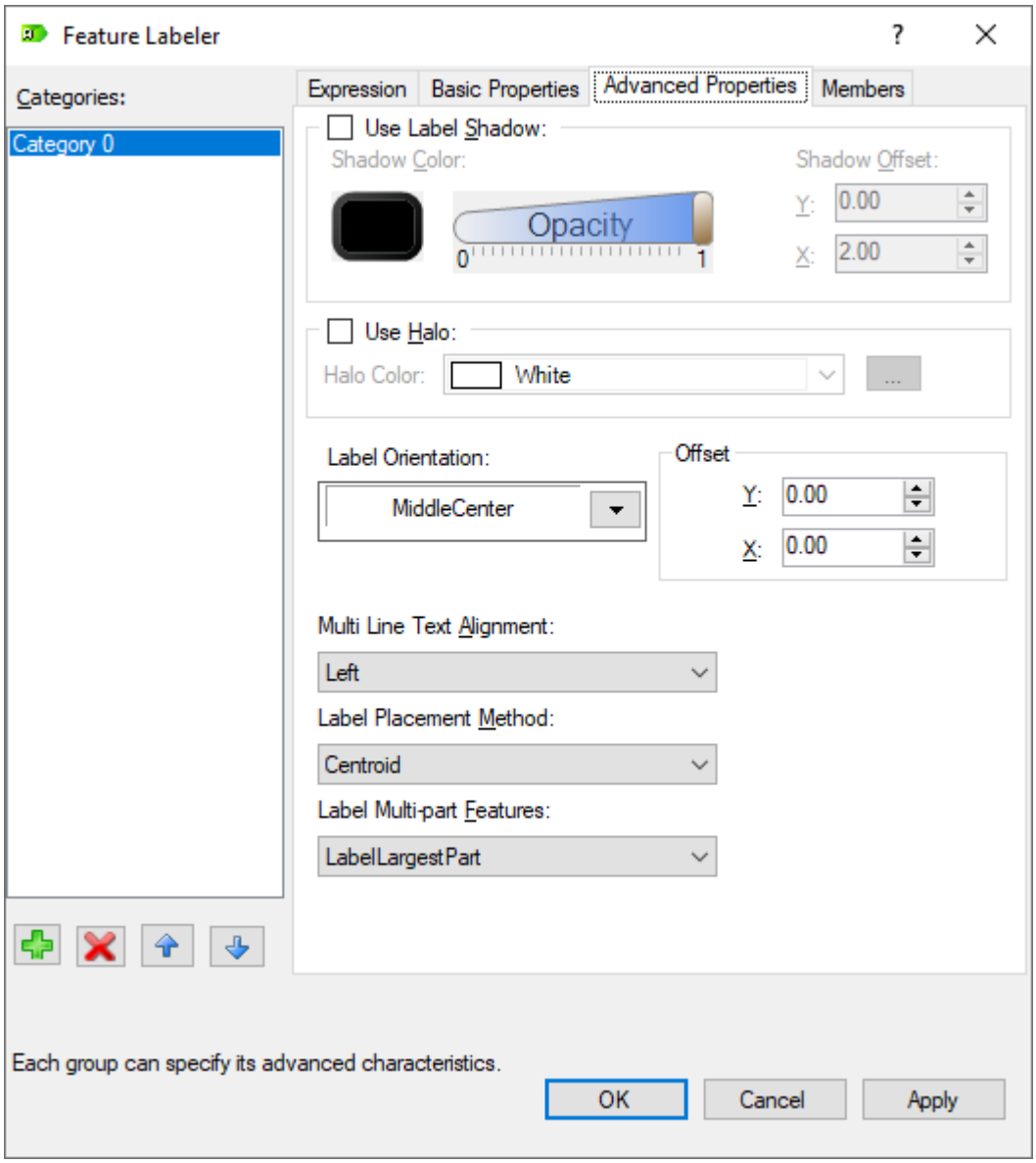
Basic Properties

The Basic Properties tab provides an interface for setting some basic labeling settings for the current label category, including font, background, border, collision handling, and label rotation:



Advanced Properties

The Advanced Properties tab provides an interface for setting more advanced labeling settings for the current label category, including shadows, halos, orientation, alignment, and offsets:



Members

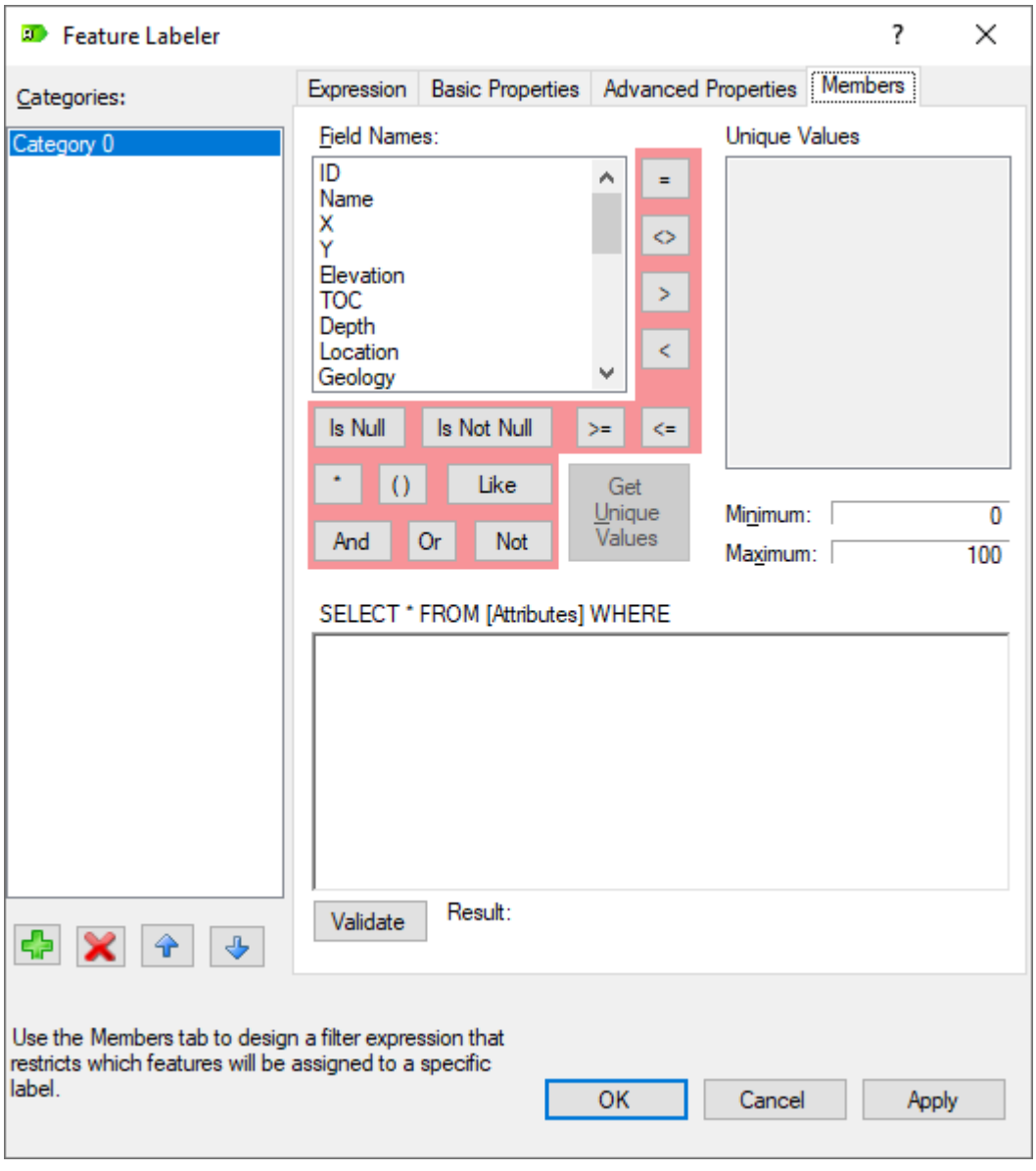
The Members tab provides an interface that helps you build a query statement that will be used to determine which features in the current label category will be labeled.

- **Field Names**: provides a list of fields in the attribute table. Clicking a field name will select it. Double-clicking a field name will add it to the statement input.
- **Unique values**: provides a list of the unique values in the currently selected field when the "Get Unique Values" button is pressed
- **Operator buttons**: provides a set of buttons(highlighted in light red) representing common keywords/operators used in SQL statements. Clicking a button will add it to

the statement input

- **Statement input**: the input form to complete the SQL statement (SELECT * FROM [Attributes] WHERE...) that determines which features will be used to determine which features in the current label category will be labeled.

- **Validate button**: allows you to test the input statement and will return an example the statement is valid and an error if not.

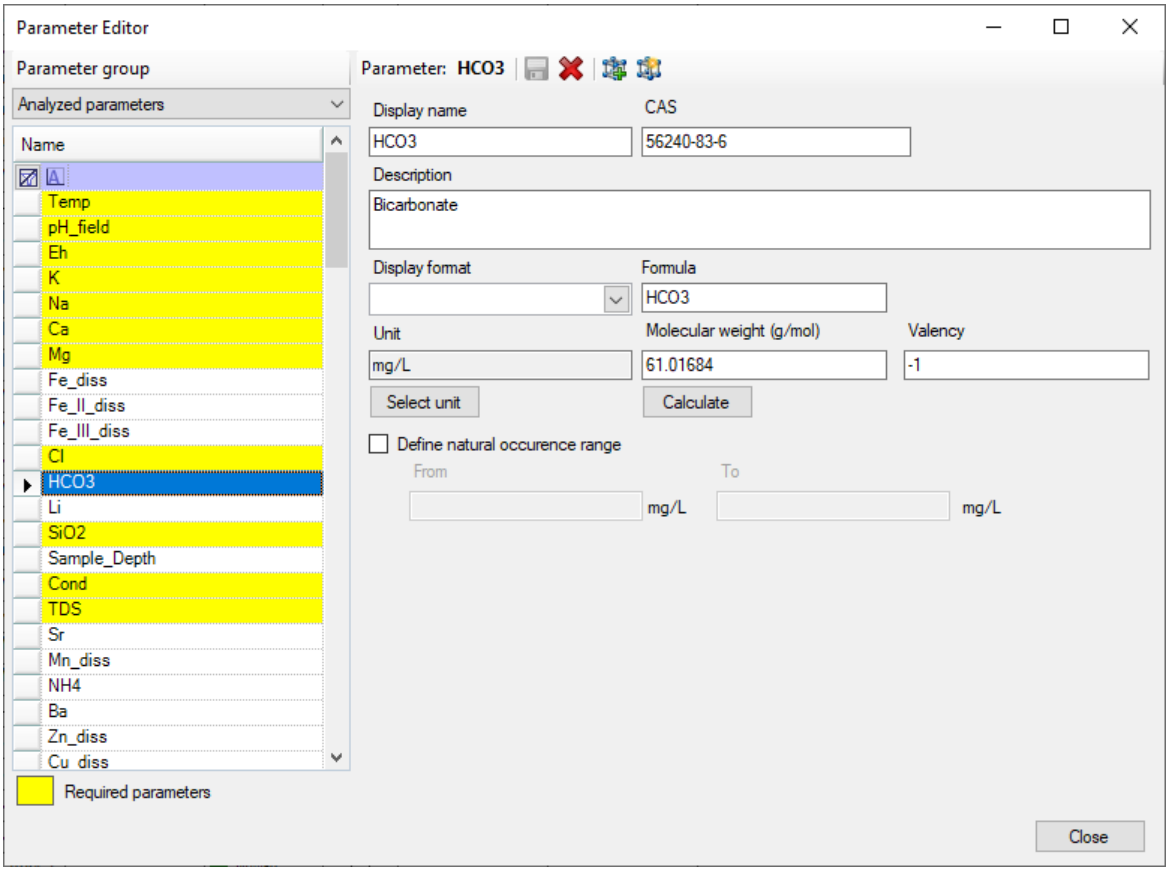


An example statement would be:

([SampleDate] > #1/1/2000 12:00 AM# AND [SampleDate] < #1/1/2010 12:00 AM#) AND [WATERTYPE] LIKE 'Ca*'

Chapter 9 Parameter Editor

The Parameter Editor allows you to create, manage, and define parameters parameters in your project. You can open the Parameter Editor from the Modules menu or click on the  button in the main toolbar. The Parameter Editor will appear as a tab in the main AquaChem view, as shown in the following example:

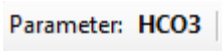


Please Note: If you make changes to any of the Parameters, AquaChem will reload your project, which includes resetting your views and prompting you to save changes to other modules.

On the left side of the tab you will find a list of parameters that can be filtered using a dropdown list of the Parameter Groups and the standard filter bar in AquaChem. The right side of the Parameter Editor window provides the tools to manage the selected parameter and its associated metadata using the relevant forms and the following buttons on the parameter editor toolbar:

Parameter Editor Toolbar

The Parameter Editor toolbar contains the following controls:

- 

Parameter: Displays the name of the currently selected parameter.
-  **Save**: saves changes to the currently selected parameter.
-  **Delete:** deletes the currently selected parameter.
-  **Add Parameter:** adds a new parameter from the Chemical List.
-  **New Parameter:** adds a new blank parameter to the project.

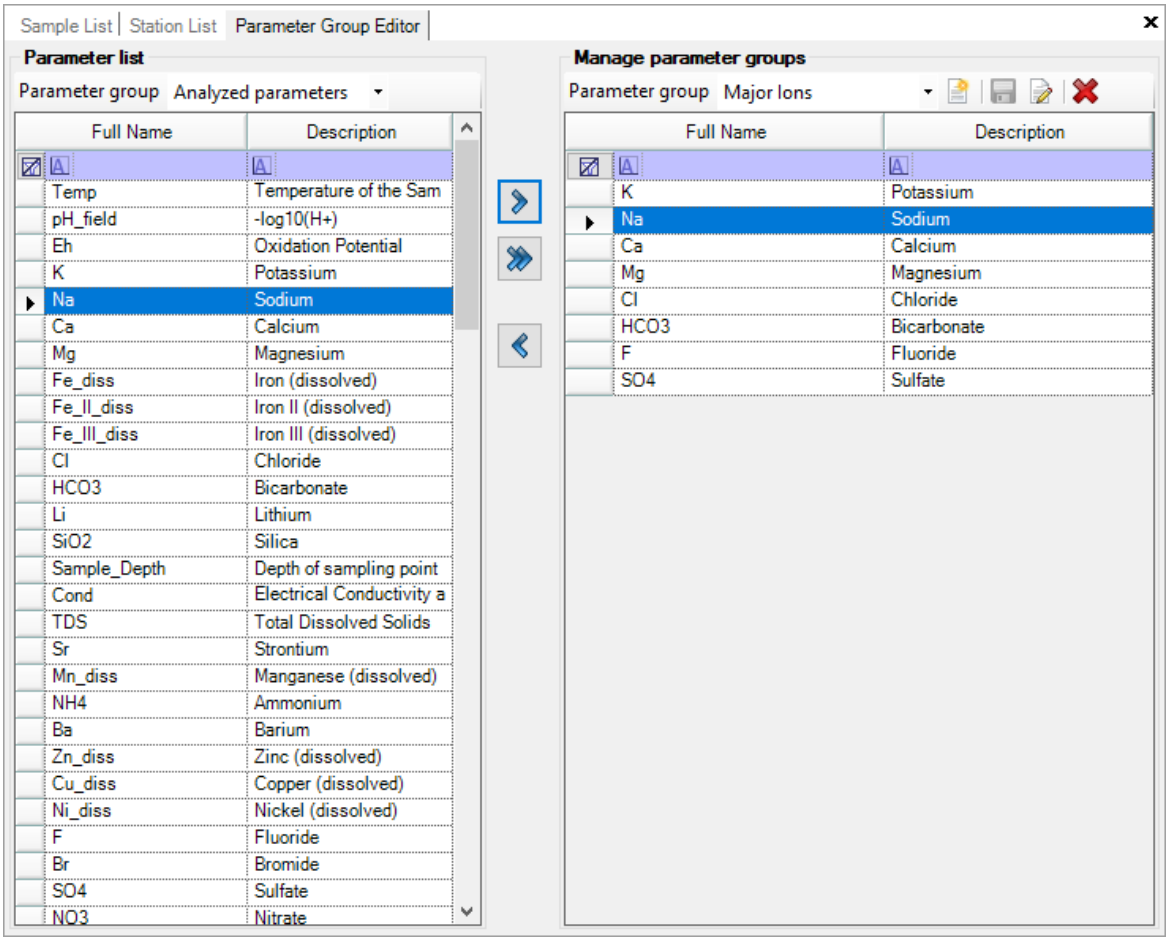
Parameter Information

Information about all measured parameters is managed below the Parameter Editor toolbar and stored in the Parameter Table. Parameter metadata information includes the relevant chemical and descriptive attributes as follows (using bicarbonate as an example):

- **Short Name**: a unique, typically short or abbreviated, name that is easily recognizable (e.g. HCO3) and used as a look up name and a primary key
- **Display Name**: a longer descriptive name (e.g. bicarbonate) used for labeling in plots and tables
- **CAS**: Chemical Abstracts Service (CAS) Registry number (e.g. 56240-83-6), a unique number assigned by CAS, a division of the American Chemical Society.
- **Description**: typically a more descriptive name that may include a list of alternate names (e.g. bicarbonate; hydrogencarbonate)
- **Formula**: chemical formula (e.g. HCO3)
- **Molecular Weight:** combined atomic weights of all constituent atoms that compose the parameter (e.g. HCO3 = 1x1.00794 + 1x12.0107 + 3x15.9994 = 61.01684 g/mol)
- **Valency:** the ionic/electric charge of the parameter in solution (e.g. -1).

Chapter 10 Parameter Group Editor

The Parameter Group Editor allows you to create and manage groupings of project parameters. Parameter groups make it easier to find and work with parameters in other modules, such as the results pane of the Sample List view, Plot Collections, and R-Console. AquaChem includes some automatic parameter groups as well as custom parameter groups.



The '**Parameter list**' (left) side of the Parameter Group Editor includes a list of parameters from which to select and build parameter groups. You can filter the parameter list using the '**Parameter group**' dropdown, which includes both automatic parameter groups and custom parameter groups. The '**Manage parameter groups**' (right) side of the Parameter Group Editor includes controls that allow you to edit parameter groups.

Automatic parameter groups

There are a number of parameter groups that are built into AquaChem. The list of parameters within each of these automatic parameter groups is dynamically generated by AquaChem as follows:

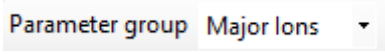
- **Analyzed Parameters:** includes measured parameters with at least one result
- **Cations:** measured parameters with a positive valence
- **Anions:** measured parameters with a negative valence
- **Ions:** measured parameters with a non-zero valence
- **Required:** measured parameters required in calculations/functions and commonly used in many of the plots
- **Used in standard:** measured parameters that are included in an active water quality standard
- **All measured parameters:** all measured parameters included in the project database

Custom parameter groups

In AquaChem, you can create and manage custom lists of parameters using the right side of the Parameter Group window. Custom parameter groups can be used to facilitate working with the sample list view, plot collections, and sample reports. Custom parameter groups can be generated using the controls described below.

Parameter Editor Toolbar

The Parameter Editor contains the following controls:

- 

Parameter group: allows you to select which parameter group is active.
-  **New Parameter Group:** creates a new empty parameter group.
-  **Save**: saves changes to the active parameter group.
-  **Rename:** allows you to rename the active parameter group.
-  **Delete:** deletes the active parameter group from the database.
-  **Remove Parameter:** removes the selected parameter(s) selected from the active parameter group on the right side of the Parameter Group Editor.
-  **Add Parameter:** adds the selected parameter(s) selected from the parameter list on the left side of the Parameter Group Editor to the active parameter list

-  **Add All Parameters:** adds all parameter(s) selected from the parameter list on the left side of the Parameter Group Editor to the active parameter list

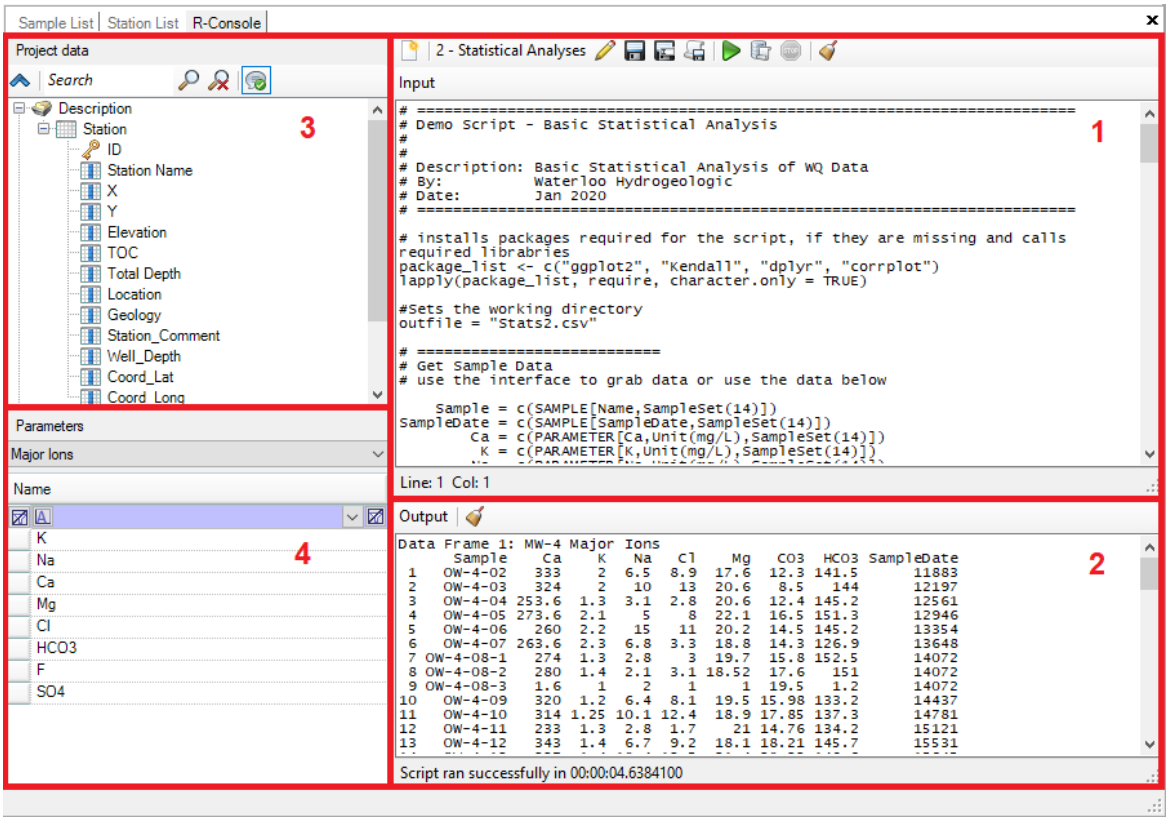
Chapter 11 R-Console

R is a freely available scripting language and environment for statistical computing developed by the R Foundation and supplemented by an active user community which provides a vast variety of statistical and graphical procedures. The R-Console has been built into AquaChem to leverage the extensive data science libraries available in R.

Please Note: The R-Console is meant to be a light-weight utility that provides a direct connection to your project data rather than a replacement for more comprehensive integrated development environments (IDE) for R such as RStudio. As the R programming language is well documented at the R-Project website and other sites, the documentation provided in this section is limited to descriptions of the functionality of the R-Console and a few distinct differences between the version of R used in the R-Console module of AquaChem and standard R.

The R-Console module is divided into four separate panes:

1. Input pane: a workspace to develop and input R scripts,
2. Output pane: outputs from scripts will appear here,
3. Project Data pane: allows you to easily add list variables containing values from a project database field from a given station group, and
4. Parameters pane: allows you to easily add list variables containing parameter values from a given sample set.



Input Pane

The Input pane provides a workspace to develop R scripts. The Input pane includes the tools described above as well as a status bar that provides a line and column counter for the location of the cursor.

R-Console Toolbar

The R-Console contains the following controls:

- **New Script:** creates a new empty script.
- **Rename:** allows you to rename the current script.
- **Save**: saves changes to the current script.
- **Save As**: saves changes as a new script.

-  **Export to File:** saves the script as an external file.
-  **Run:** runs the entire script.
-  **Parse:** parses AquaChem-specific commands (e.g. the list constructors built using the interface) into the raw data that can be run in native R interfaces such as RGui or RStudio.
-  **Stop:** stops a running script.
-  **Clear:** clears variables in active memory from previous script runs

Differences between R-Console scripts and standard R scripts

There are several differences between the R scripts available in the AquaChem R-Console and standard R-scripts:

- **Multi-line commands:** multi-line commands in many implementations of R do not require a line-continuation character. In the case of R-Console, a '+' must be placed in the first column of each continued line. To facilitate this, you can press <SHIFT>+<ENTER> to continue a line and a '+' will be added for you. An example of a continued line from the second script in the AquaChem Demo Project tutorial is shown below:

```
chart1 <- ggplot(df, aes(x=X, y=Y)) +
+    geom_point() +
+    ggtitle("Monitoring Well Coordinates") +
+    labs(x = "Easting (m)", y = "Northing (m)")
```

- **Comments:** similar to standard R, the '#' symbol defines a code comment and text following this character will not be interpreted as part of the script. furthermore, comments in the R-Console can also be in any column of the script; however, unlike other implementations of R they cannot interrupt multi-line commands without causing an error.

- **Output**: by default, most implementations of R echo commands from the script. Given the potential for large datasets in AquaChem, the echo has been disabled in R-Console so that script performance is not degraded. The output pane only displays information that is passed through the `print()` command.

- **Project Data variables:** R-Console includes custom commands that allow AquaChem to inject project data into R. In this process, each script is interpreted in two passes, the first by AquaChem to convert these custom commands (this is equivalent to the parse  button), the second pass is the interpretation of the R script itself. An example from the second script in the AquaChem Demo Project tutorial is shown below:

R-Console script with project data

```
Sample = c(SAMPLE[Name,SampleSet(14)])
```

Equivalent Parsed R-script with project data

```
Sample = c("OW-4-02", "OW-4-03", "OW-4-04", "OW-4-05", "OW-4-
06", "OW-4-07", "OW-4-08-1", "OW-4-08-2", "OW-4-08-3", "OW-4-
09", "OW-4-10", "OW-4-11", "OW-4-12", "OW-4-13", "OW-4-14",
"OW-4-15", "OW-4-16", "OW-4-17", "OW-4-18")
```

For more information, see the sections on the Project Data pane and the Parameter Pane.

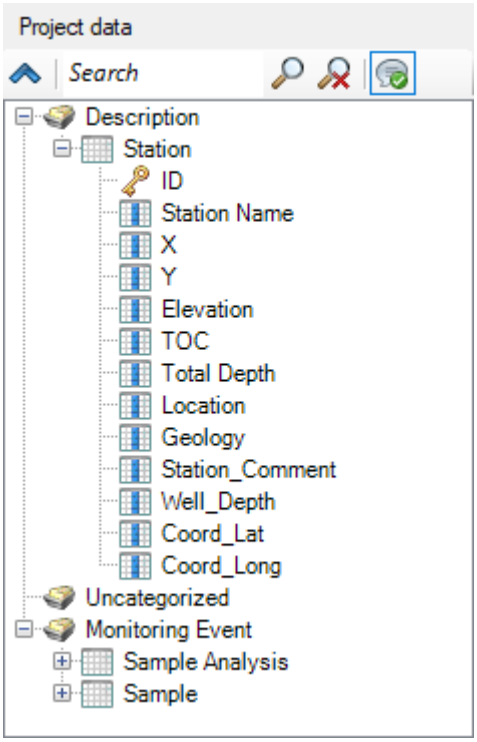
Output Pane

The Output pane displays output from R scripts that have run. The Output pane contains one button, (the Clear button), which clears any output from the pane, and a status bar at the bottom of the pane which provides information (e.g. whether a script is running or how long scripts have taken to run). As described above, in order to improve the performance and runtimes of scripts, the Output pane only broadcasts information from `print()` commands.

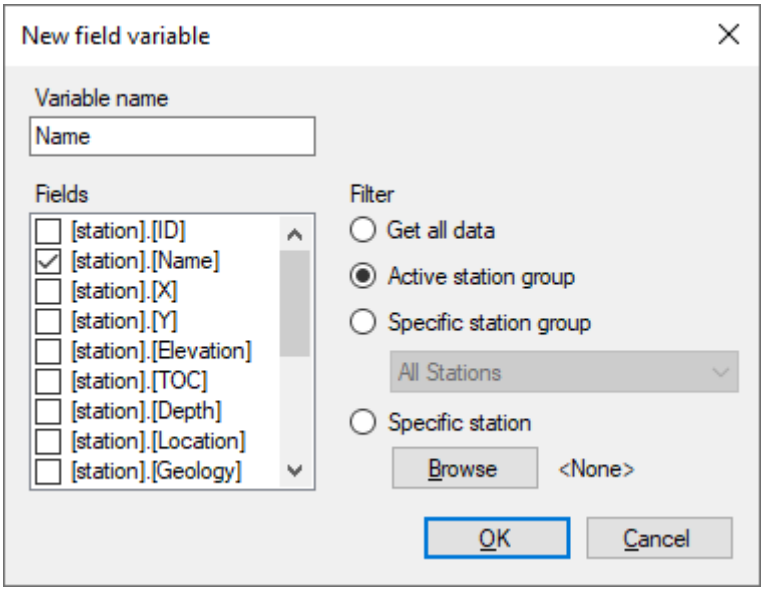
Project Data Pane: **Adding a Project Data Variable**

The Project data pane includes a hierarchical tree of the database structure organized by data categories > tables > fields. The pane also includes controls:

- **Collapse tree:** collapses the Project data tree
- **Search:** searches the project database using the search term in the input box to the left
- **Clear Search:** clears the search bar
- **Show Tooltips:** toggles whether tooltips are shown when hovering the mouse pointer over a given entry in the tree



Double-clicking a field in the project tree opens the New field variable window:



The following inputs are included in the window:

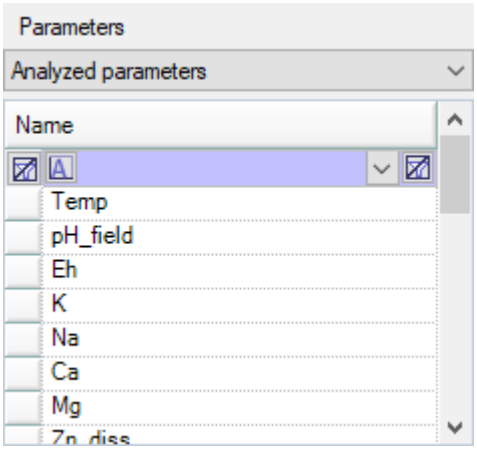
- **Variable name:** the name that will be used in the script, by default, this will be the name of the selected field
- **Fields:** allows you to select a field that will be

- **Filter:** allows you to constrain the data using one of the following options:
  - *Get all data:* returns all data in the table from the selected field
  - *Active Station Group:* data will be limited to the active station group
  - *Specific Station Group:* data will be limited to the selected station group in the Project Explorer using the accompanying dropdown menu
  - *Specific station:* data will be limited to the selected station; the browse button will invoke a Station picker

Click the OK button to add the new list variable subject to the constraints listed above.

Parameter Pane: **Adding a parameter variable**

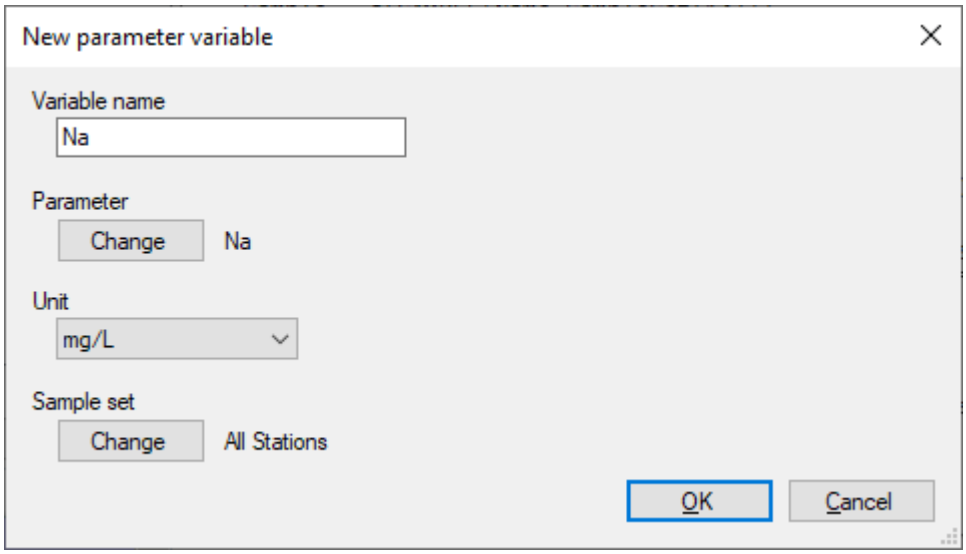
A parameter picker is included in the R-Console module to facilitate adding a list variable to your script that includes the values of the selected parameter for a specified sample set.



The parameter picker includes a parameter group dropdown menu containing:

- **Automatic parameter groups:** station parameters, sample parameters, analyzed parameters, cations, anions, ions, calculated parameters, and parameters used in a standard; and
- **Custom parameter groups:** parameter groups created in the Parameter Group Editor

If you wish to add a parameter variable, use the parameter group dropdown menu and/or the filter bar to find the desired parameter. Once you've located the parameter, you can select it by double-clicking it and the new parameter variable window will appear:



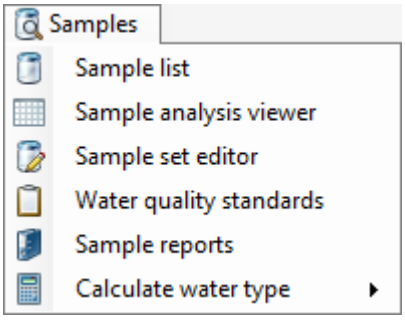
The following inputs are included in the window:

- **Variable name:** the name that will be used in the script, by default, this will be the name of the selected parameter
- **Parameter:** the parameter that you selected; you can change the parameter if you need to by selecting the Change button
- **Unit:** the unit that will be used for the parameter (from the same unit category as the parameter)
- **Sample Set:** allows you to select the sample set for which the variable applies

Click the OK button to add the new parameter list variable to your script at the current cursor location in the Input window.

Chapter 12 Sample Module

Modules specifically related to Samples in AquaChem 10.0 can be found in this menu. Each module is summarized below and explained in further detail in following sections:



Sample List

The Sample List provides an interface for managing samples and results. The following features are available:

- Adding, deleting, and editing samples
- Adding, deleting, and editing results for the active sample
- Comparing results to active Water Quality Standards
- Creating static sample sets

For more details, please refer to the Sample List section.

Sample Analysis Viewer

The Sample Analysis Viewer provides an interface for viewing and filtering analytical results for selected samples or for the active station or sample set. The following features are available:

- View sample results from a Sample Set, Station Group, a Selected Station or Selected Samples
- View and filter data based on one or more criteria
- Optionally view associated fields from the Station and/or Sample tables in the same record

For more details, please refer to the Sample Analysis Viewer section.

 Sample Set Editor

The Sample Set Editor provides the tools create dynamic sample sets and station groups based on one or more user-defined conditions. The following features are available:

- Save, edit, load, and delete a sample set
- Create station groups based on the current sample set
- Define, edit, and delete sample set conditions that are based on the values of:
  - station parameters (e.g. station name)
  - sample parameters (e.g. analysis date)
  - sample results (e.g. concentration of a specified parameter)
  - sample results relative to water quality standards

For more details, please refer to the Sample Set Editor section.

 Water Quality Standards

The Water Quality Standards tab allows you to work with water quality standards in your project. The following features are available:

- Save, edit, and delete a water quality standard
- Import a Water Quality Standard from Excel or delimited text files
- Add, edit, delete water quality criteria for given parameters

For more details, please refer to the Water Quality Standards section.

 Sample Reports

The Sample Reports tab allows you to create custom tabulations of your samples and their results based on one or more criteria including: station, sample date ranges, parameters or groups, and/or exceedances of one or more active Water Quality Standards. The report can also produce general statistics for samples included in the report.

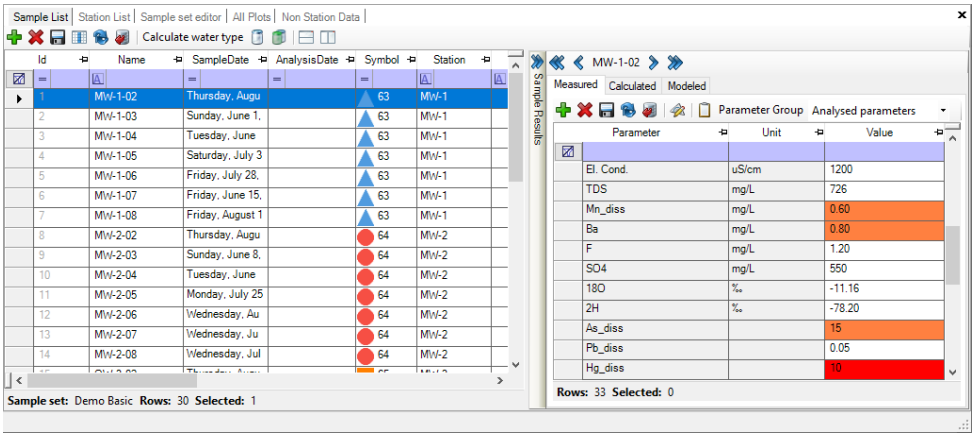
For more details, please refer to the Sample Report section.

 Calculate Water Type

The Calculate Water Type menu item allows you to determine the major ionic constituents in your sample(s) based on the results and specified parameters. For more details, please refer to the Calculate Water Type section.

12.1 Sample List

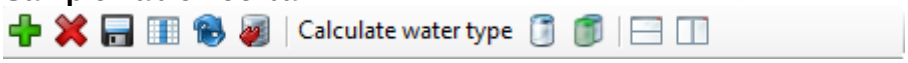
The Sample List tab provides an overview of the samples in the selected Sample Set or Station Group. This tab displays fields from the Sample table (left) and also displays results for the active sample, as denoted by the ▶ symbol in the sample table (right). Note that results with values that exceed an active Water Quality Standard will be color coded.



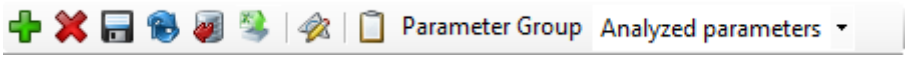
Toolbars

The Sample table and results viewer toolbars in the Sample List tab contain the following controls:

Sample Table Toolbar

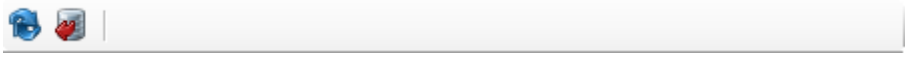


Measured Sample Results Toolbar



Calculated Sample Results Toolbar

Modeled Sample Results Toolbar



 Adds a new record to the appropriate (i.e. sample or result) table.

 Deletes the currently selected record(s) from the project database.

 Saves the changes you have made to the project database.

 Allows you to select which columns you want to show or hide in the sample table.

 Refreshes the data from the project database.

 Exports the data from the applicable table.

 Calculates the water type for the selected record(s).

 Calculates the water type for all records in the sample list.

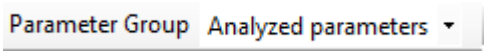
 Splits the sample table and results viewer horizontally.

 Splits the sample table and results viewer vertically.

 Exports the data from the applicable table to a selected Excel Template file.

 Provides the option to display concentration results using a single/consistent unit for all applicable parameters in the results viewer.

 Provides the option to display the active water quality standards.



Allows you to filter displayed results to the selected parameter group.

 Writes the active calculated field (denoted by ) to a selected numeric field in the Sample List.

 Opens the calculation settings for the project.

Working with the Data

The first line shown on the sample table in the Sample List Tab contains field names/column headers; below this is the filter line, which is highlighted in light blue and denoted by the clear filter button () in the left-most column. The filter line can be used to restrict records to display based on the values in one or more field and is described in detail in the Data Filtering section.

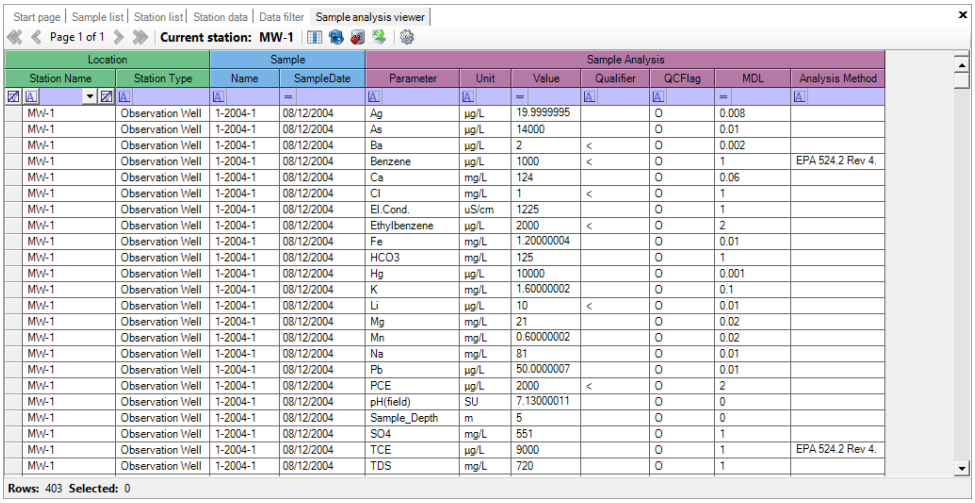
You can select one or more records (that will turn bright blue) in the data table by clicking on the buttons on the left-hand side of the grid (using the <SHIFT> and <CRTL> keys for selecting multiple records). You can perform the several actions by right-clicking on the selected record(s) in the currently displayed table, including showing/hiding fields and

records, copy, paste, adding the selected station(s) to a new/existing station group, refreshing the data from the project database, and resizing the columns to fit the station list table within the current workspace.

Values in the data fields may be modified for a selected sample (simply click in the cell you wish to edit); or a new sample may be created here (selecting the ✚ icon), and the values for these fields may be defined. The Sample List tab may be used to quickly enter numerous samples and their results.

12.2 Sample Analysis Viewer

The Sample Analysis Viewer tab provides information about all of the samples collected samples in the selected Sample Set or Station Group. This tab displays fields from the Sample table (left) and also displays results for the active sample, as denoted by the ▶ symbol in the sample table (right). Note that results with values that exceed an active Water Quality Standard will be color coded.



Toolbar

The Sample table and results viewer toolbars in the Sample List tab contain the following controls:

Sample Analysis View Toolbar

Navigates data pages; skipping to the first page (in the sort order), to the previous page, to the specified page, to the next page or to the last page.

 Allows you to select which columns you want to show or hide in the sample analysis table.

 Refreshes the data from the project database.

 Exports the data from the applicable table.

 Exports the table to a selected Excel workbook based on a selected template.

 Allows you to configure the view including the data source, whether or not to display fields from the station or sample tables, and pick highlight colors for column headers.

Working with the Data

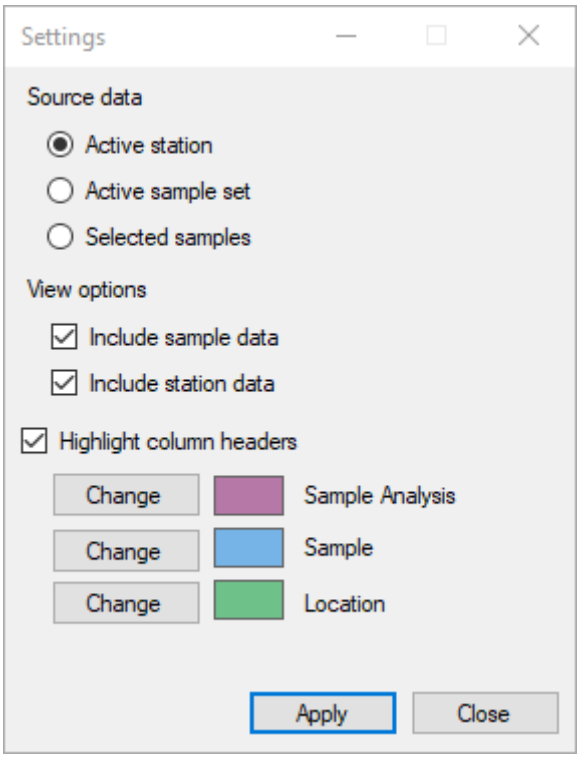
The first line shown on the sample table in the Sample List Tab contains field names/column headers; below this is the filter line, which is highlighted in light blue and denoted by the clear filter button () in the left-most column. The filter line can be used to restrict records to display based on the values in one or more field and is described in detail in the Data Filtering section.

You can select one or more records (that will turn bright blue) in the data table by clicking on the buttons on the left-hand side of the grid (using the <SHIFT> and <CRTL> keys for selecting multiple records). You can perform the several actions by right-clicking on the selected record(s) in the currently displayed table, including showing/hiding fields and records, copy, paste, adding the selected station(s) to a new/existing station group, refreshing the data from the project database, and resizing the columns to fit the station list table within the current workspace.

Values in the data fields cannot be modified in this view. You must modify values in the Sample List, Station List, or Station Data tabs.

Configuring the Sample Analysis View

Selecting the settings  button in the Sample Analysis View will open the Settings dialog (shown below), which has the following options:



- **Source Data:** choose which data are shown in the Sample Analysis view table. Available data sources are the active station, active sample set, or selected samples. These can be selected using the Sample Picker or Station Picker as appropriate.

- **View Options:** show/hide fields from the Sample table and/or the station table.

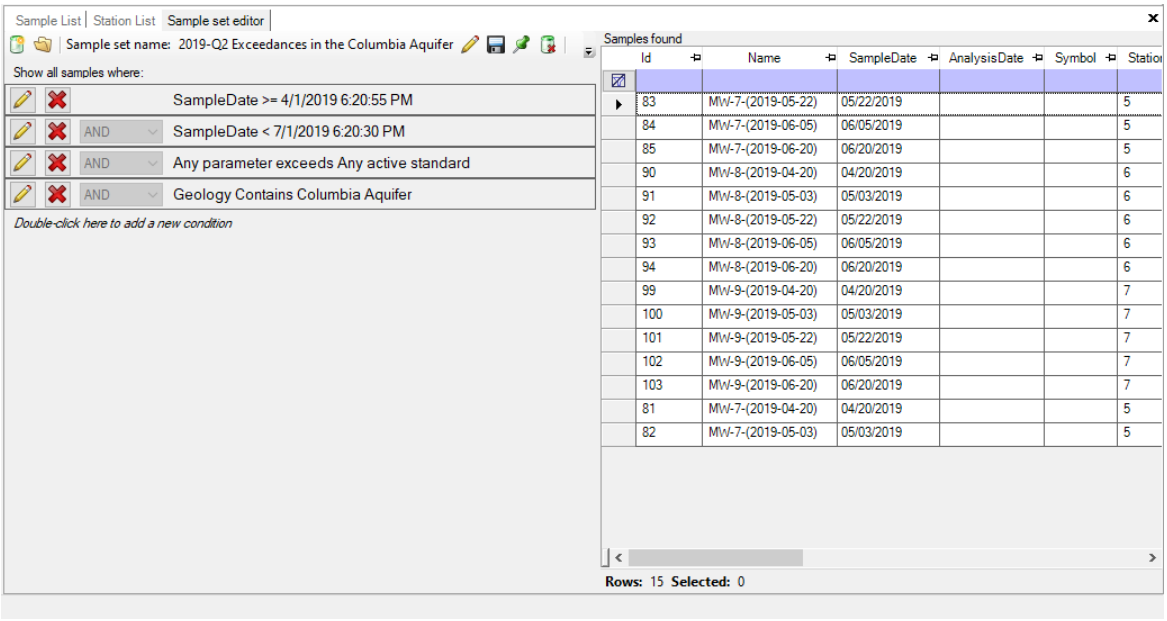
- **Highlight column headers:** optionally define highlight colors for the Sample Analysis, Sample, and Station (location) tables.

12.3 Sample Set Editor

The Sample Set Editor allows you to build dynamic sets of samples that meet one or more specified conditions. You can use the Sample Set Editor to quickly find samples of interest, such as:

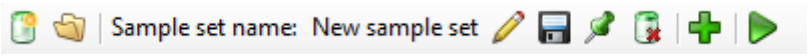
- *Samples that were collected during a specified time range (e.g. 2019-Q2 samples);*
- *Samples with exceedances of a particular water quality standard; and/or*
- *Samples collected from a particular stream or aquifer*

The Sample Set Editor allows you to build these types of conditional statements into a query as shown below:



Sample Set Editor Toolbar

The Sample Set Editor toolbar contains the following controls:



- **New Dynamic Sample Set:** create a new dynamic sample set.
- **Open:** Open an existing dynamic sample set.
- **Rename:** Allows you to rename the current dynamic sample set
- **Save:** saves changes to the current dynamic sample set.
- **Dynamic Station Group:** creates a dynamic station group that is tied to the current sample set, so that the station group includes the stations where at least one sample is included in its parent sample set. Modifying the conditions of the dynamic station group's parent sample set will similarly modify the results of the dynamic station group.
- **Delete:** deletes the current dynamic sample set.
- **Add Condition:** adds a new condition to the current dynamic sample set.

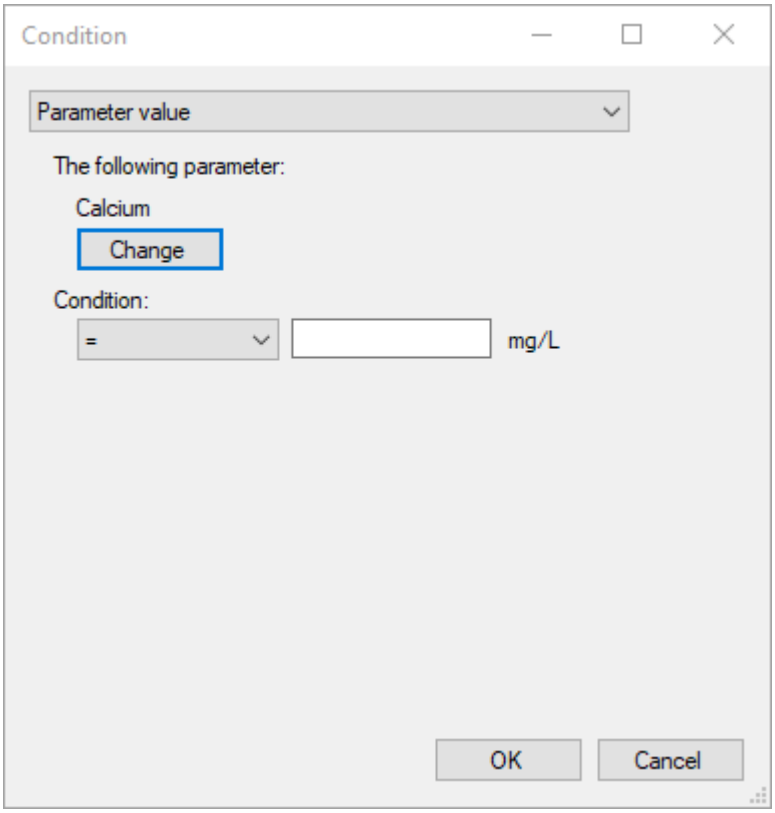
- **Test Sample Set:** creates a preview of the samples that belong to current dynamic sample set based on the current set of conditions.

Adding Sample Set Conditions

When adding a condition to the current sample set, the Condition dialog will be shown. The Condition dialog provides options to build the condition you wish to use to constrain/build a dynamic sample set. The dropdown at the top of the window provides two options:

Parameter value

When using this option, the condition will be based on a comparison between the value of a station, sample, or analytical parameter and a specified constant:

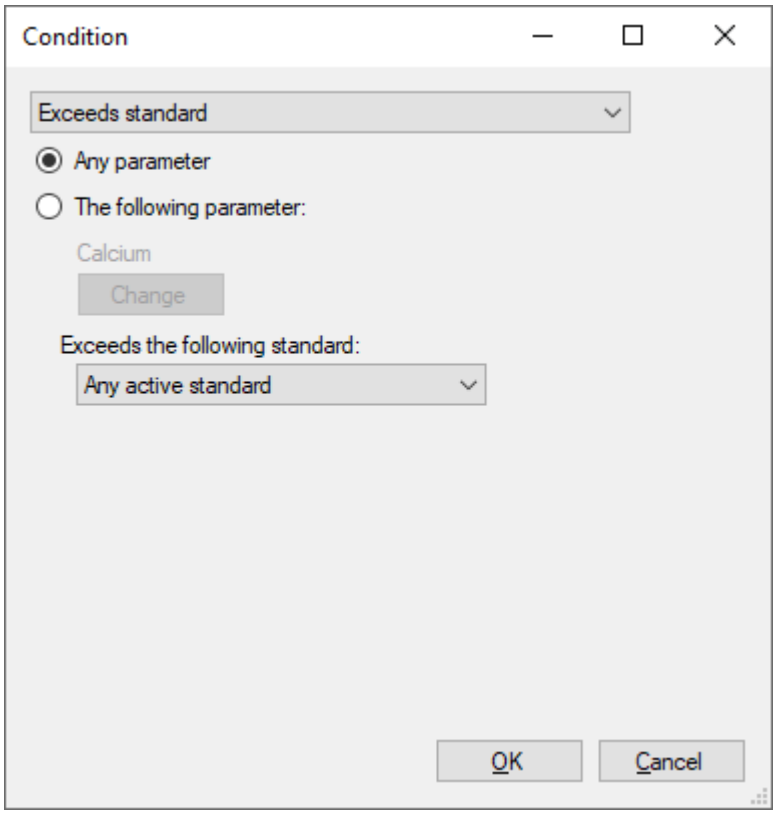


Depending on the parameter data type, you will provided with different conditional operators:

Numeric Parameter	String Parameter
>	=
>=	Starts with
<	Ends with
<=	Contains
=	Does not contain

Exceeds standard

When using this option, the condition will be based on whether one or any analytical parameter exceeds one or any of the active Water Quality Standard(s):



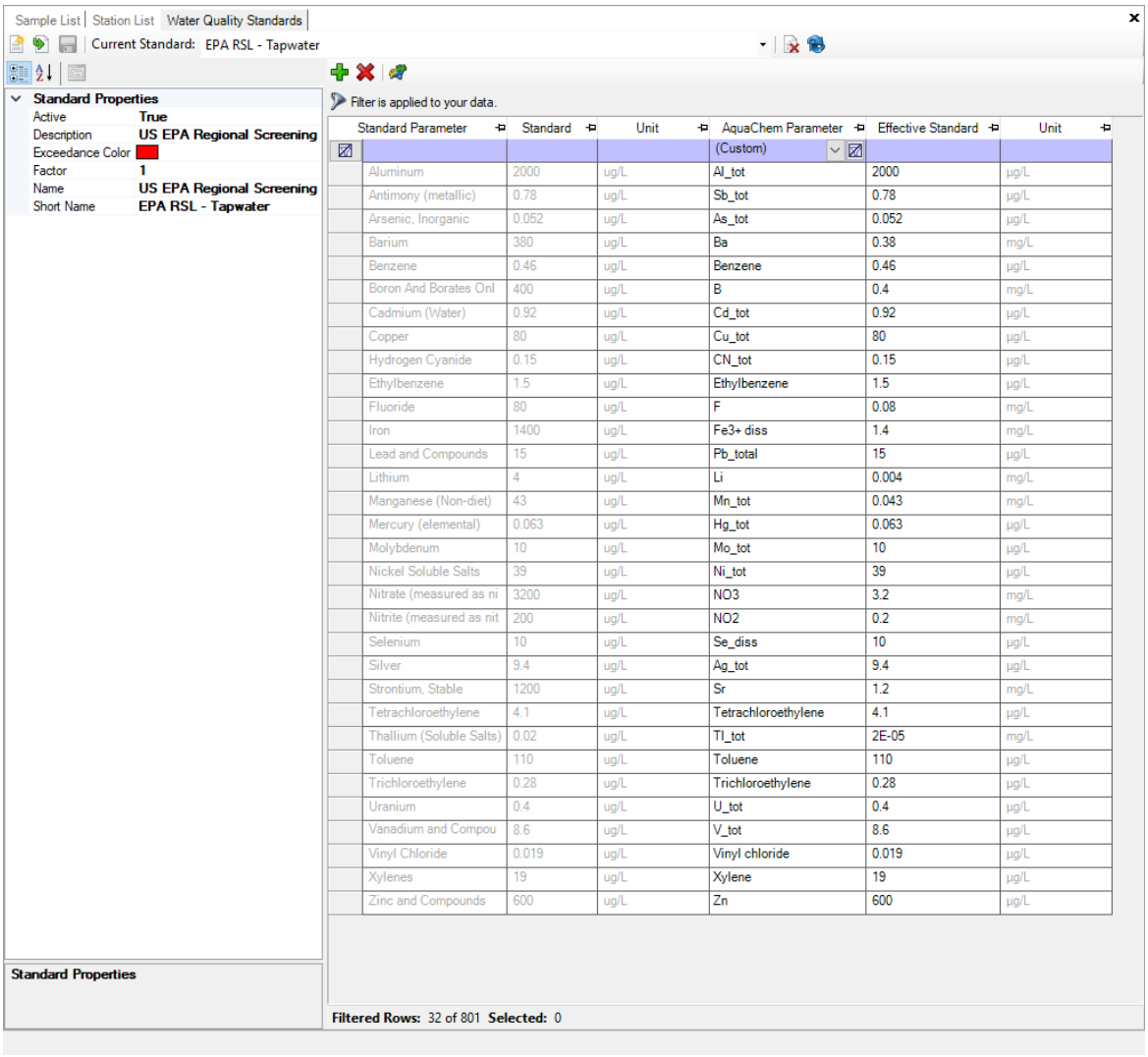
12.4 Water Quality Standards

The Water Quality Standards view allows you to manage Water Quality Standards in the current project in AquaChem. The options in this view allow you to see and modify water quality standard criteria and create or import new sets of standards. These standards are used throughout AquaChem, including in the Results pane of Sample List view, when adding conditions to the Sample Set Editor, building a Sample Report, and adding Plots. Multiple standards can be made active in the project, allowing you to check values against a mix of criteria across jurisdictions (Federal, State/Provincial, local) or target receptors (human health: drinking water, dermal contact, etc. or the environment: aquatic fish, agricultural receptors, etc.).

Parameter values exceeding their respective water quality standards will be highlighted using a color code specific to each water quality standard when displaying the data throughout AquaChem. Measured parameters which exceed these pre-defined levels are highlighted in predefined colors depending upon specified preferences. This allows you to quickly identify

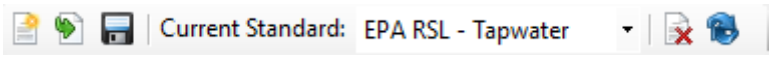
sample exceedances and water samples which may be harmful to human health and the environment.

The Water Quality Standard view can be accessed by selecting **Samples > Water Quality Standards** from the Main Menu.



Toolbar

The main toolbar of the Water Quality Standard view contains the following controls:

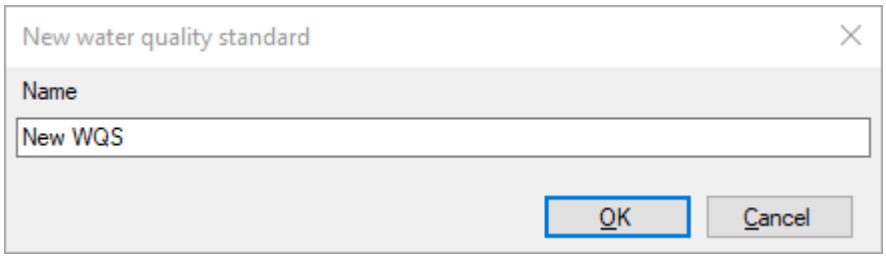


- **Create a new standard:** create a new water quality standard.

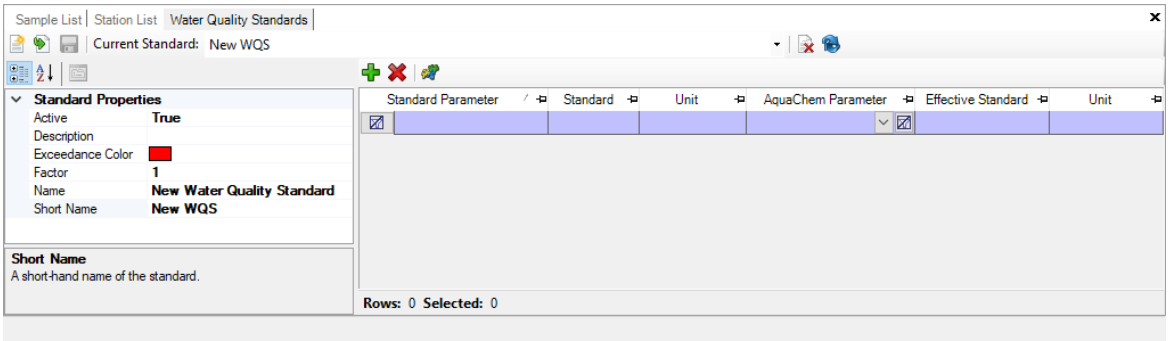
- **Import:** imports a water quality standard from an existing file.
- **Save changes:** saves changes to the current water quality standard.
- Current Standard: EPA RSL - Tapwater **Standard Dropdown Menu:** Allows you to specify the current selected water quality standard, which will be shown in the Water Quality Standard viewer to view and/or modify.
- **Delete standard:** deletes the currently selected water quality standard.
- **Refresh:** refreshes the currently selected water quality standard from the database and discards any unsaved changes.

Creating a New Water Quality Standard

To create a new water quality standard, select the **Create a new standard** button. You will first be prompted to provide a (short) name for the standard that will be used to identify the standard in the database and in the Standard Dropdown Menu (e.g. New WQS):



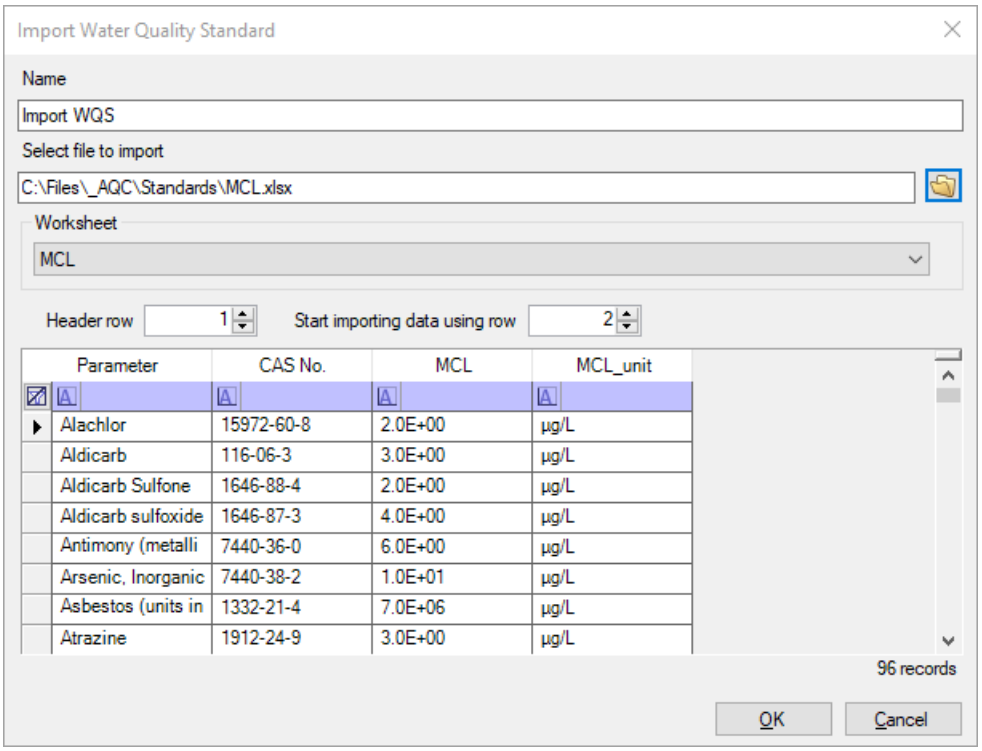
Once you have entered a name, Click OK and AquaChem will create a new blank water quality standard that you can edit:



For more information, see the section on editing existing water quality standards.

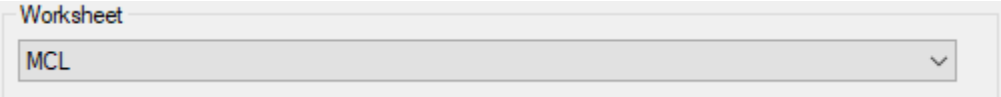
Importing a Water Quality Standard

To create a new water quality standard by importing the standards from an external file, select the **Import** button to open the Import Water Quality Standard window:

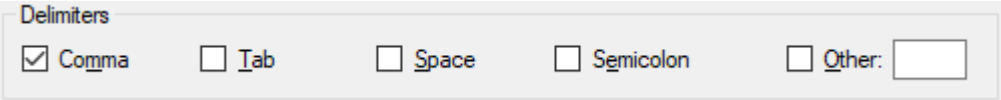


At the Import Water Quality Standard window, you must enter the following information to complete the import:

- **Name:** a (short) name for the standard that will be used to identify the standard in the database and in the Standard Dropdown Menu;
- **Select file to import:** enter the full path of the file to be imported or select the button to navigate to the file. Note that excel (.xlsx, .xls) and comma delimited text files (.csv) are supported;
- **Worksheet** (shown if importing an Excel file) allows you to select which worksheet to import;



- **Delimiter** (shown if importing a text file) allows you to select which delimiter(s) separate the data fields to be imported;

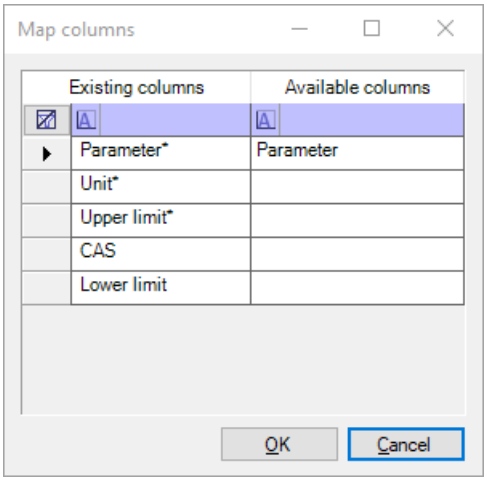


- **Header row:** the row containing headers for the data fields to be mapped
- **Start Importing data using row:** the row where the data starts (default = 2)

Below these inputs, you will be shown a preview of the data to be imported. Click OK to proceed.

Map Columns

At this step in the import process, you will be asked to map the following fields in the standard to be imported:



- **Parameter*:** the parameter to which the standard applies
- **Unit*:** the unit of measurement of the standard for the given parameter. If the unit is different from the specified of the parameter in the project but of the same unit category, it will be converted at the edit window.
- **Upper limit*:** the value above which the parameter will exceed the standard
- **CAS:** the Chemical Abstract Service (CAS) number of the parameter. The CAS number will be used to match parameters where the project parameter and imported standard parameter name do not match exactly.
- **Lower Limit:** the value below which the parameter will not comply with the standard. If not specified, the lower limit will not be considered in the project.

Please Note: fields marked by an asterisk (*) are required, you must map these fields in order to finish importing the standard.

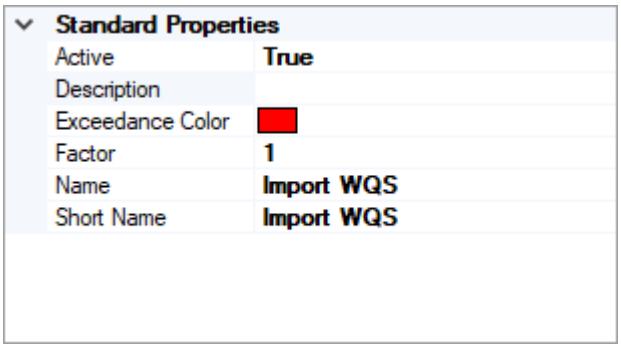
Click OK to finish the import. Once the standard has been imported, it will be shown in the Water Quality Standard view and you can review and edit the standard as necessary.

Editing an Existing Water Quality Standard

The currently selected water quality standard (i.e. the standard that is selected in the **Standard Dropdown Menu**) will be shown in the Water Quality Standard view, which consists of two parts: the left side contains a list of the properties of the currently selected standard, while the right side contains a list of the criteria of the currently selected standard.

Standard Properties

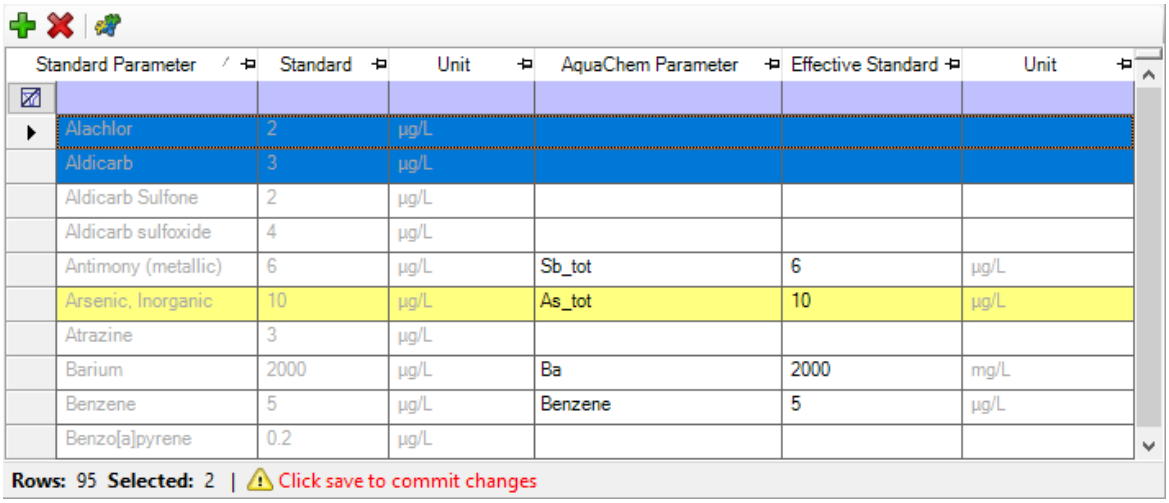
The left side of the Water Quality Standards view shows the properties of the currently selected standard:



- **Active**: a Boolean *(True/False)* variable that allows you to specify if the standard is *active*. Standards that are active (i.e. Active = True) in the project will be available throughout AquaChem including in the results pane of the Sample List, when adding conditions to the Sample Set Editor, building a Sample Report, and adding Plots. Standards that are inactive (i.e. Active = False) will be unavailable in these features
- **Description:** a description of the Standard. You may include pertinent information about the standard in this field such as the data of applicability, references, promulgating agency, etc.
- **Exceedance color:** a color picker control. The color you chose will be used to highlight cells where parameter values exceed the standard.
- **Factor:** a value from 0 to 1 (default =1). All values in the standard will be multiplied by this value, which can be used to add a factor of safety when evaluating parameter values against the selected standard
- **Name:** the name of the water quality standard
- **Short Name:** an abbreviated name for the water quality standard

Standard Parameter Values

The right side of the Water Quality Standards view shows the standard criteria table and a toolbar:



Standard Parameter	Standard	Unit	AquaChem Parameter	Effective Standard	Unit
Alachlor	2	µg/L			
Aldicarb	3	µg/L			
Aldicarb Sulfone	2	µg/L			
Aldicarb sulfoxide	4	µg/L			
Antimony (metallic)	6	µg/L	Sb_tot	6	µg/L
Arsenic, Inorganic	10	µg/L	As_tot	10	µg/L
Atrazine	3	µg/L			
Barium	2000	µg/L	Ba	2000	mg/L
Benzene	5	µg/L	Benzene	5	µg/L
Benzo[a]pyrene	0.2	µg/L			

Rows: 95 Selected: 2 | Click save to commit changes

Standard Criteria table

The standard criteria table includes the following six columns that describe the criteria in the standard:

Imported Standard Criteria Fields - the following columns are populated when importing a standard and are not editable:

- **Standard Parameter:** the name of the imported parameter
- **Standard:** the value of the criteria for the given imported parameter
- **Unit:** the measurement unit of the imported parameter

AquaChem Standard Criteria Fields - the following columns are editable and are the actual standards that your project will use:

- **AquaChem Parameter:** the name of the parameter in the project. Only mapped parameters in this column will be used elsewhere in the application. To map a parameter, click in the cell and you can select the parameter using the parameter picker.
- **Effective Standard:** the value of the criteria for the given project parameter. Values will only be shown for mapped parameters using the project parameter units
- **Unit:** the measurement unit of the project parameter; can only be edited in the Parameter Editor.

Edited criteria will be highlighted yellow ( ), while selected criteria will be highlighted in blue ( ).

Toolbar

The toolbar includes the following controls:

- **Add a parameter:** adds a new row to the standard. If selected, a new row will appear in the standard. You can click in the new row to select a parameter using the parameter picker.
- **Remove selected parameters:** removes the selected parameter(s) from the standard.
- **Auto-map selected parameters:** maps selected parameters.

12.5 Sample Report

The Sample Report provides you with the tools to build a customized summary of sample results for a select set of samples that includes optional statistics and comparisons to one or more active standards.

The Sample Report view can be accessed by selecting **Samples > Sample Report** from the Main Menu.

Toolbar

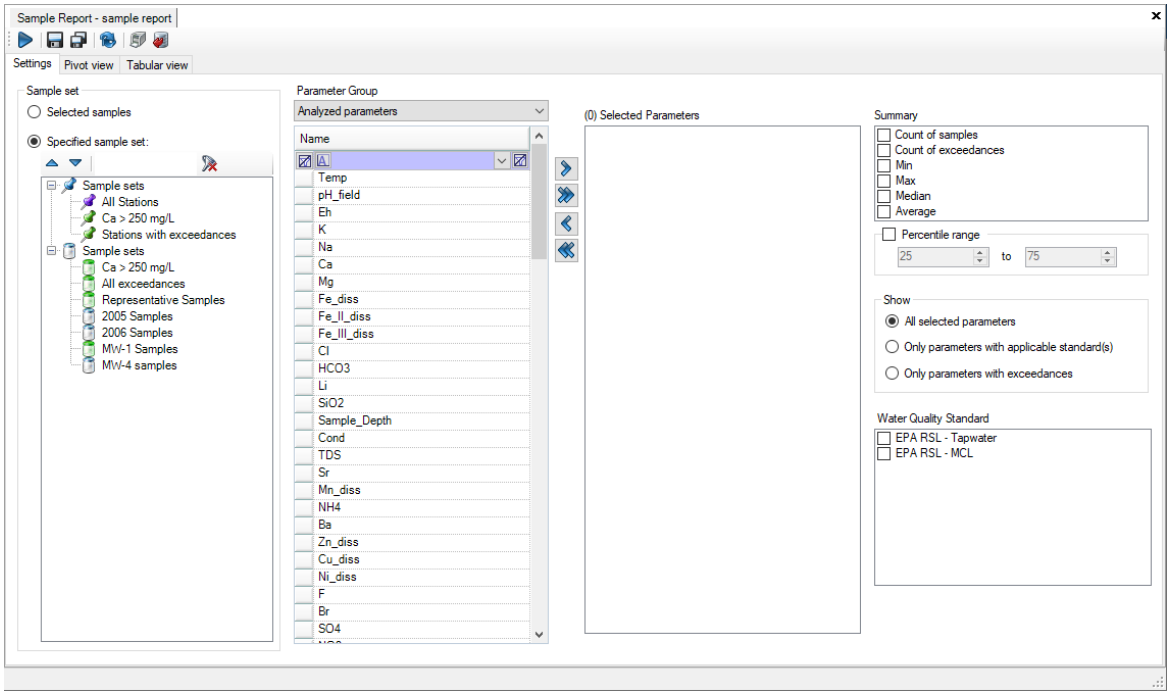
The main toolbar of the Sample Report view contains the following controls:

- **Execute:** builds the sample report based on the current criteria.
- **Save:** saves the sample report.
- **Save As:** saves a new copy of the sample report.
- **Refresh:** refreshes the sample report and project database and discards any unsaved changes
- **Print Preview:** provides a print preview of the sample report when viewing the Pivot View or the Tabular View.

- **Export Data:** exports the Pivot View or the Tabular View, whichever is active.

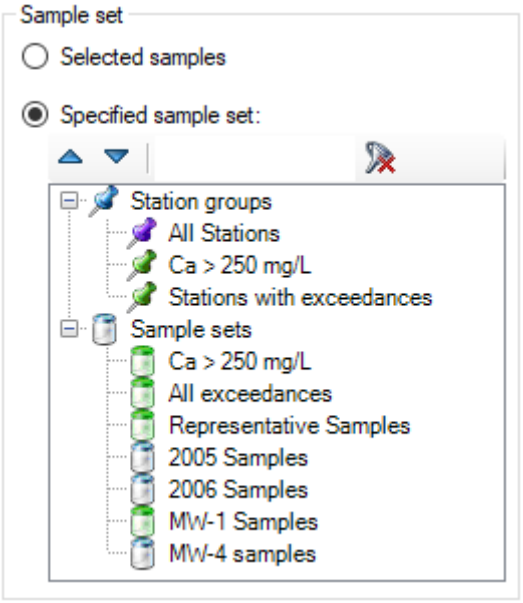
Settings View

The Settings View allows you to build the Sample Report by selecting a set of samples and a group of parameters. The report may also include statistics about the set of samples for each parameter and comparisons to one or more water quality standards.



Sample Selection

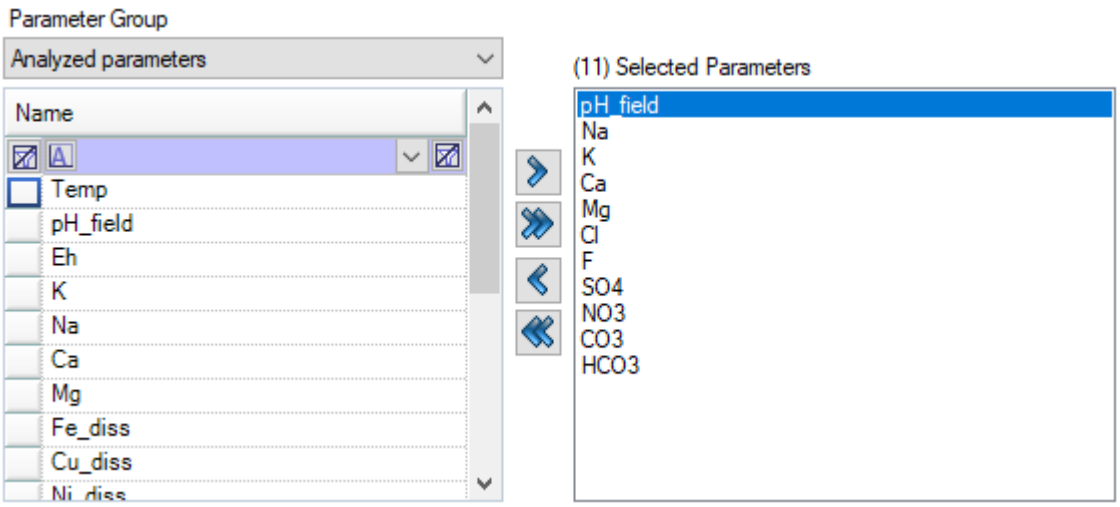
The left-most portion of the settings tab contains options to include the selected samples or a selected sample set or station group.



Parameter Selection

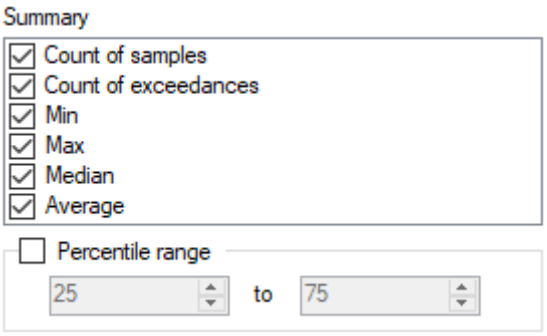
The middle portion of the Settings tab contains a parameter picker. Parameters can be selected for use in the Sample Report by using the directional arrows:

- add selected parameters to the Sample Report
- add all parameters in the sample picker to the Sample Report
- remove selected parameters from the Sample Report
- remove all parameters from the Sample Report



Statistics

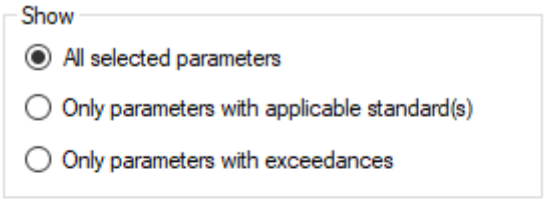
The following statistics may be included in the Sample Report:

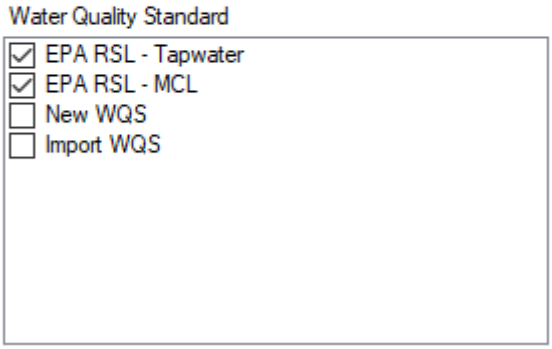


Standards

As part of the Sample Report, you may select one or more Water Quality Standards to include in the report. Options include:

- **All selected parameters:** all parameters will be included in the sample report
- **Only parameters with applicable standard(s):** only parameters with an applicable standard will be included in the sample report.
- **Only parameters with exceedances:** only parameters that exceed an



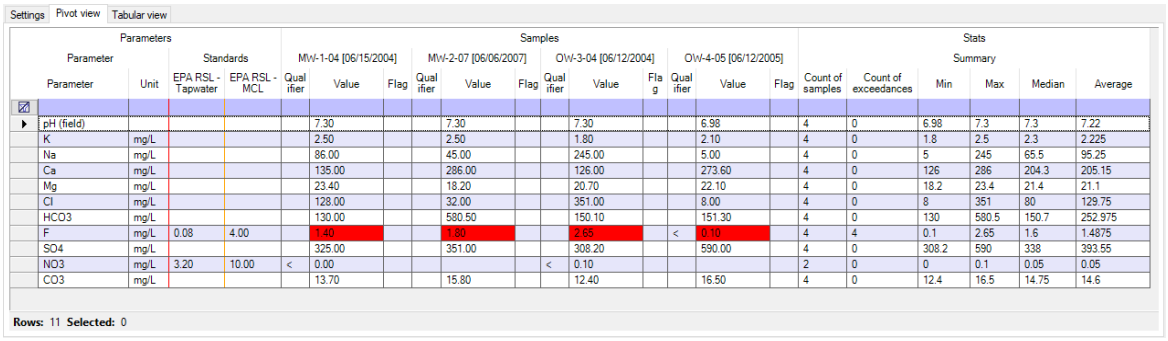


Only active water quality standards will be shown in the list of available standards.

Pivot View

The Pivot view provides a structured view of the Sample Report. Columns will be shown in the following order:

- **Parameters:** the names of parameters selected in the settings
- **Unit:** units of the project parameters
- **Standards:** water quality standards selected in the settings
- **Samples:** samples selected in the settings. A column for the qualifier, value, and data flags will be shown for each sample. Values that exceed a standard will be highlighted using the exceedance color of that standard
- **Statistics:** statistics selected in the settings



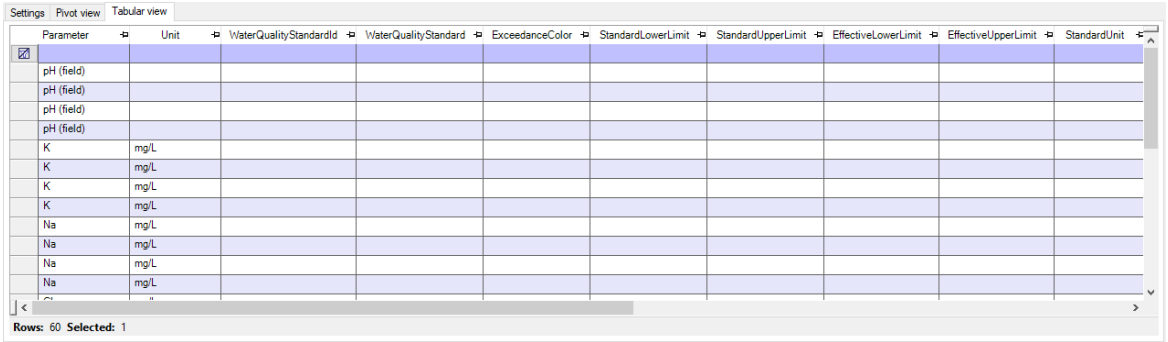
Settings | Pivot view | Tabular view

Parameters		Standards		Samples											Stats					
Parameter				MW-1-04 [06/15/2004]			MW-2-07 [06/06/2007]			OW-3-04 [06/12/2004]			OW-4-05 [06/12/2005]		Summary					
Parameter	Unit	EPA RSL - Tapwater	EPA RSL - MCL	Qualifier	Value	Flag	Qualifier	Value	Flag	Qualifier	Value	Flag	Qualifier	Value	Flag	Count of samples	Count of exceedances	Min	Max	Median	Average
pH (field)					7.30			7.30			7.30			6.98		4	0	6.98	7.3	7.3	7.22
K	mg/L				2.50			2.50			1.80			2.10		4	0	1.8	2.5	2.3	2.225
Na	mg/L				86.00			45.00			245.00			5.00		4	0	5	245	65.5	95.25
Ca	mg/L				135.00			286.00			126.00			273.60		4	0	126	286	204.3	205.15
Mg	mg/L				23.40			18.20			20.70			22.10		4	0	18.2	23.4	21.4	21.1
Cl	mg/L				128.00			32.00			351.00			8.00		4	0	8	351	80	129.75
HCO3	mg/L				130.00			580.50			150.10			151.30		4	0	130	580.5	150.7	252.975
F	mg/L	0.08	4.00		1.40			1.30			2.65		<	0.10		4	4	0.1	2.65	1.6	1.4875
SO4	mg/L				325.00			351.00			308.20			590.00		4	0	308.2	590	338	393.55
NO3	mg/L	3.20	10.00	<	0.00					<	0.10					2	0	0	0.1	0.05	0.05
CO3	mg/L				13.70			15.80			12.40			16.50		4	0	12.4	16.5	14.75	14.6

Rows: 11 **Selected:** 0

Tabular View

The tabular view provides a "flat" database view of the Sample Report that may be useful for exporting to other applications.



Settings | Pivot view | Tabular view

Parameter	Unit	WaterQualityStandardId	WaterQualityStandard	ExceedanceColor	StandardLowerLimit	StandardUpperLimit	EffectiveLowerLimit	EffectiveUpperLimit	StandardUnit
pH (field)									
pH (field)									
pH (field)									
pH (field)									
K	mg/L								
K	mg/L								
K	mg/L								
K	mg/L								
Na	mg/L								
Na	mg/L								
Na	mg/L								
Na	mg/L								

Rows: 60 **Selected:** 1

12.6 Calculate Water Type

The Calculate Water Type sub-menu that is accessible through the Samples item in the Main menu (and related functions in toolbar of the Sample List) allow you to calculate the Water Type of a sample.

Theory

The Water Type, also known as the water facies, of a sample describes its major ionic constituents. The Water Type of a given sample will be influenced by the interaction of the water with the minerals that it has been in contact with. These types of interactions include precipitation, dissolution, ion exchange, geological structure, and the mineralogy of watershed/aquifer.

The Water Type is determined by calculating the percent contribution of each cation and anion to the total concentration of ions in solution on a equivalents per liter basis. In AquaChem, you can calculate a "short" water type or a "long" water type. The "short" water type is calculated by concatenating the cation and anion with the highest equivalent concentrations. The "long" water type is calculated by concatenating cations and anions with concentrations above a specified percent contribution threshold.

The threshold for determining if an ion is major is normally 10%; however in some countries 12.5% is more common. the higher the threshold, the smaller number of parameters that may exceed this threshold is. Usually, only major ions (Na, Ca, Mg, HCO3, Cl, SO4) will have a concentration that allows them to exceed the defined threshold. If you want to make sure, that other important elements such as potassium or nitrate appears in the water type expression, then you can achieve this by lowering the threshold value. Examples of short and long water calculations are shown in Table 1 below.

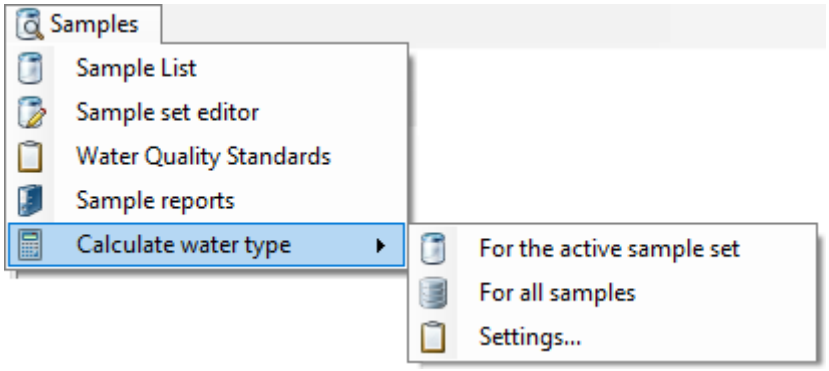
Table 1. Major Ions and Water Type for Example Samples

		SAMPLE			
		MW-1-04	**MW-2-07**	**OW-3-04**	**OW-4-05**
Cations					
	Na^+	3.74 (15%)	1.96 (5%)	10.66 (28%)	0.22 (1%)
	K^+	0.06 (0.2%)	0.06 (0.2%)	0.05 (0.1%)	0.05 (0.1%)
	Ca^{2+}	6.74 (26%)	14.72 (40%)	6.29 (17%)	13.65 (34%)
	Mg^{2+}	1.93 (8%)	1.50 (4%)	1.70 (4%)	10.81 (27%)
Anions					
	Cl^-	3.61 (14%)	0.90 (2%)	9.90 (26%)	0.23 (1%)
	HCO_3^-	2.13 (8%)	9.51 (26%)	2.46 (6%)	2.48 (6%)
	CO_3^{2-}	0.46 (2%)	0.53 (1%)	0.41 (1%)	0.55 (1%)
	SO_4^{2-}	6.77 (27%)	7.31(20%)	6.42 (17%)	12.28 (30%)

	SAMPLE			
	MW-1-04	MW-2-07	OW-3-04	OW-4-05
Water Type				
Short	Ca-SO4	Ca-HCO3	Na-Cl	Ca-SO4
Long (20%)	Ca-SO4	Ca-HCO3-SO4	Na-Cl	Ca-SO4
Long (10%)	Ca-Na-SO4-Cl	Ca-HCO3-SO4	Na-Ca-Cl-SO4	Ca-SO4

Menu Commands

The options in the menu include:



Calculate the water type:

- **For the active sample set:** calculates the water type for the active sample set, that is the sample set shown in the sample list
- **For all samples:** calculates the water type for all samples in the project database
- **Settings...:** opens the Water Type tab in the project settings window and allows you to configure how the water type will be calculated.

Water Type Toolbar Commands in the Sample List

The Sample List view also contains buttons to help you calculate the water type for samples in the active sample set:

Calculates the water type for the selected record(s).

Calculates the water type for all records in the sample list.

Chapter 13 Plot Module

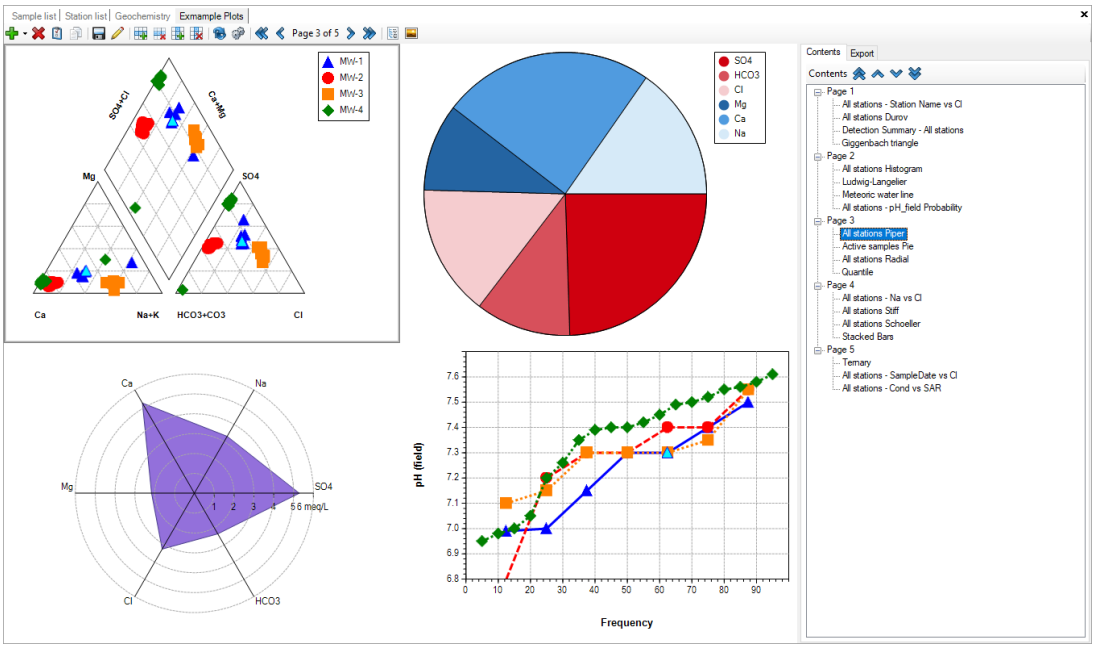
In AquaChem, you can easily create collections of plots to visualize, analyze, summarize, and report on your data. Plot collections consist of one or more plots. There are nineteen different plot types available. When you select Plots from the main menu and then New Plot Collection, a new plot collection will be created and you can add () any of the available plot types:

- Box and Whisker
- Detection Summary
- Durov Plot
- Giggenbach Triangle
- Histogram
- Ludwig-Langelier Plot
- Meteoric Water Line (MWL) Plot
- Pie Chart
- Piper Diagram
- Probability Plot
- Quantile Plot
- Radial Plot
- Scatter Plot
- Schoeller Plot
- Stacked Bars Plot
- Stiff Plot
- Ternary Plot
- Time Series
- Wilcox Plot

AquaChem allows you to create multiple plots for the same data set and view these plots simultaneously within the Windows environment. Each of these plots is explained in greater detail later in this chapter. The following sections also describe some of the features that are common to all plots and how to organize your plots into plot collections.

13.1 Plot Collections

Plots in AquaChem are organized into plot collections, which consist of one or more individual plots. The layout of a plot collection can be adjusted using the main toolbar of the Plot Collection view and reordered using the table of contents. The plot collection can be shown in as a print preview mode and exported the plots to an image or a report template using the export layout.



Toolbar

The Plot Collection toolbar is contains the following controls:

 Add a new plot at the end of the Plot Collection

 Delete the currently selected plot

 Open the plot settings dialog for the currently active plot

 Clone the current plot

 Save the plot collection configuration

 Rename the plot collection

 Add a row to the page layout of the plot collection

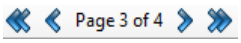
 Remove a row from the page layout of the plot collection

 Add a column to the page layout of the plot collection

 Remove a column from the page layout of the plot collection

 Refresh plots

 Open the plot settings dialog

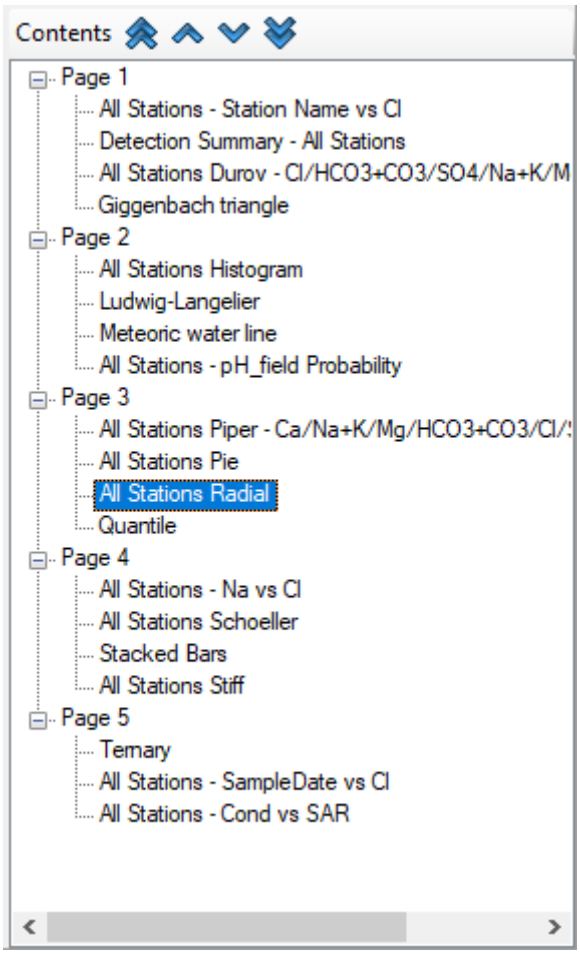
 Page Navigation controls

 Open/close the plot collection Table of Contents

 Open/close the plot collection Export Layout

Table of Contents

The table of contents in the plot collection displays a list of the plots that belong to the collection. If the plot layout includes multiple plots per page (using the add rows  or columns ), then the table of contents is displayed as a tree with a node for each page and subnodes for each plot on a given page - plots will be drawn in order from left to right and then top to bottom. For example, the radial plot that is selected in the table of contents below and shown in the image above is the third item on the page and is located in first column of the second row.



You can navigate to any plot in the collection by clicking on its title. You can also reorganize/reorder plots using the toolbar.

The tool bar buttons move the selected plot within the plot collection as follows:

 top/beginning of the collection

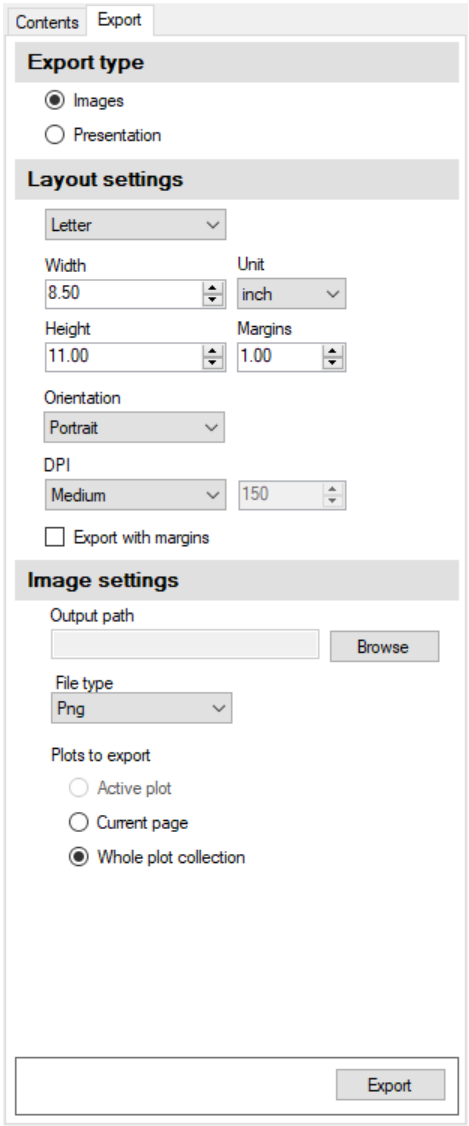
 up/backward one position

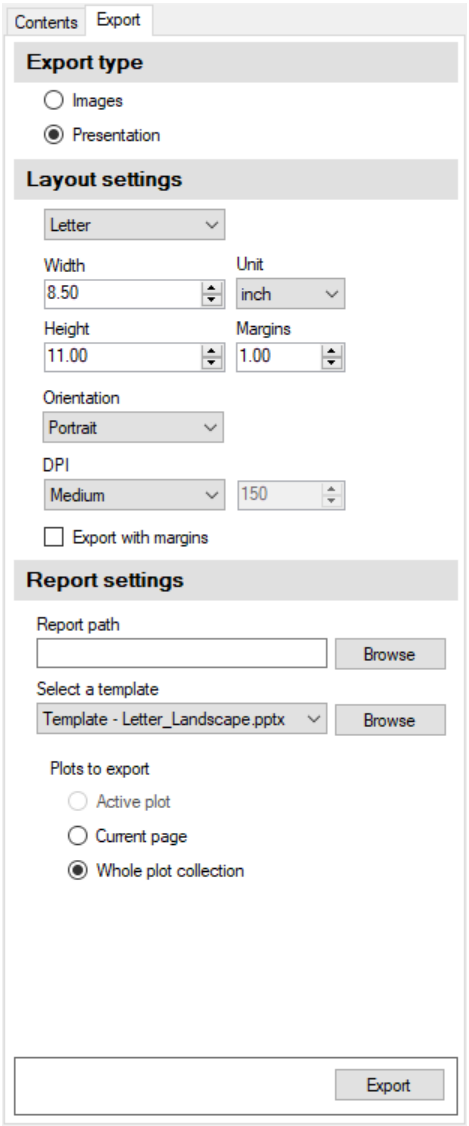
 down/forward one position

 bottom/end

Export Layout

The Export tab (available in the plot collection by clicking the button) displays opens to generate a print preview of the plot collection as it will appear when exported to a set of images or to a PowerPoint template.





Export Type

The export type section pane allows you to select the format to be exported:

- **Image:** the plots will be exported as one or more images based on the Image Settings
- **Presentation:** the plot collection will be exported to a PowerPoint template based on the Report Settings.

Layout Settings

The layout settings pane allows you to define the settings for the page layout:

- **Layout dropdown menu**: allows you to select a predefined page layout (e.g. letter, legal, A4), a custom layout, or no layout (i.e. none). Available layouts include:
  - **Letter:** a page layout 8.5" in width and 11" in height
  - **Legal:** a page layout 8.5" in width and 14" in height
  - **Tabloid:** a page layout 11" in width and 17" in height
  - **A4:** a page layout 21 cm in width and 29.7 cm in height
  - **Custom:** a custom page size defined using the other controls within this section
  - **None:** no defined page layout will be used. The plot collection will fill the available workspace.

  Note selecting a page layout other than the "none" layer, the two-way interactivity between the plots is disconnected - you will not be able to select data points.

- **Width:** the width of the layout
- **Height:** the height of the layout
- **Unit:** the measurement units of the layout (cm or inches ["])
- **Orientation:** orientation of the page layout: landscape or portrait
- **DPI:** the scaling of image relative to the page layout. A value of 100 will reproduce dimensions presented on the screen. Smaller values will produce larger drawing elements with a more coarse resolution; while larger values will produce smaller elements with a more fine resolution.

Image Settings

The image settings pane (shown if the export type is set to Image) allows you to define:

- **Output Path:** the output folder where the exported image(s) will be saved
- **File Type:** the image format: *.PNG, *.TIF, *.JPG, *.EMF

- **Plots to Export:** the scope of the export:
  - **Current Page:** only the page currently displayed in the plot collection will be exported
  - **Whole Plot Collection:** all pages in the plot collection will be exported as separate files. One image will be exported per page and the resulting files will include an appended page number in the file name

- **Export Button:** one or more images will be generated based on the Layout and Image settings

Report Settings

The report settings pane (shown if the export type is set to Presentation) allows you to define:

- **Report Path:** the output file name and location (note, if the Reports subfolder of the project is selected as the path (default)
- **Template:** a PowerPoint template selected from the Office reports > PPT Plots folder of the project tree

- **Plots to Export:** the scope of the export:
  - **Current Page:** only the page currently displayed in the plot collection will be exported
  - **Whole Plot Collection:** all pages in the plot collection will be exported into the template with one plot collection page per slide

- **Export Button:** the plot collection will be exported to the selected PowerPoint template based on the Layout and Report settings

13.2 Common Plot Features

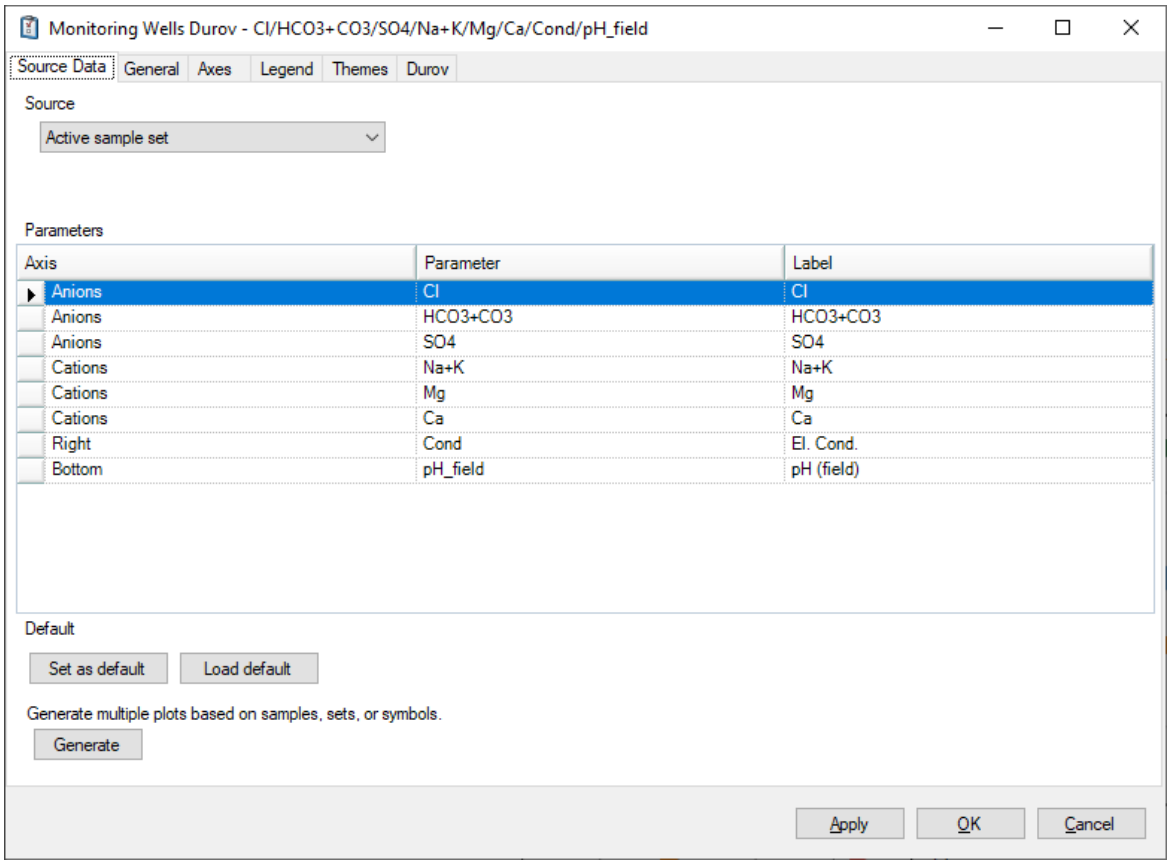
Although each of the available plot types has unique characteristics, there are also many graphical features and options that they have in common. When you select any of the plot types to include in the plot collection, a Plot Options dialogue will appear with default settings for data sources, parameters and other plot settings. Settings common to all plots include:

- Source Data
- General
- Axis
- Legend
- Themes

Many plots also support the addition of custom Lines and plot-specific settings, which are described where applicable in the discussion of each individual plot type.

Source Data

The source data selection will determine which sample/station data are included in the plot:



Source

While the parameter data to be plotted in each of the plots can vary significantly between plot types, the source of the data can be based on dynamic data:

- **Active Sample Set**: the sample set that is currently active in the station picker
- **Active Samples**: the sample(s) currently selected in the sample picker/sample list
- **Active Station**: the sample(s) associated with the currently selection station

or static data:

- **Sample Set**: a specific sample set or station group
- **Station**: a specific station
- **Sample**: a specific sample
- **Symbol**: a specific symbol

Parameters

Once you have selected a data source, you can select parameters to be plotted. The plot type will determine which parameters (and sometimes how many) are to be plotted. Clicking a value within the Parameter column will open the parameter selection window.

Many of the plot types (e.g. Piper plot and Stiff diagrams) have specific parameters that are most commonly used with them. These are described in each of the individual Plot Type sections.

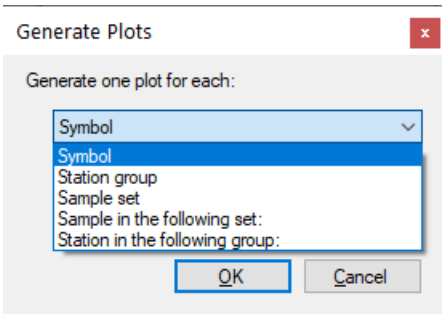
Default

The following options are available for working with default plot settings:

- **Set as default**: sets the current source, parameters, and style settings as the default for the current plot type in the current project
- **Load default**: applied the default settings to the current plot

Generate multiple plots

You can generate multiple plots based on a common set of parameters and style settings using the Generate button, which when clicked opens the following dialog:

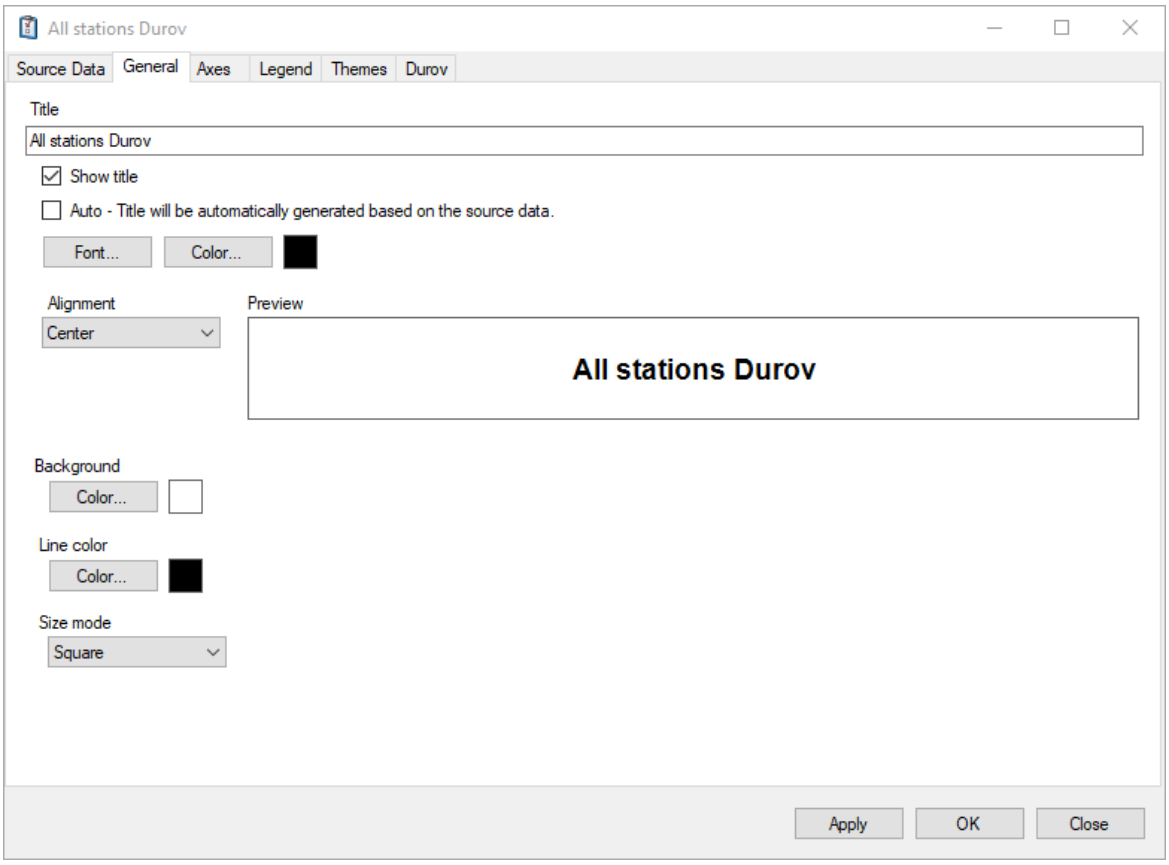


- **Symbol**: generates one plot for each symbol in the active symbol group
- **Station Group**: generates one plot for each station group listed in the project tree
- **Sample Set**: generates one plot for each sample set listed in the project tree
- **Sample in the following set**: generates one plot for each sample in a sample set selected using the sample set picker
- **Station in the following group**: generates one plot for each station in a station group selected using the station group picker

Once the multiple plots have been generated each plot will have distinct plot settings, so it is generally easier to set up the plot style prior to generating multiple plots to minimize having to make adjustments to each plot individually.

General

The General tab provides options for setting the title of the plot and formatting for the general style of the plot:

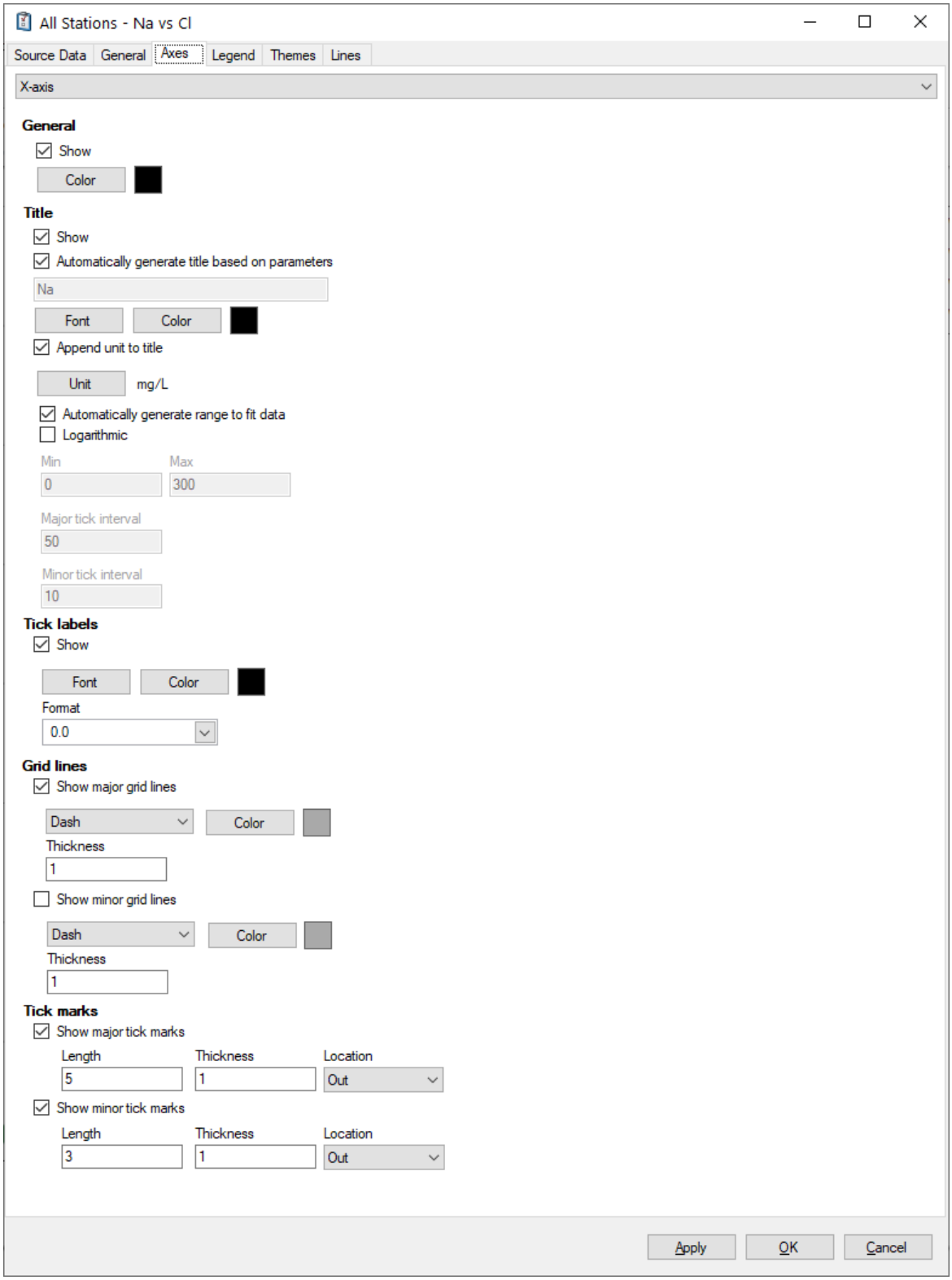


- **Title**: a text input form for the Title of the plot; disabled if Auto is checked on
- **Show title**: if checked will display the title above the plot
- **Auto**: if checked will automatically generate a plot-specific title based on the plot type, data source, and/or input parameters
- **Font**: sets the font, size, and style of the plot title
- **Color**: sets the color of the plot title font
- **Alignment**: specifies the alignment of the plot title relative to the plot: left, center, or right
- **Background**: specifies the background color of the entire plot
- **Line Color**: specifies the color of the plot frame. Note that axes are drawn on top of the plot outline
- **Size Mode**: specifies if the plot should be stretched to fill the available space in the plot collection or if the X/Y axes should have equal lengths. This feature is only available for rectangular plots (e.g. scatter, probability, quantile, etc.)

Axes

The Axes tab provides options for formatting the plot axes. All axis settings are described below; however not all axis settings are available/applicable for axes in each of the plot types (for example the concentration axis on Stiff diagrams does not have a Units setting as units are fixed to meq/L). Similarly, in some case, multiple axes will share settings; for example,

ternary plots and plots that contain one or more ternary plots (i.e. Durov, Piper, and Giggenbach) have one ternary axis with common settings.



A drop down menu is available at the top of the Axes tab which allows you select the axis to review and specify the following settings:

General

- **Show**: if checked, shows the axes and related settings will be shown on the plot
- **Color**: specifies the color of the axes

Title

- **Show**: if checked, shows the axis title
- **Automatically generate title based on parameters**: if checked, the text of the axis title will be generated by AquaChem based on the current set of parameters
- **Title Input**: a text input box for the title; disabled if the title is set to auto-generate
- **Font**: specifies the font, size, and style of the axis title
- **Color**: specifies the color of the axis title
- **Append unit to title**: if checked, the parameter measurement unit will be appended to the axis title
- **Unit**: if clicked you will be prompted to select a measurement unit from the same measurement category as the parameter.
- **Logarithmic**: if checked, the axis scale will be transformed to a base-10 logarithm scale
- **Min**: the minimum value of the axis
- **Max**: the maximum value of the axis
- **Major Tick Interval**: the spacing between major tick marks, gridlines, and tick labels for the axis
- **Minor Tick Interval**: the spacing between minor tick marks and gridlines for the axis

Tick Labels

- **Show**: if checked, shows value labels at the major tick marks
- **Font**: specifies the font, size, and style of the axis tick labels
- **Color**: specifies the color of the axis tick labels
- **Format**: allows you to specify the numerical format of the axis tick labels. If the dropdown is selected, you may choose from standard formats numeric or date/time formats, based on the axis value type. You also have the option of clearing the format to use a general/automatic format and AquaChem will automatically format each label for you based on the type and magnitude of the number or date.

Grid lines

The following options are available for the major and minor gridlines:

- **Show**: if checked, axis major/minor gridlines will be shown on the plot
- **Type**: specifies the line type in a dropdown menu: solid, dot, dash, dash dot, dash dot dot
- **Color**: specifies the color of the axis major/minor gridlines
- **Thickness**: specifies the thickness of the major/minor gridlines in point units

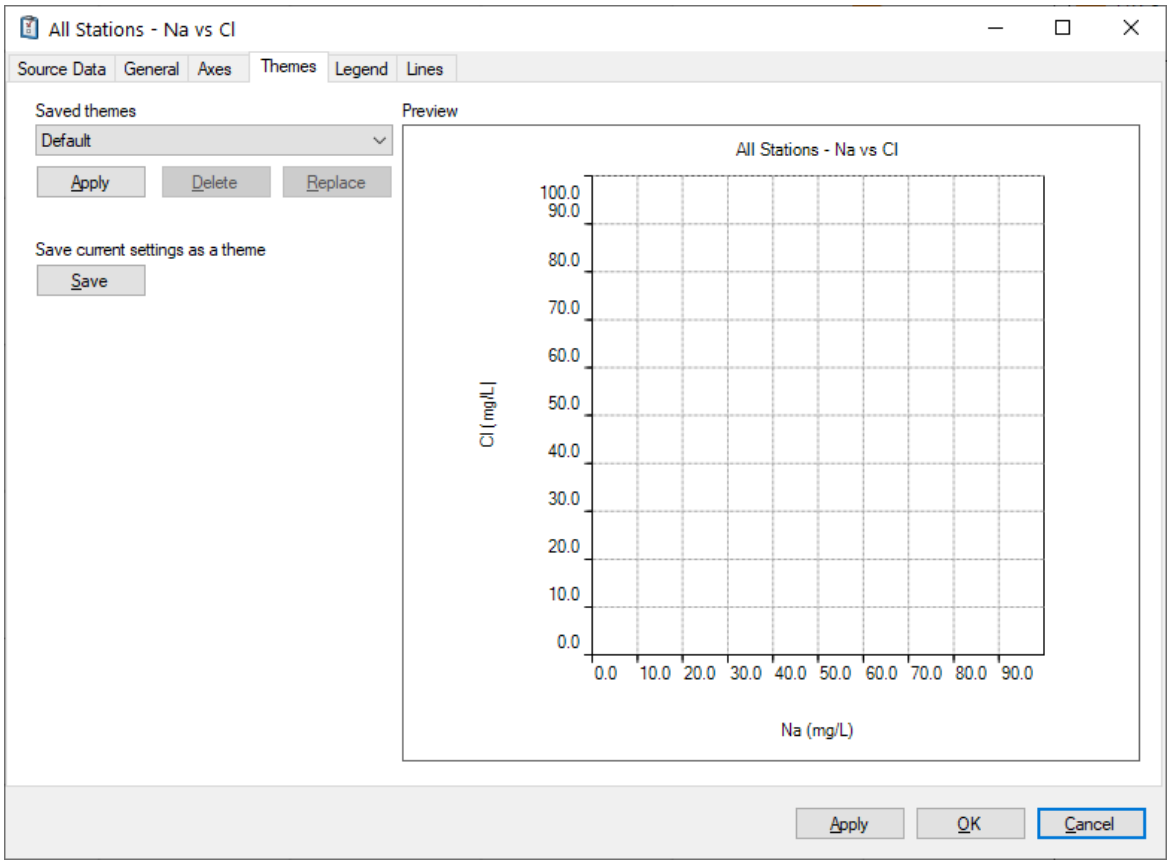
Tick Marks

The following options are available for the major and minor tick marks:

- **Show**: if checked, axis major/minor tick marks will be shown along the axis
- **Length**: specifies the length of the tick mark perpendicular to the axis
- **Thickness**: specifies the thickness of the major/minor gridlines in point units
- **Location**: a dropdown with the following options: In, Out, and Cross

Themes

The Themes tab provides options for managing plot themes. Plot themes are style settings that can be shared across plot types and collections within a given project, including axis and plot title fonts, line colors and styles. Plot themes allow you to develop a common style for plots so that you can quickly generate plots that have a common design style to help you develop professional looking plots.



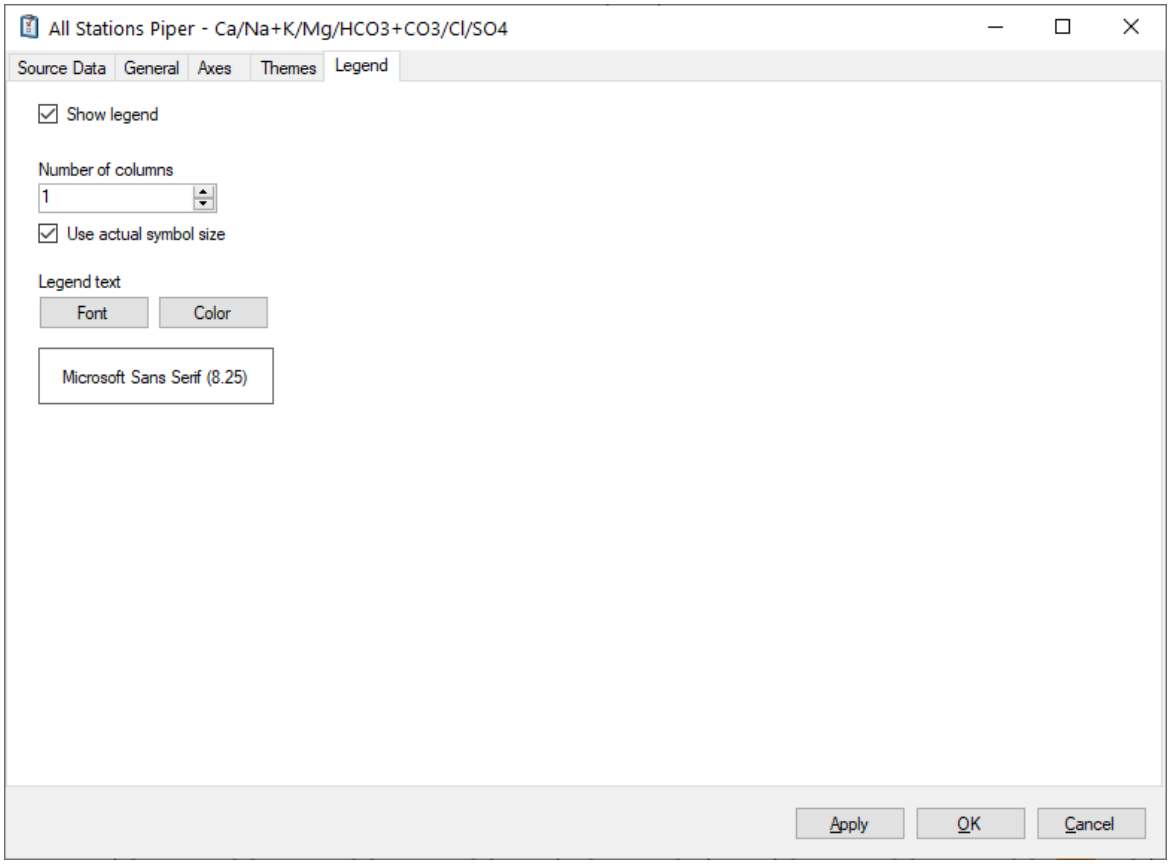
- **Saved Themes** (dropdown): allows you to select one of the plot themes saved in the current project
- **Apply**: formats the current plot using the selected plot theme
- **Delete**: deletes the selected plot theme from the project. Note: the default plot theme cannot be deleted

- **Replace**: replaces/updates the settings of the selected plot theme with those of the current plot
- **Save**: saves the settings of the current plot as a new theme

Note that certain plot elements including data formats, number ranges and tick mark intervals are not included in plot themes as these rely on the data sources which can vary widely across various plot types; however, these settings can be saved using the plot defaults.

Legend

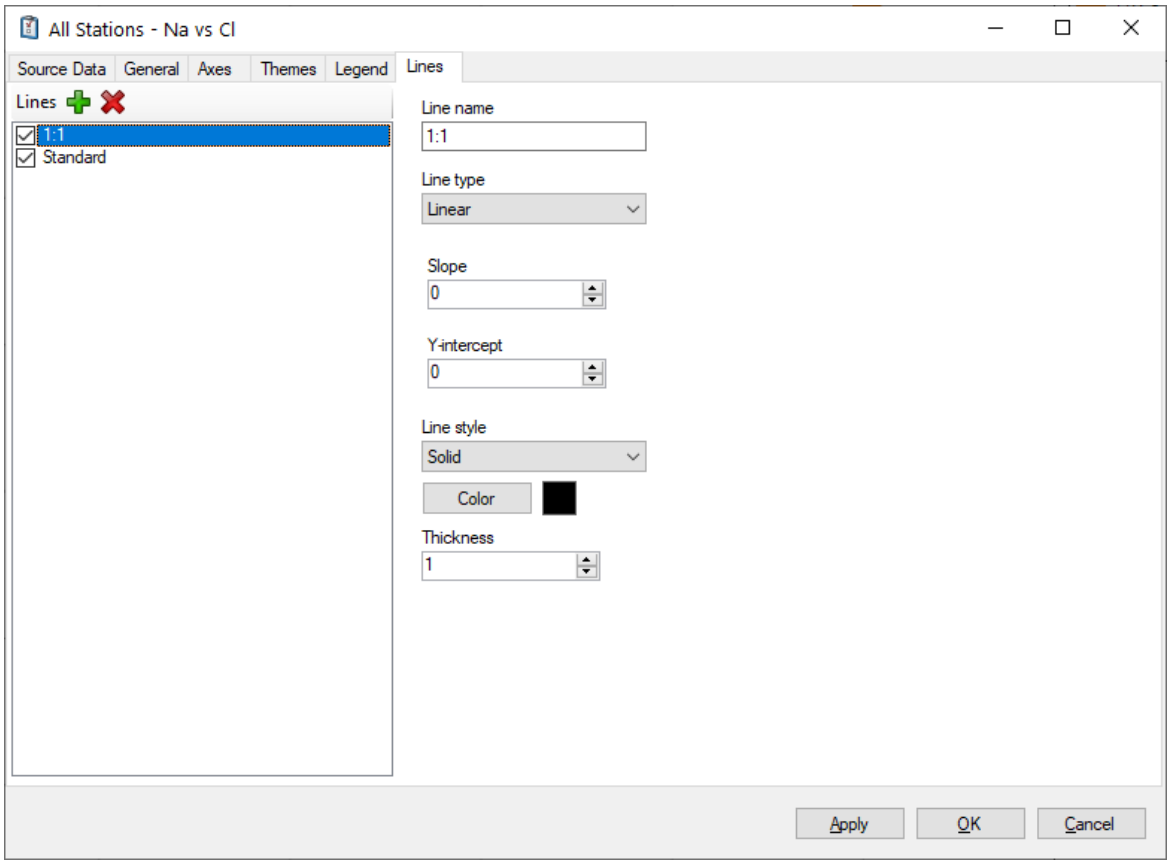
The Legend tab provides options for setting the format and style of the legend:



- **Show legend**: if checked, the legend will be displayed on plot
- **Number of columns**: an integer, the legend will be divided into this many columns
- **Use actual symbol size**: if checked, symbols in the legend will be the same size as on the plot, otherwise they will be the same size as the legend font
- **Font**: specifies the font, size, and style of the legend item labels
- **Color**: sets the color of the text in the legend

Lines

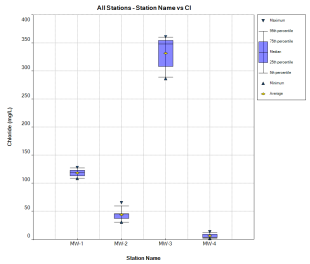
The Lines tab is available for many plot types and provides options for adding and formatting custom lines to the current plot:



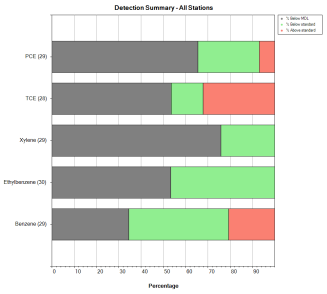
- adds a new custom line to the plot
- removes the currently selected line from the plot
- **Line Name**: a text input to provide a name for the line that is used for the legend
- **Line Type**: a dropdown to select the line type: Horizontal, Vertical, Linear, Time Series, Standard
- **Slope**: the slope of the line (if the line type is linear)
- **Every**: the time unit for slope (if the line type is Time Series)
- **Y-intercept**: y-intercept of the line (if the line type is linear)
- **X-intercept**: x-intercept of the line (if the line type is Time Series)
- **X-Value**: constant value of the line if the line type is vertical
- **Y-Value**: constant value of the line if the line type is horizontal
- **Water Quality Standard**: the water quality standard to use (if the line type if Standard)
- **Parameter**: the parameter to use (if the line type if Standard)
- **Line Style**: specifies the line type in a dropdown menu: solid, dot, dash, dash dot, dash dot dot
- **Color**: sets the color of the line
- **Thickness**: sets the weight of the line in font points

13.3 Plot Types

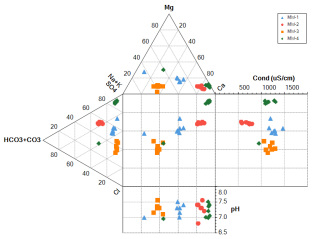
This section describes each of the AquaChem plots and the options available for each plot:



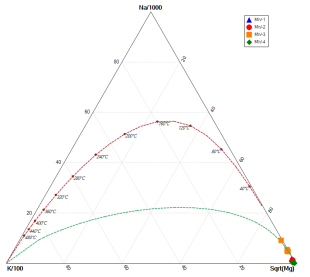
Box and Whisker



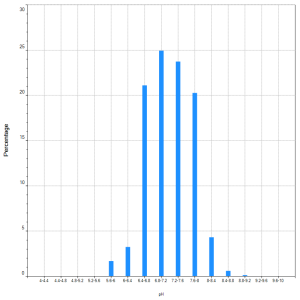
Detection Summary



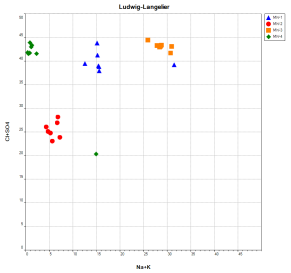
Durov Plot



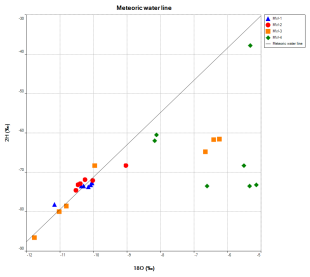
Giggenbach Triangle



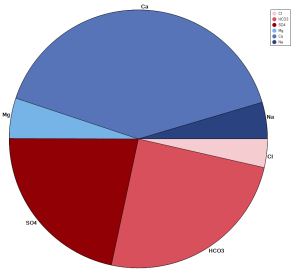
Histogram



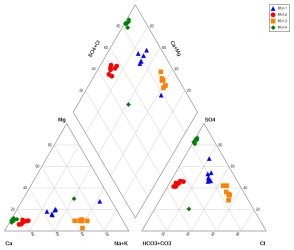
Ludwig-Langelier Plot



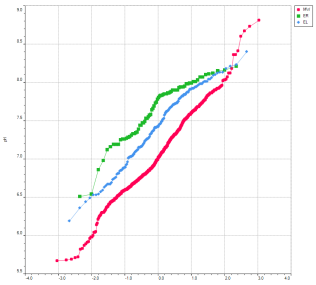
Meteoric Water Line (MWL) Plot



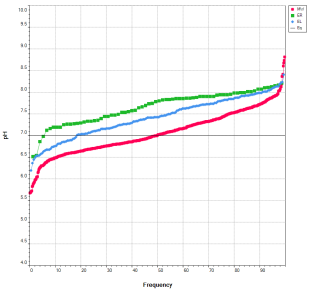
Pie Chart



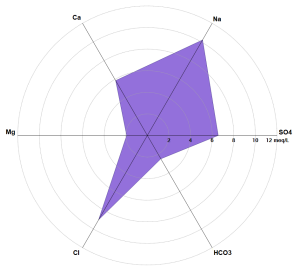
Piper Diagram



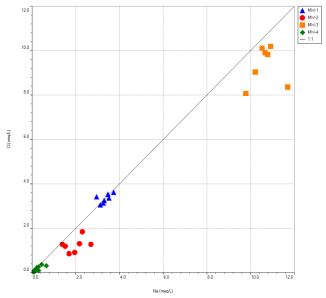
[Probability Plot](#)



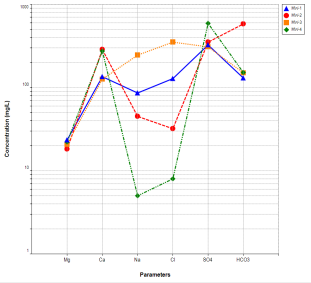
[Quantile Plot](#)



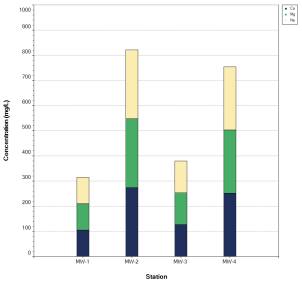
[Radial Plot](#)



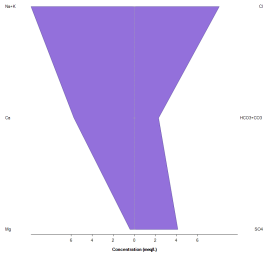
[Scatter Plot](#)



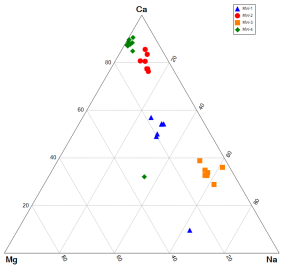
[Schoeller Plot](#)



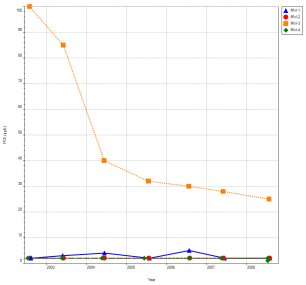
[Stacked Bars](#)



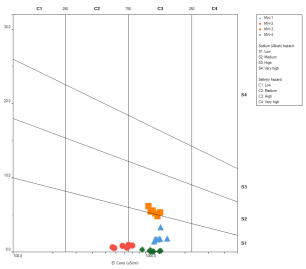
[Stiff Plot](#)



[Ternary Plot](#)



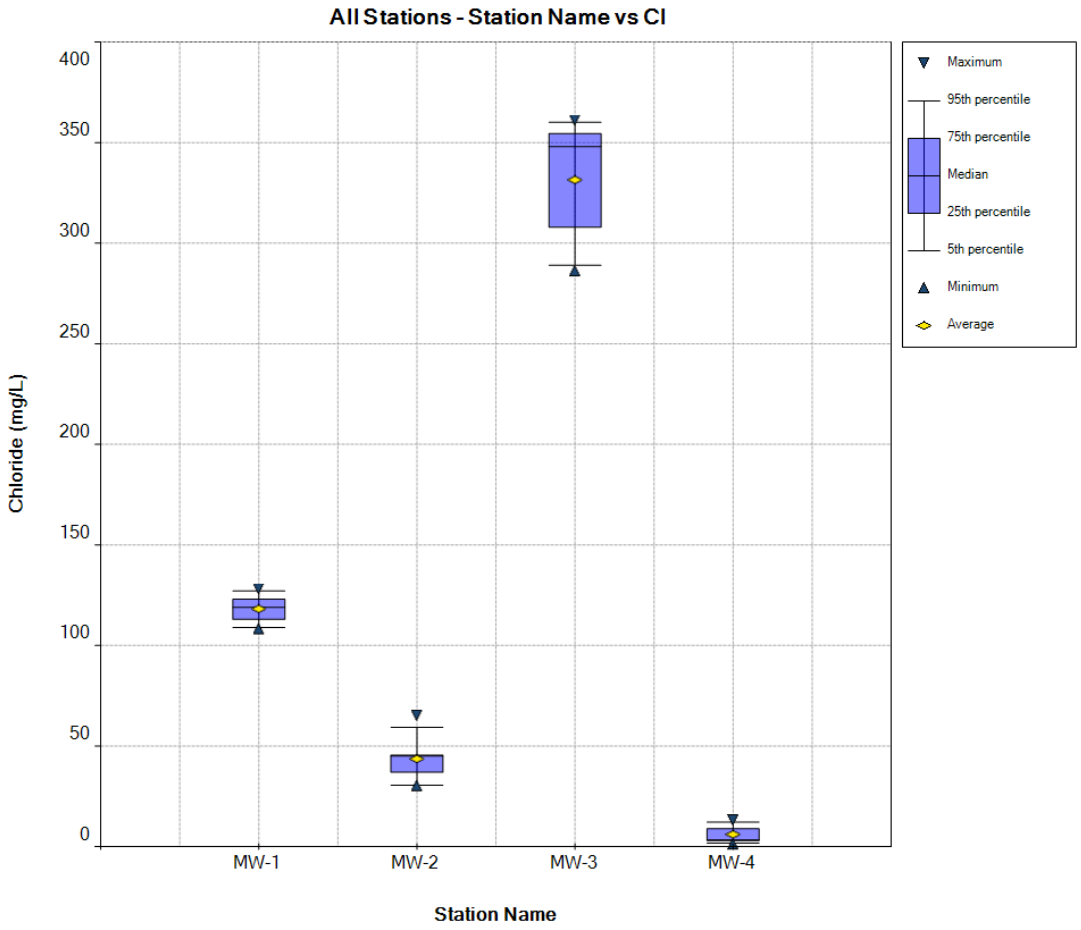
[Time Series](#)



[Wilcox Plot](#)

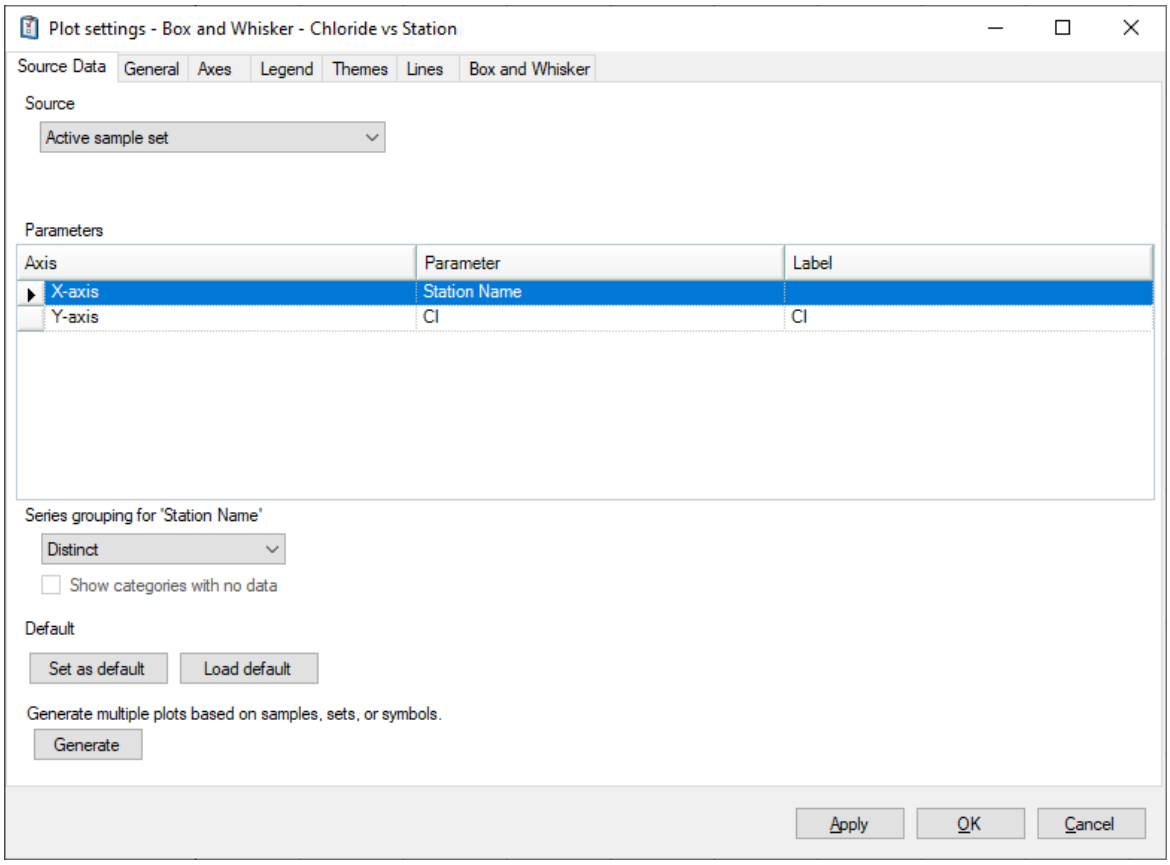
13.3.1 Box and Whisker

The Box and Whisker plot displays a statistical summary of any measured database parameter(s). It is composed of a central box, showing the spread of the bulk of the data (typically the 25th-75th quantile range), and a pair of whiskers, showing the range of the tails (typically the 5th-95th quantile range). AquaChem supplements this chart type by allowing you to add the min, max, median, and average values to the plot:



Source Data Tab

Data are specified in a Box and Whisker Plot as follows:



Source

See common plot settings.

Parameter

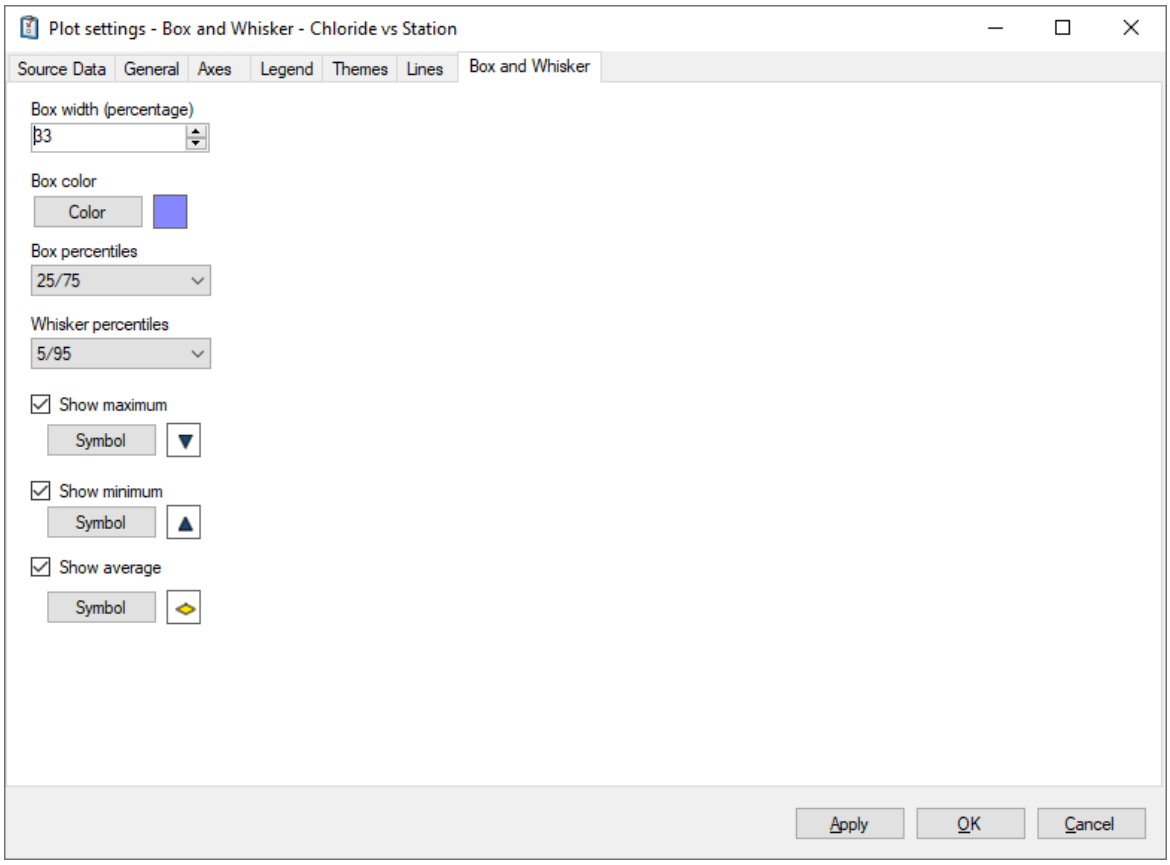
Parameters in a Box and Whisker plot are specified for the category (X) axis and for the value (Y) axis. The X-axis (category) data source is used to group the data and (Y-axis) value statistics are calculated for each category.

Box and Whisker Settings

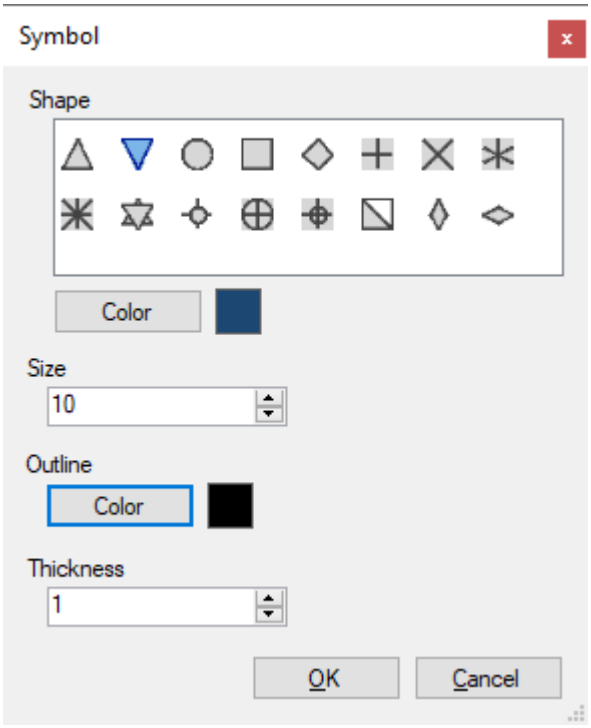
The following settings can be applied to the Box and Whisker plot:

- **Box width:** width of the box and whisker relative to each x-axis category
- **Box color**: fill color of each box
- **Box percentiles**: quantile range for each box (defaults in bold): **25/75**, 10/90, 5/95, 1/99
- **Whisker percentiles**: quantile range for each set of whiskers (defaults in bold): 25/75, 10/90, **5/95**, 1/99
- **Show Maximum**: toggles the visibility of the maximum data point of each category
- **Symbol (Maximum)**: style controls for the maximum symbol of each category

- **Show Minimum**: toggles the visibility of the minimum data point of each category
- **Symbol (Minimum)**: style controls for the minimum symbol of each category
- **Show Average**: toggles the visibility of the average of the values data for each category
- **Symbol (average)**: style controls for the average of the values for each category



The symbol picker allows you to customize the shape and color of the select symbol type (min, max, average) as well as the color and thickness of its outline:

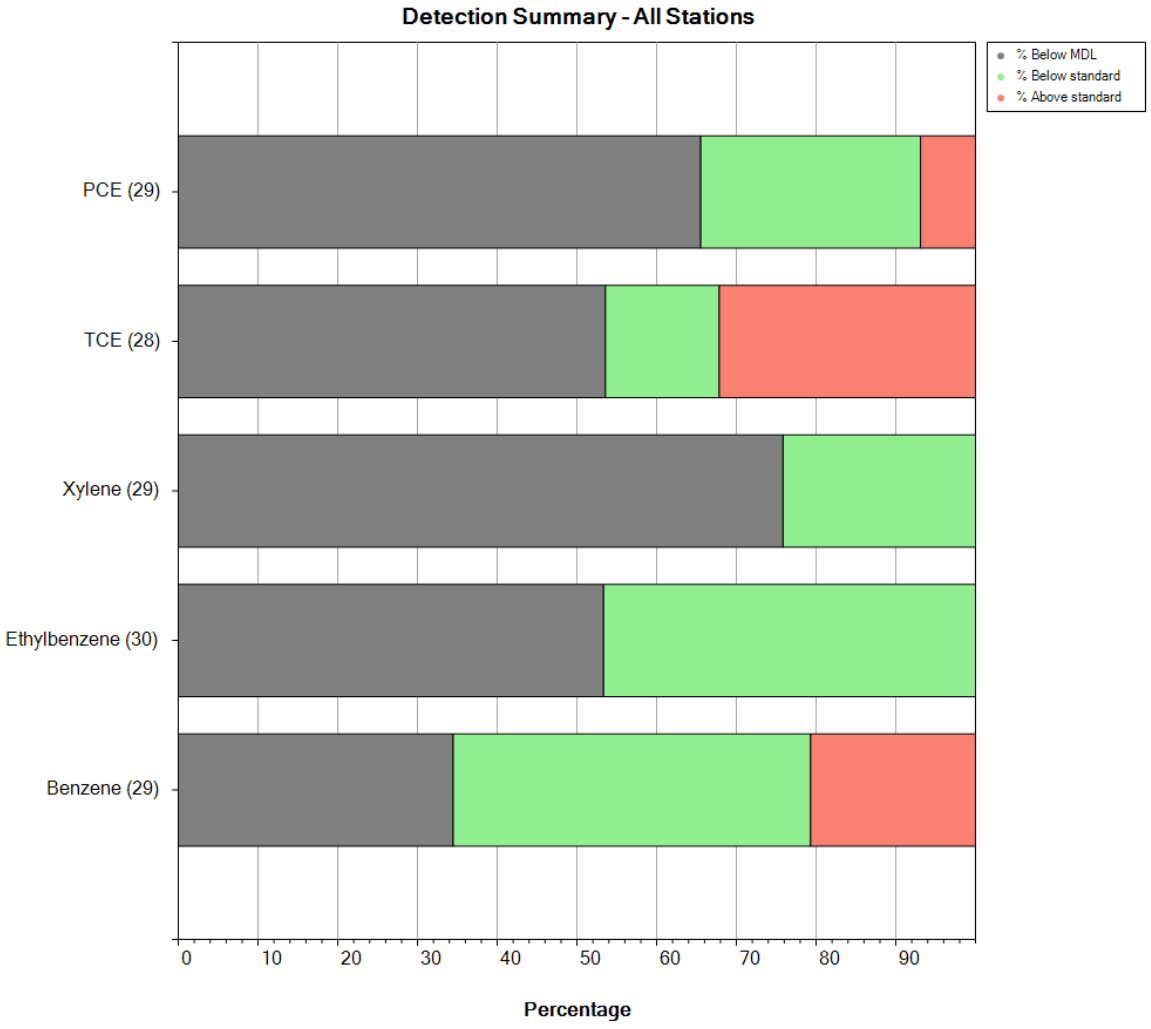


13.3.2 Detection Summary

The Detection Summary plot is used to visualize the relative proportions of samples above the active Water Quality Standards. The plot shows a summary bar for every parameter with the percentage of values where the constituent concentration is:

- below the detection limit,
- between the detection limit and an active water quality standard, and
- exceeds an active water quality standard

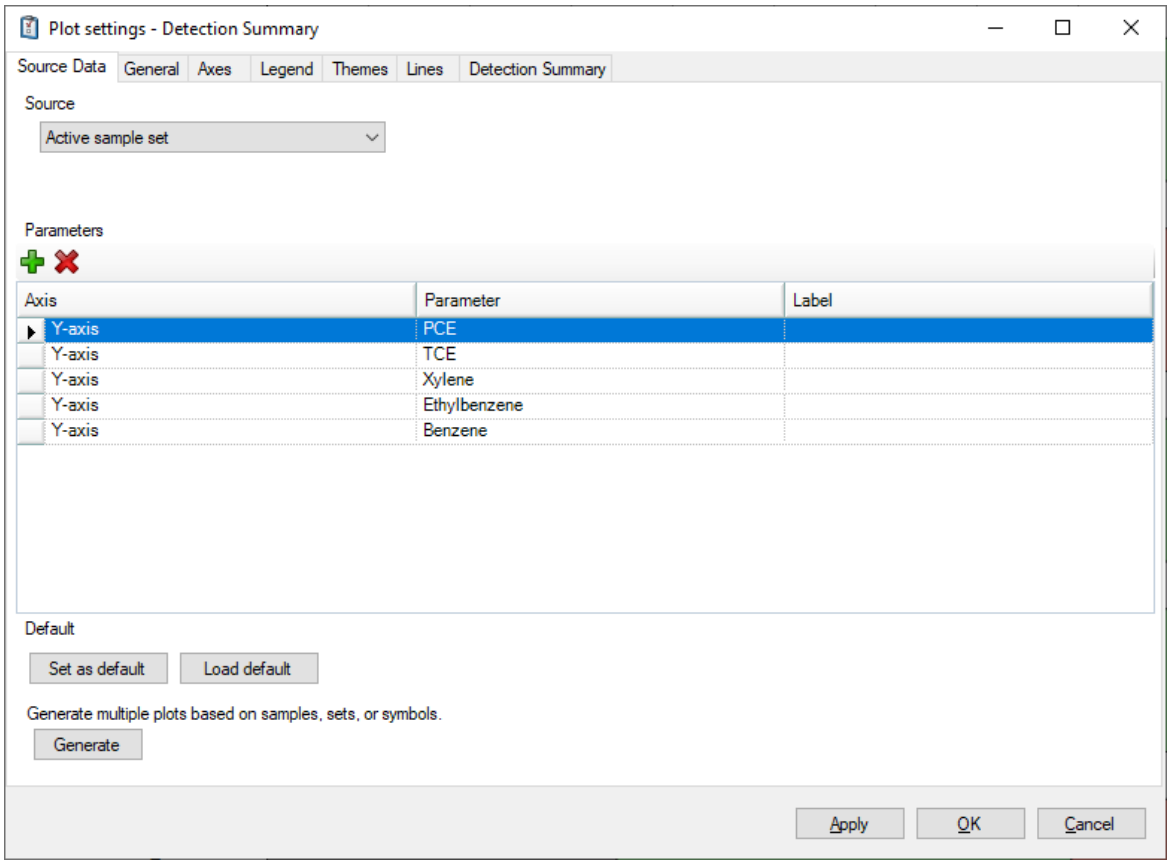
An example the Detection Summary plot based on the demo project is shown below:



The X-axis of the Detection Summary plot spans from 0 to 100 percent of samples. The name of each parameter is listed on the left side of the plot for the applicable detection summary bar. The number of samples for each parameter is also (optionally) displayed.

Source Data Tab

Data are specified in a Detection Summary Plot as follows:



Source

See common plot settings.

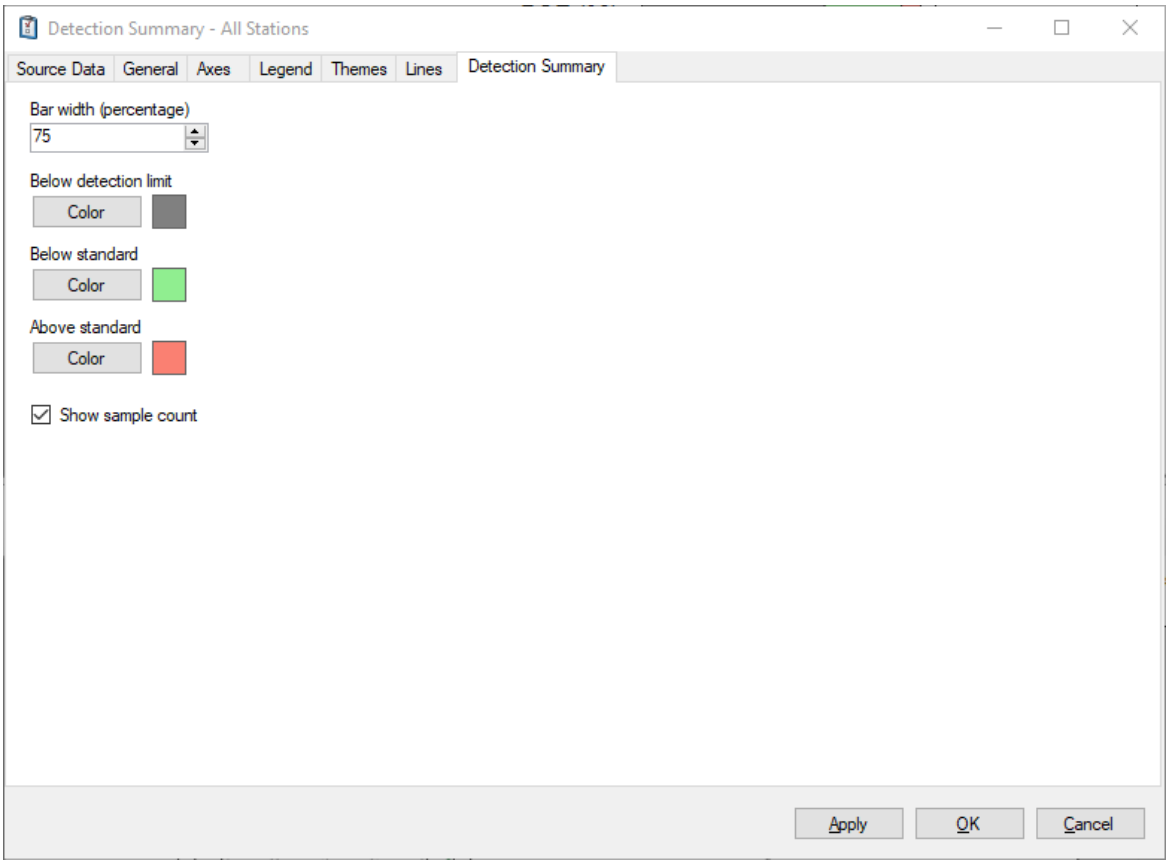
Parameter

In a Detection Summary plot, you may add one or more parameters, which are plotted in the order listed along the Y-axis.

Detection Summary Tab

The following settings can be applied to the Detection Summary plot:

- **Bar Width**: allows you to set the width of each bar as a percentage of the category; a value of 100% will leave no gap between categories
- **Color:** three color boxes allow you to specify the fill color of the bars for data based on values:
  - **Below Detection Limit**
  - **Below standard** (but above detection limit)
  - **Above standard**

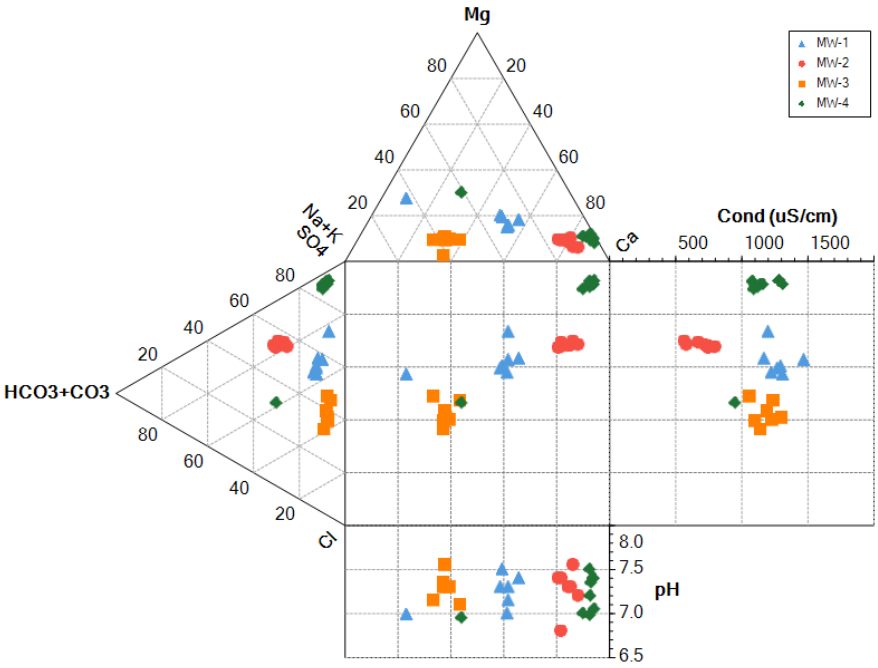


13.3.3 Durov Plot

The trilinear Durov plot is a composite plot based on the percentage of major ion milliequivalents and two (optional) additional water quality parameters (Durov, 1948). Major cation and anion values are plotted on two separate triangular plots and the data points are projected onto a shared rectangular grid at the base of each triangle. The Durov plot also allows for the direct comparison of two other groundwater parameters, typically pH and the total dissolved solids (TDS) or electrical conductivity. The Durov plot is an alternative to the Piper Diagram which is described later in this chapter.

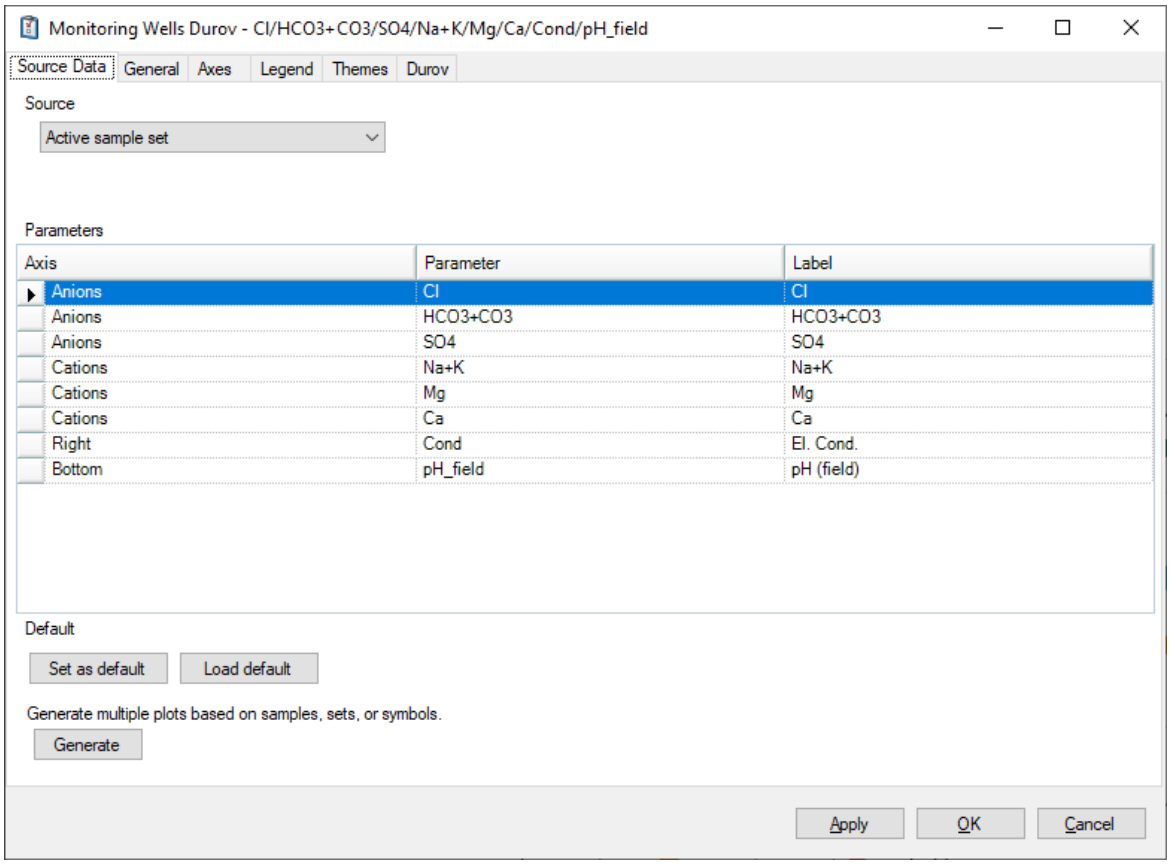
Since the data points are projected along the base of the triangle, which lies perpendicular to the third axis in each triangle, information about the concentration of the vertex element (the third element) is lost in the square grid. Changing the orientation of parameters in both triangles may improve your ability to detect distinct groups.

An example Durov Plot Options based on the Demo project is shown in the figure below:



Source Data Tab

Data are specified in a Durov Plot as follows:



Source

See common plot settings.

Parameters

Durov Plots have a total of eight required parameters:

- three major **anions**, typically: chloride (Cl), bicarbonate (HCO3) and carbonate (CO3), and sulfate (SO4);
- three major **cations**, typically: sodium (Na) and potassium (K), magnesium (Mg), and calcium (Ca);
- right frame parameter, typically: conductance or total dissolved solids; and
- bottom frame parameter, typically: pH

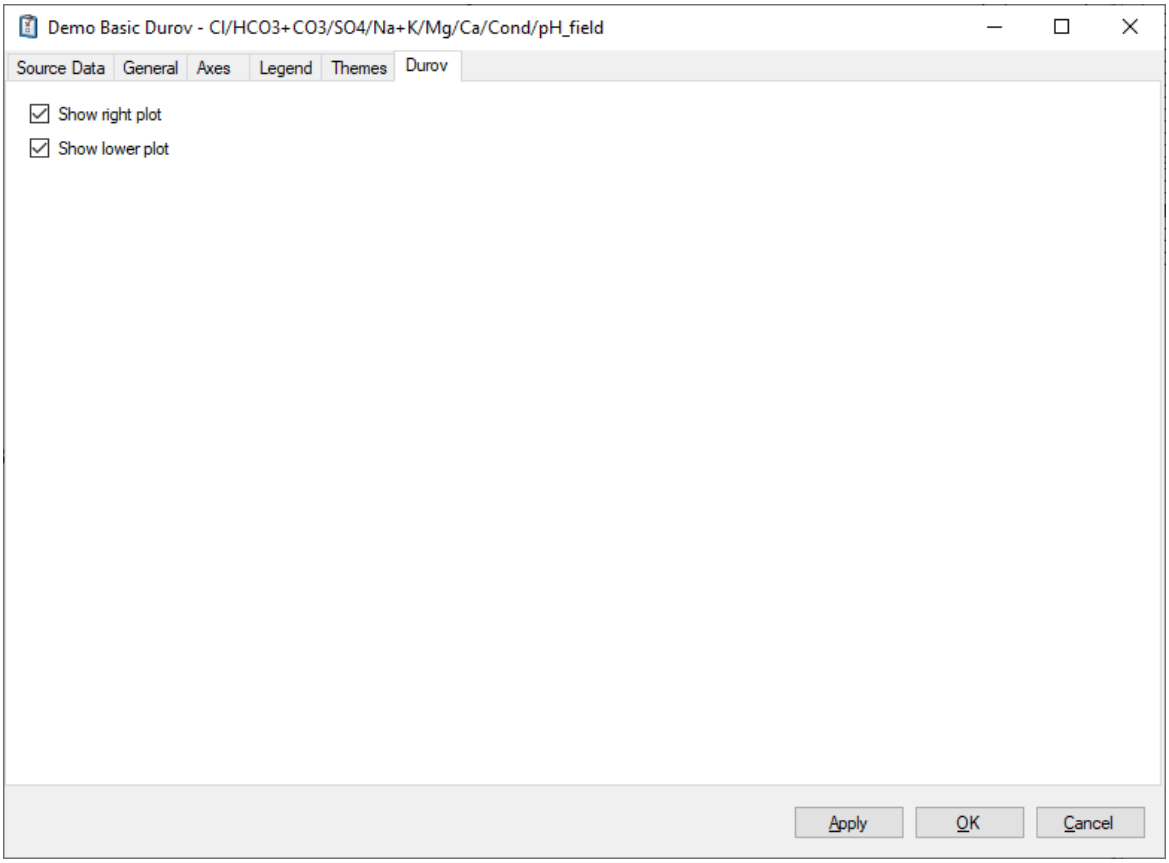
The cations specify the parameters that are presented in the left triangle. Default settings are the major cations Na+K, Ca, and Mg; however the parameters can be reordered or any other parameter can be selected (e.g. gas composition, trace elements etc.). The anions generally specify the parameters for the upper triangle. Default settings are the major anions Cl, SO4, and HCO3+CO3 and, as with cations, anions can be reordered or substituted with other suitable parameters. Note that measured or calculated Alkalinity may be a valid anion

parameter. If using the alkalinity in the anion triangle, you would typically change the respective displayed label field to HCO3+CO3.

Each of the parameters also contain a matching Label field. This allows customization of the parameter labels on the plot diagram. For example the parameter `Ca' can be edited in the Label field to displayed as `Calcium'.

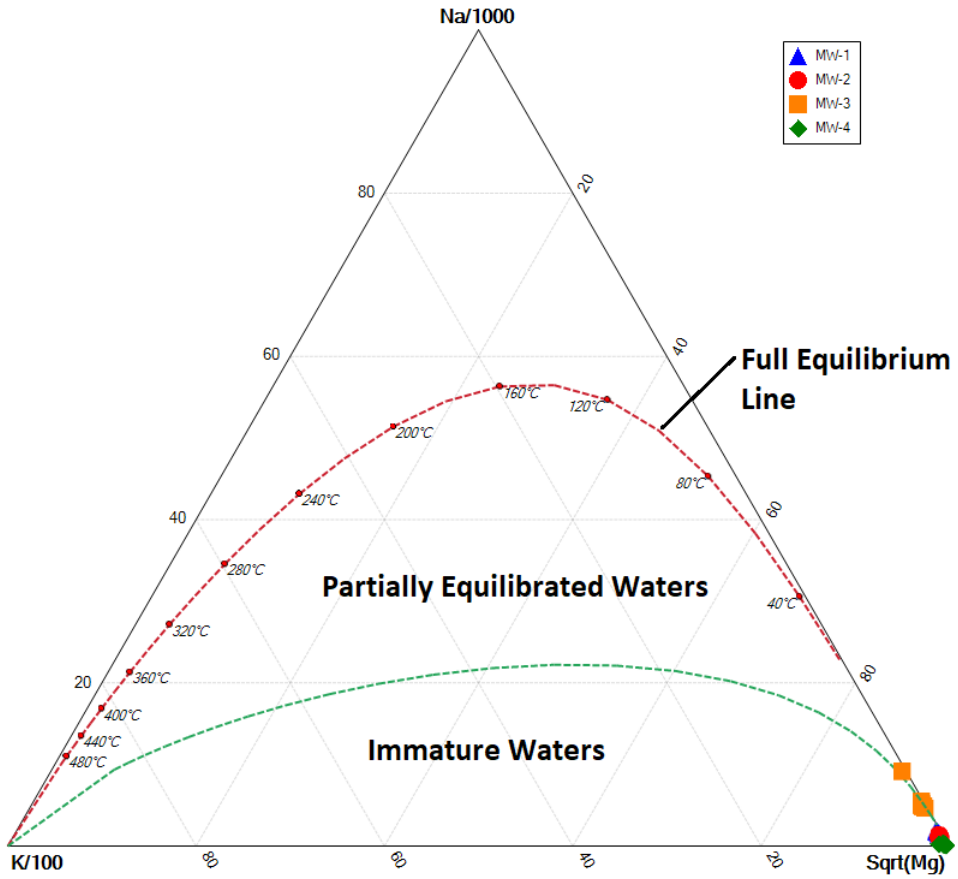
Durov Settings Tab

The Durov tab contains options to show or hide the right (conductance/TSS) and/or lower (pH) plot.



13.3.4 Giggenbach Triangle

The Giggenbach triangle (1988) provides a visual aid to determine the water-rock equilibrium. An example of the Giggenbach Triangle plot and the corresponding Giggenbach Triangle Options dialogue is shown in the figure below.



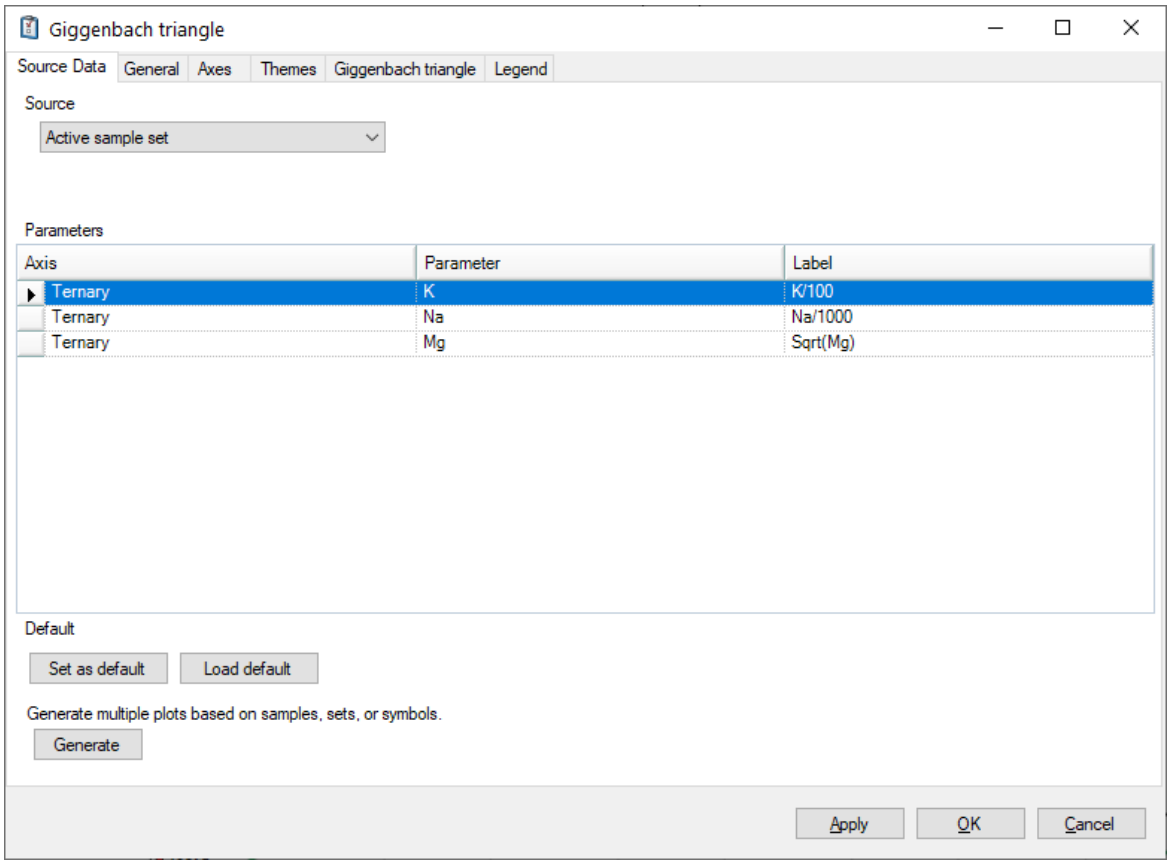
The Giggenbach Triangle (K-Mg-Na Triangle) representation allows you to verify the extent to which water-rock equilibrium has been attained. The triangle is comprised of three zones:

- Immature waters (at the base);
- Partially equilibrated waters (in the middle); and
- Fully equilibrated waters (along the curve).

Depending on where the composition of a given sample lies within this triangle, you can estimate the extent of rock-water equilibrium. For mature waters falling near the upper curve, you can estimate the temperature as well.

Source Data Tab

Data are specified in a Giggenbach plot as follows:



Source

See common plot settings.

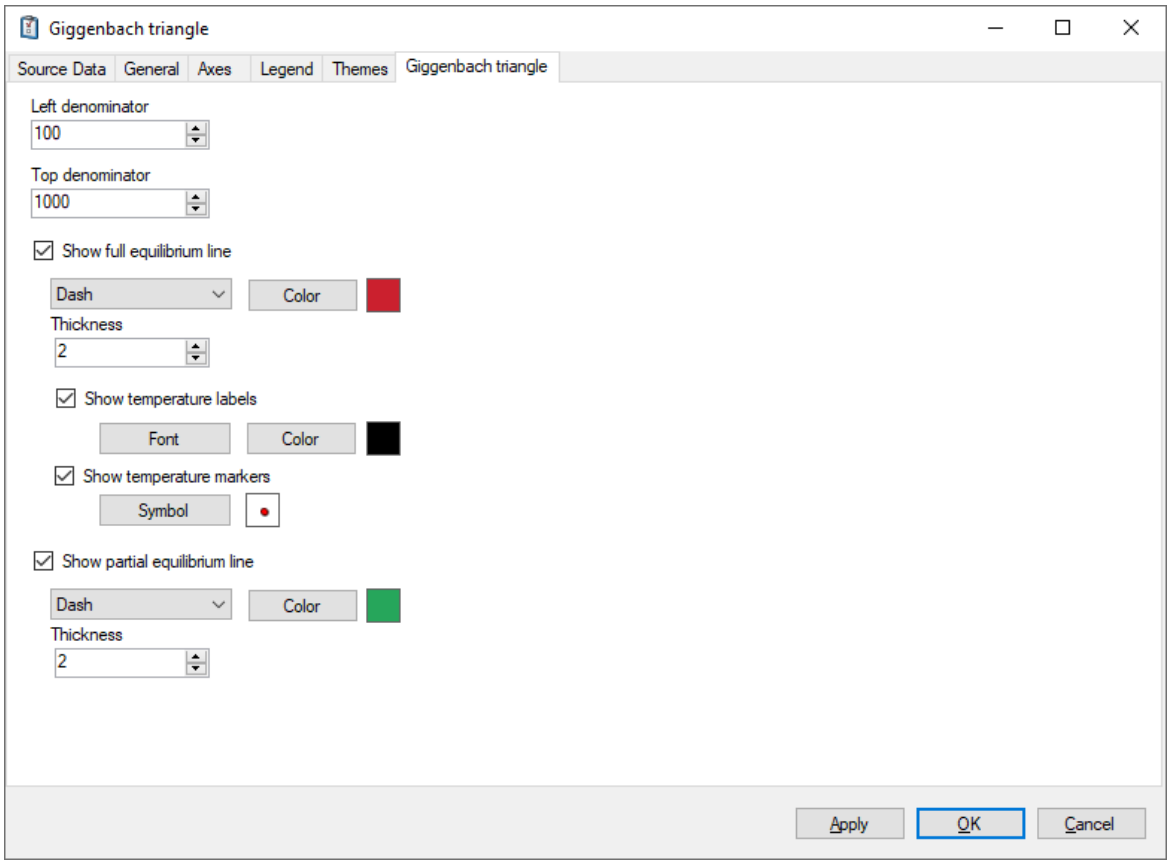
Parameters

Giggenbach plots have a total of three required parameters:

- Potassium (K);
- Sodium (Na); and
- Magnesium (Mg)

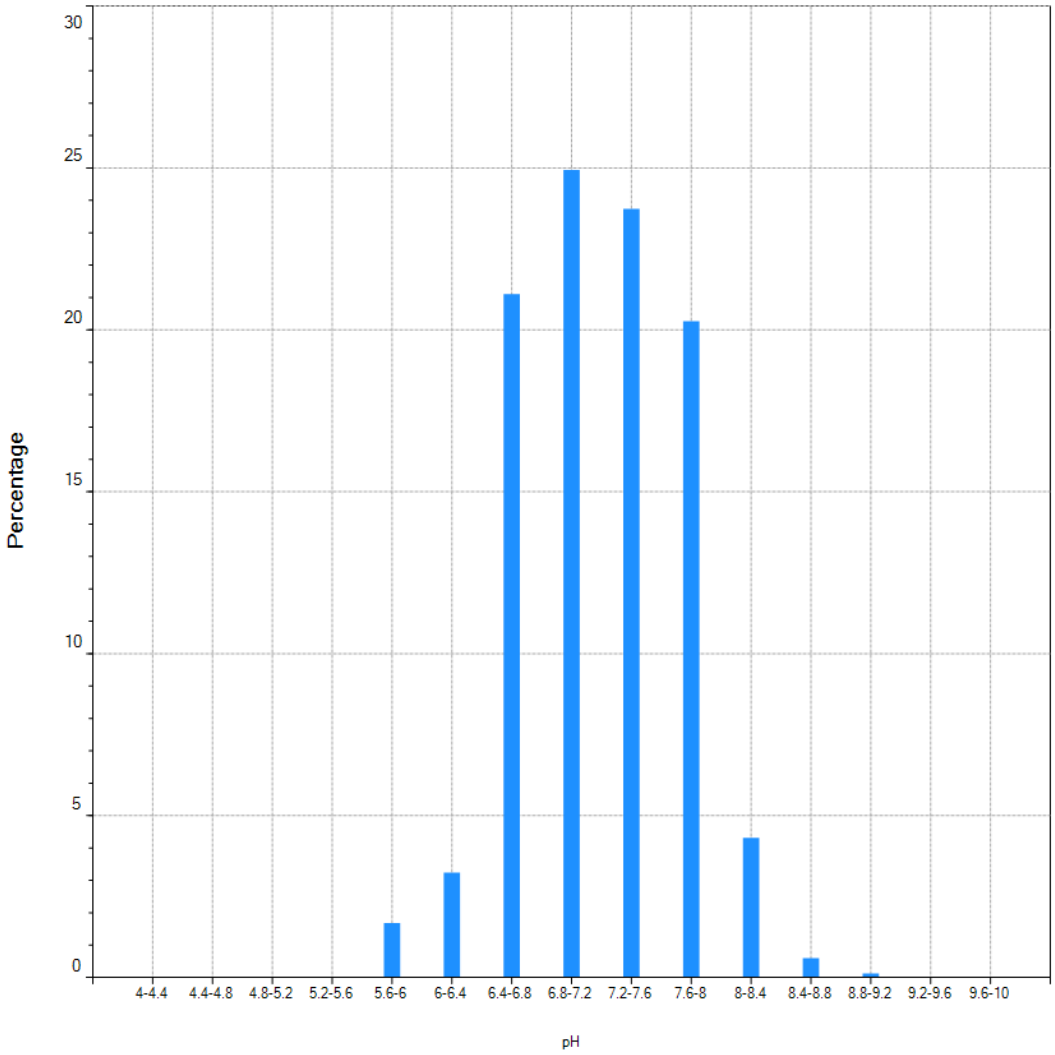
Giggenbach Triangle Settings Tab

The Giggenbach triangle tab contains options to enter division factors for K (left denominator) and Na (right denominator) in the fields provided. The default values for the plot are K/100 and Na/1000. There also options to show/hide and format the full equilibrium line, the partial equilibrium line, and the temperature markers for the full equilibrium line.



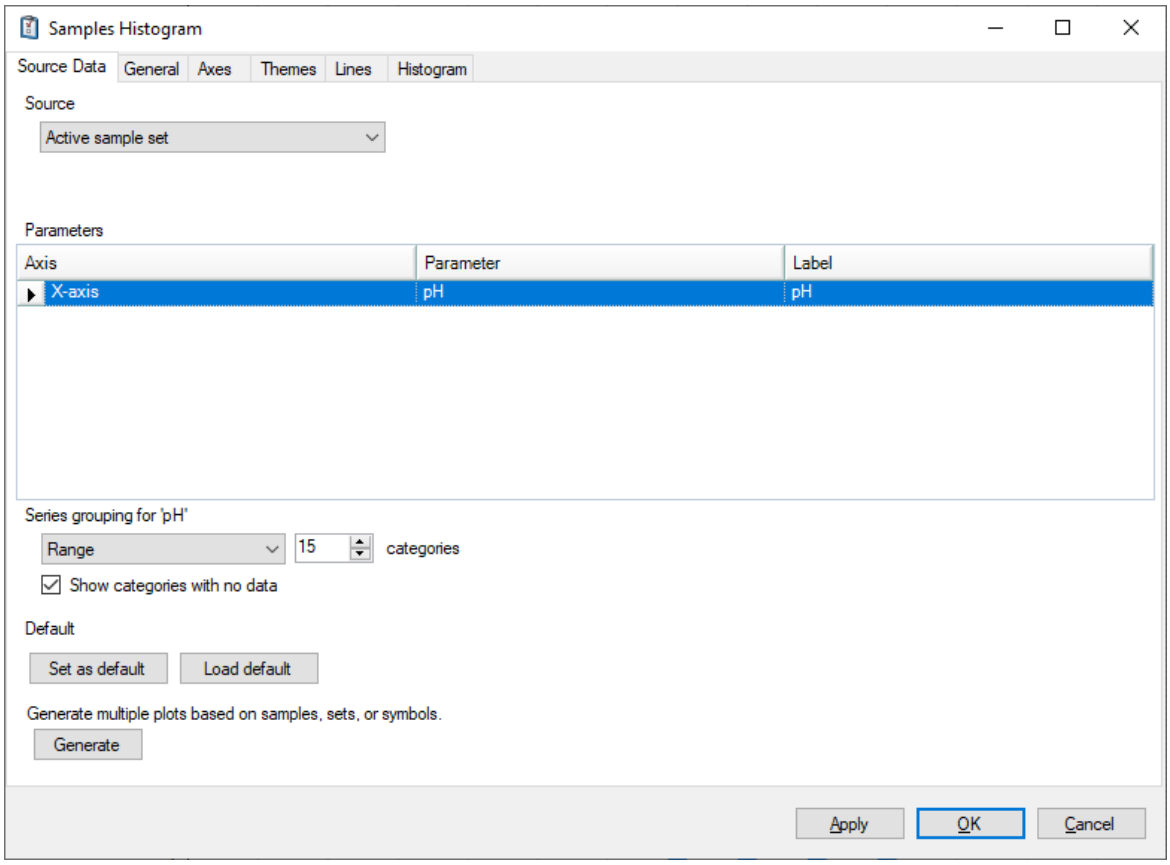
13.3.5 Histogram

One of the oldest methods for summarizing data distributions is the histogram plots. A histogram is constructed by dividing the data range into bins, which consist of ranges of values, counting the number of samples within the bins and displaying the counts in each bin using a bar graph. An example of a Histogram plot is shown in the figure below.



Source Data Tab

Data are specified in a Histogram plot as follows:



Source

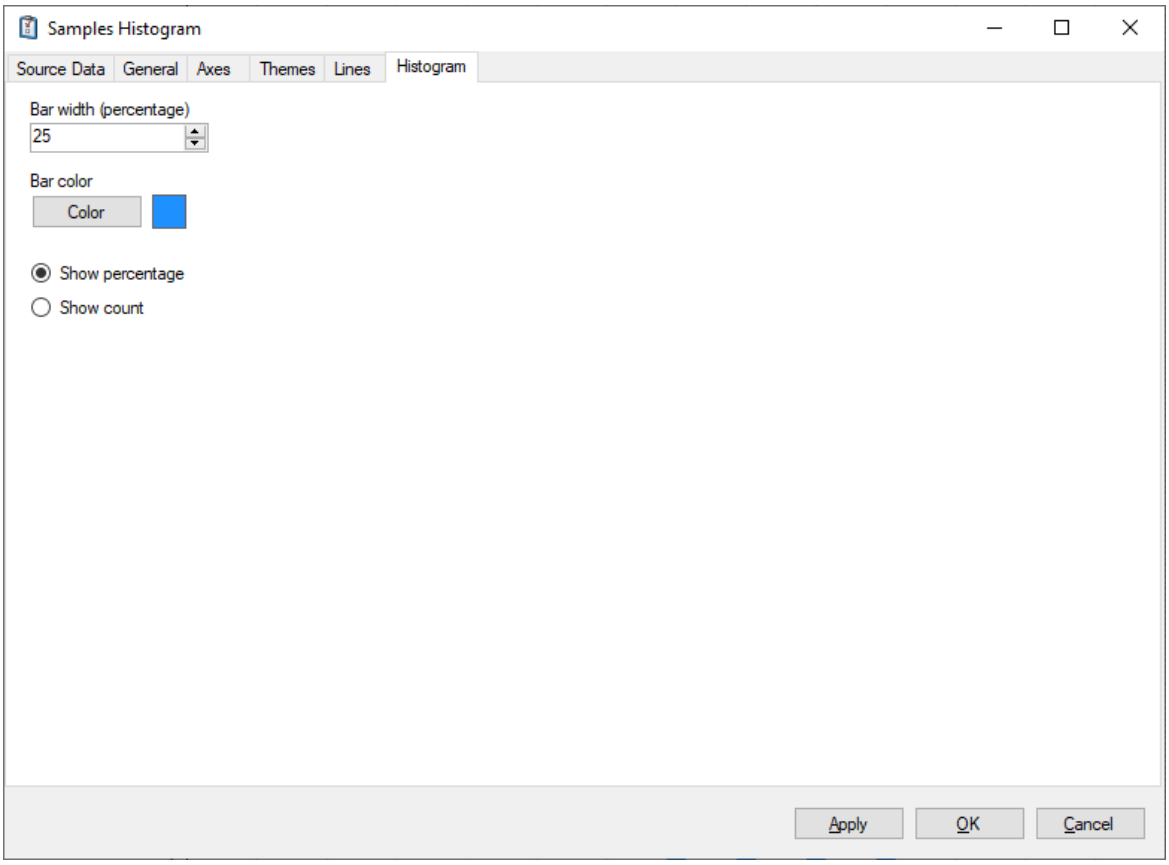
See common plot settings.

Parameters

Histogram plots have a single parameter which must contain numeric values.

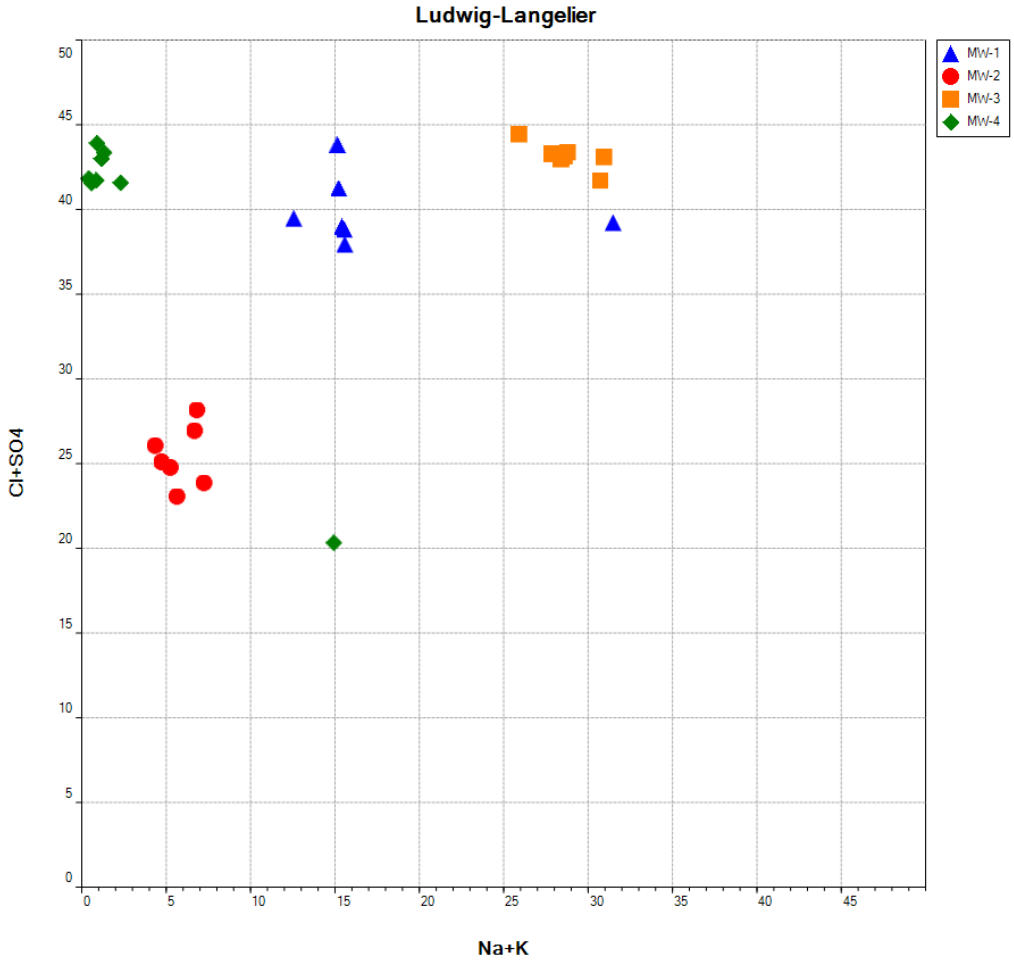
Histogram Settings Tab

The Histogram tab contains options to set the width of the bar as a percentage of their category (i.e. a value of 100 will produce bars with no gaps). There also options to format the bar color and whether to show the distribution as a percentage or as a count.



13.3.6 Ludwig-Langelier Plot

The Ludwig-Langelier plot allows you to quickly see patterns and correlations between the major cations and anions for multiple samples. An example of the Ludwig-Langelier plot and the corresponding Ludwig-Langelier Plot Options dialogue is shown in the figure below.



The Ludwig-Langelier square plot is similar to the (central) projection areas of the Piper and Durov plots. By convention, the sums of selected cations are plotted on the X-Axis and the sums of selected anions are plotted on the Y-Axis. Each axis typically ranges from 0 to 50 meq%. Suitable groupings of cations and anions are selected and plotted as percentages. Generally, this type of graph is used to plot %(Cl+SO4) versus %(Na+K). Sample points are calculated (by default) on a forced ion balance basis as follows:

$$\%(Na+K) = \frac{[Na]+[K]}{\sum[C_i]} \times 50\%$$

where: %(Na+K) = percent sodium and potassium in %meq
[Na] = concentration of sodium in meq/L
[K] = concentration of potassium in meq/L
$\sum[C_i]$ = sum of cations (see functions)

$$\%(Cl + SO_4) = \frac{[Cl] + [SO_4]}{\sum[A_i]} \times 50\%$$

where: $\%(Cl+SO_4)$ = percent chloride and sulfate in %meq
$[Cl]$ = concentration of chloride in meq/L
$[SO_4]$ = concentration of sulfate in meq/L
$\sum[A_i]$ = sum of anions (see functions)

Sample points may alternatively be calculated without a forced ion balance:

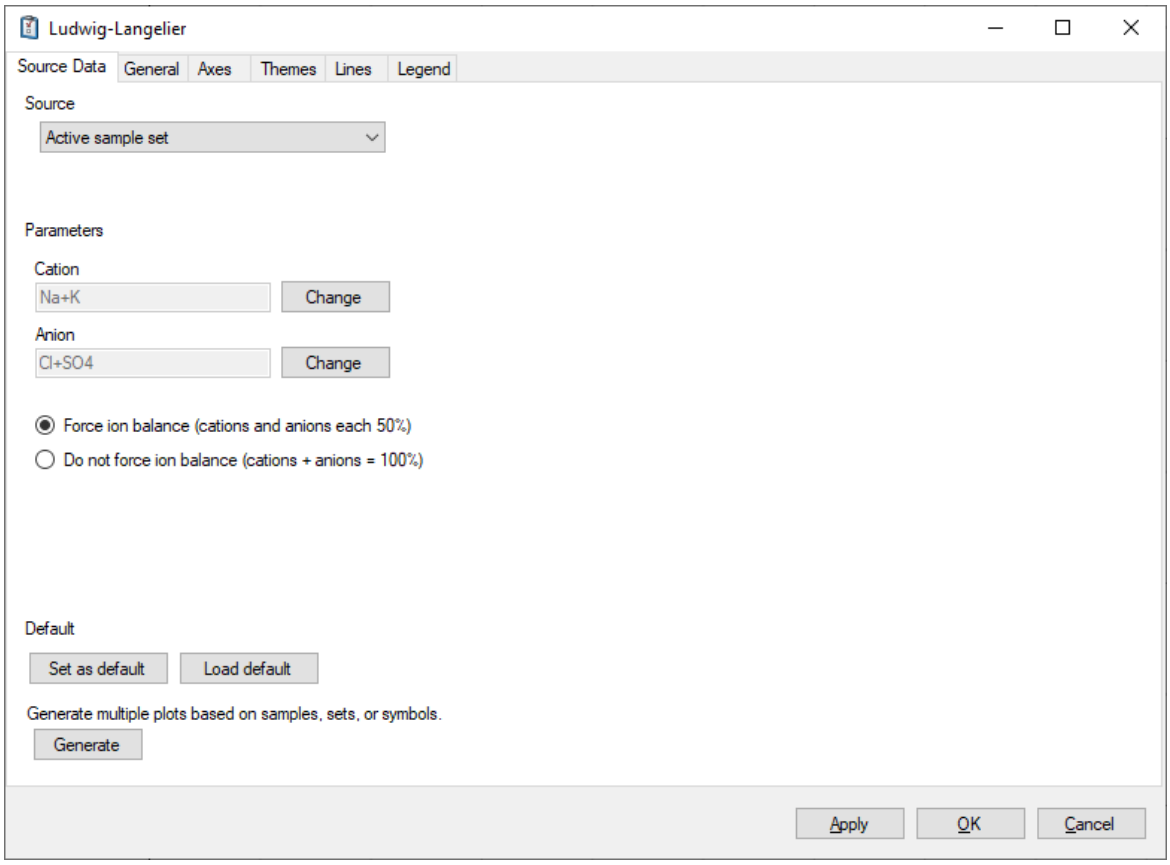
$$\%(Na + K) = \frac{[Na] + [K]}{\sum[C_i] + \sum[A_i]} \times 100\%$$

$$\%(Cl + SO_4) = \frac{[Cl] + [SO_4]}{\sum[C_i] + \sum[A_i]} \times 100\%$$

Major ions can be displayed in one plot with the Ludwig-Langelier plot; however, like the Piper and Durov plots, the Ludwig-Langelier plot displays relative ratios rather than absolute concentrations.

Source Data Tab

Data are specified in a Ludwig-Langelier plot as follows:



Source

See common plot settings.

Parameters

Ludwig-Langelier Plots two input parameters:

- **Cation**: one or more cations, typically: Na+K;
- **Anion**: one or more anions, typically: Cl+SO_4

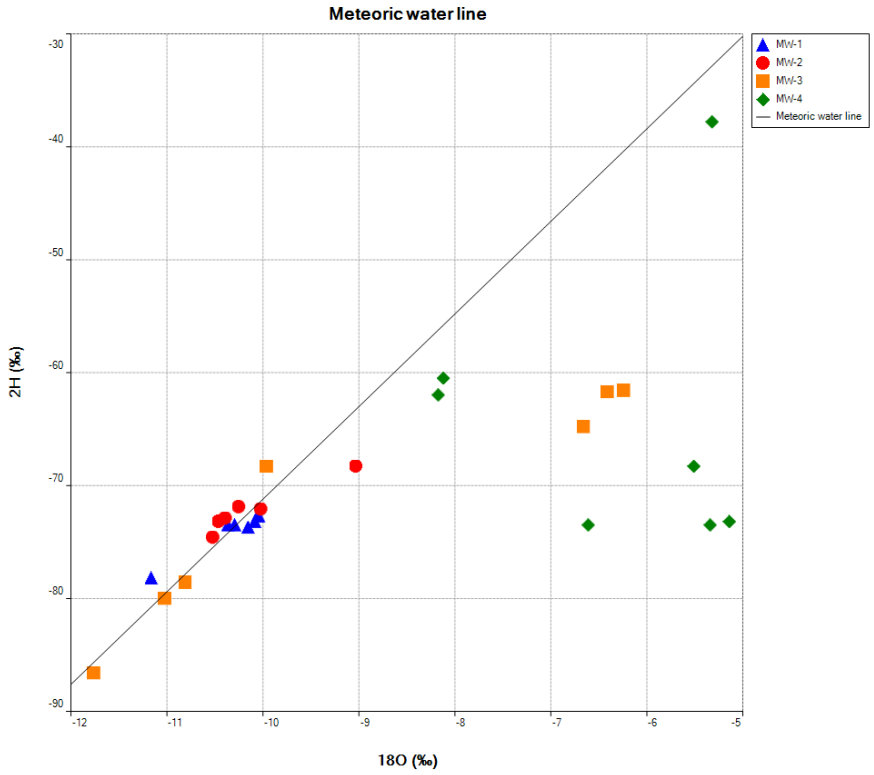
Note: that multiple parameters can be selected by holding the <CTRL> key while left-clicking to add/remove parameters from the parameter picker.

13.3.7 Meteoric Water Line (MWL) Plot

The Meteoric Water Line plot is the standard way to portray measurements of stable isotopes in water (18O and 2H). It consists of a scatter plot showing 18O on the X-axis and 2H on the y-axis. The global meteoric water line is typically defined by the following equation:

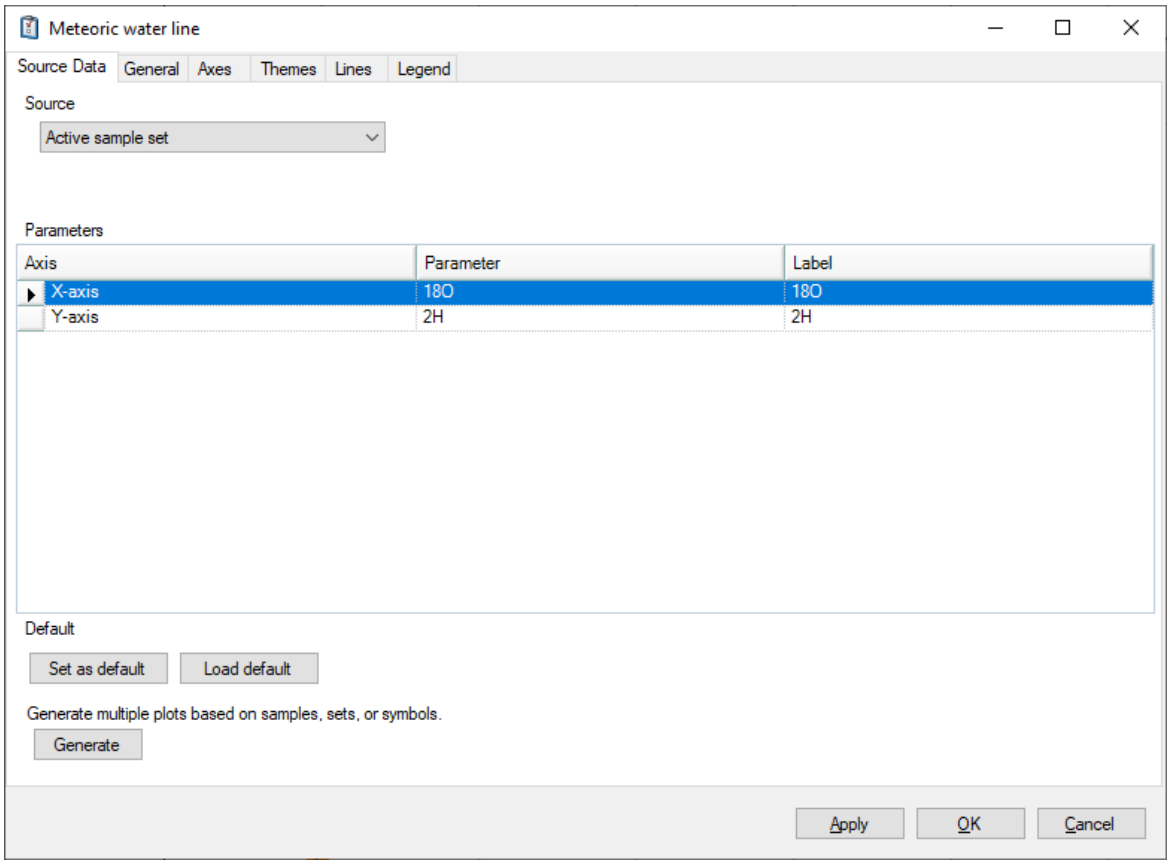
$$2H = 8.2 \times 18O + 10.8$$

Most groundwater and precipitation samples plot close to the line. In cases where the measured values are shifted from this line, the type of shifting provides important information regarding the process leading to the observed shift (e.g. rock-water interaction, evaporation, mixing with seawater, etc.).



Source Data Tab

Data are specified in a Meteoric Water Line plot as follows:



Source

See common plot settings.

Parameters

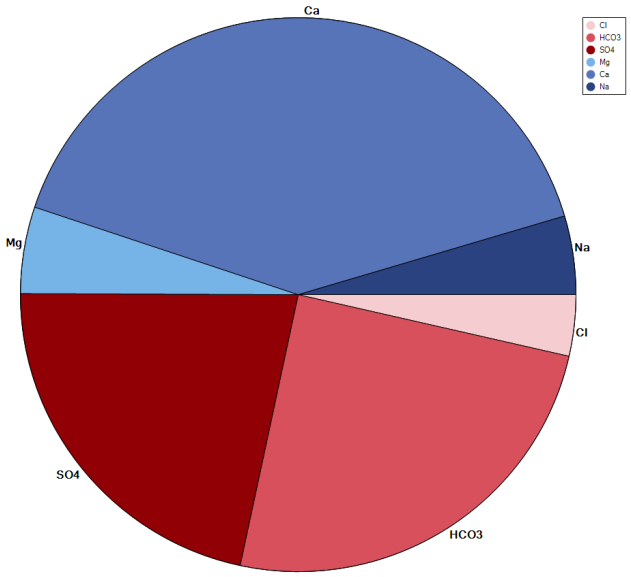
Meteoric Water Line Plots have a total of two required parameters:

- X-Axis: typically the Oxygen-18 (18O) parameter
- Y-Axis: typically the Deuterium (2H) parameter

Note: the Meteoric Water Line is added as a custom line and the default values of the slope (8.2) and intercept (10.8) in the Meteoric Water Line fitting equation can be changed to match regional variations in the line. You can change the default values in the regional chemistry tab of the project settings or you can add a custom regional line in the plot settings.

13.3.8 Pie Chart

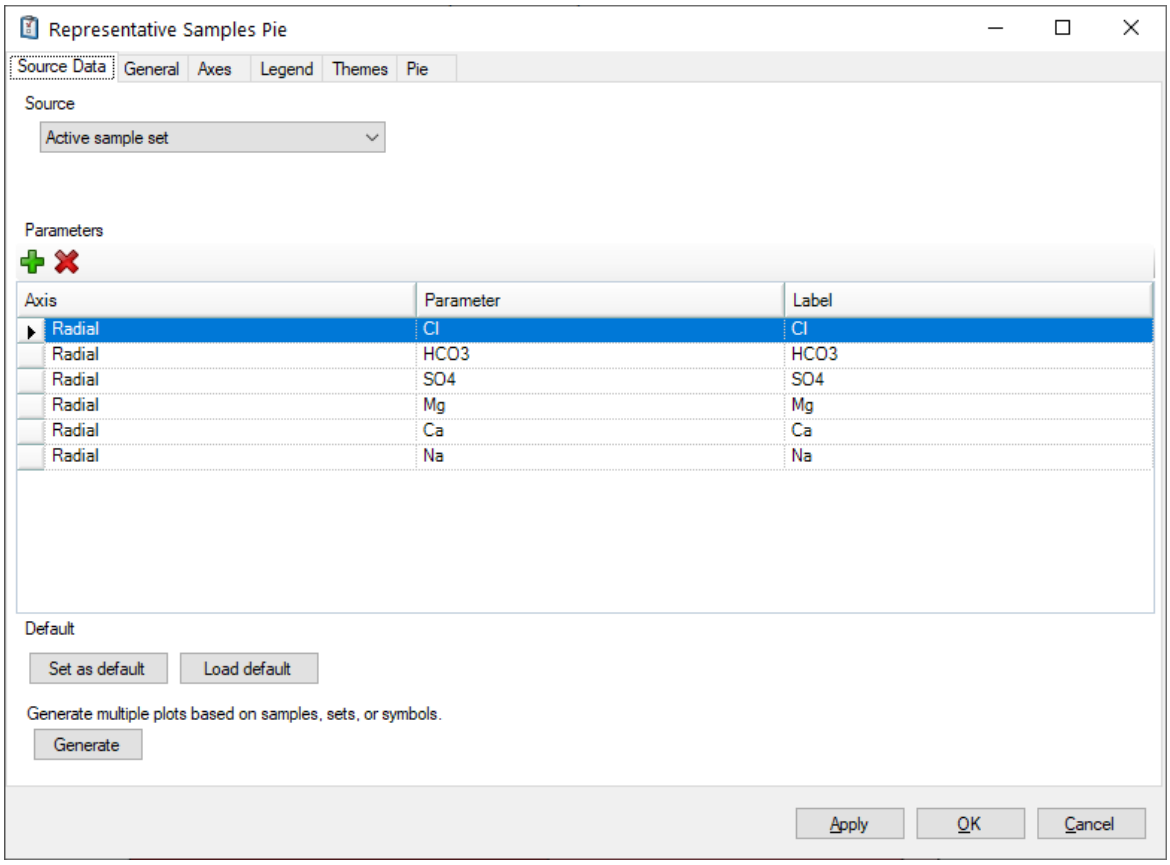
Pie charts are simple plots for showing parameter portions in a sample. An example of the Pie chart is shown in the figure below.



When a Pie chart is based on multiple samples, the average parameter values of the applicable samples will be plotted. If one or more of the parameters in a given sample are missing, that particular sample will not be included in the average. If you want to create a series of individual plots for samples in a particular sample set or station group, you can use the generate multiple plots option.

Source Data Tab

Data are specified in a Pie chart as follows:



Source

See common plot settings.

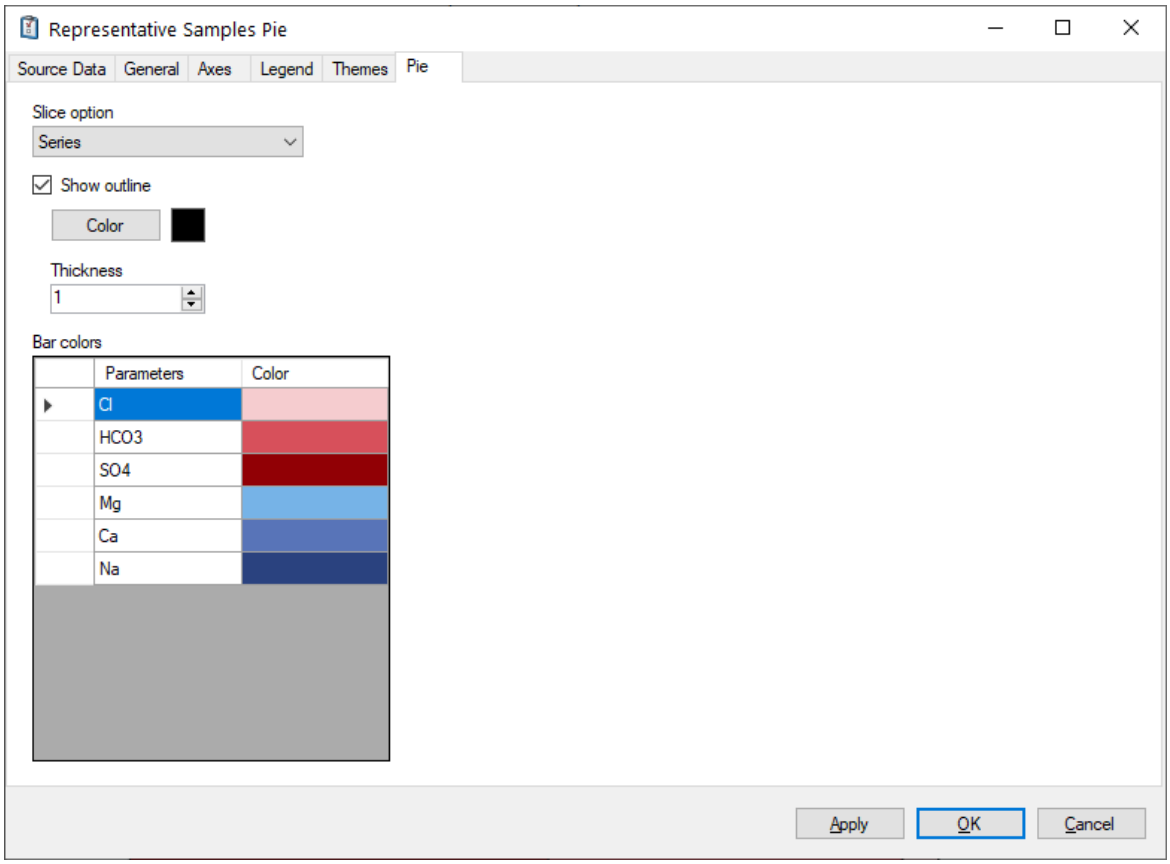
Parameters

Pie charts can have any number of numeric parameters as input.

Pie Chart Settings Tab

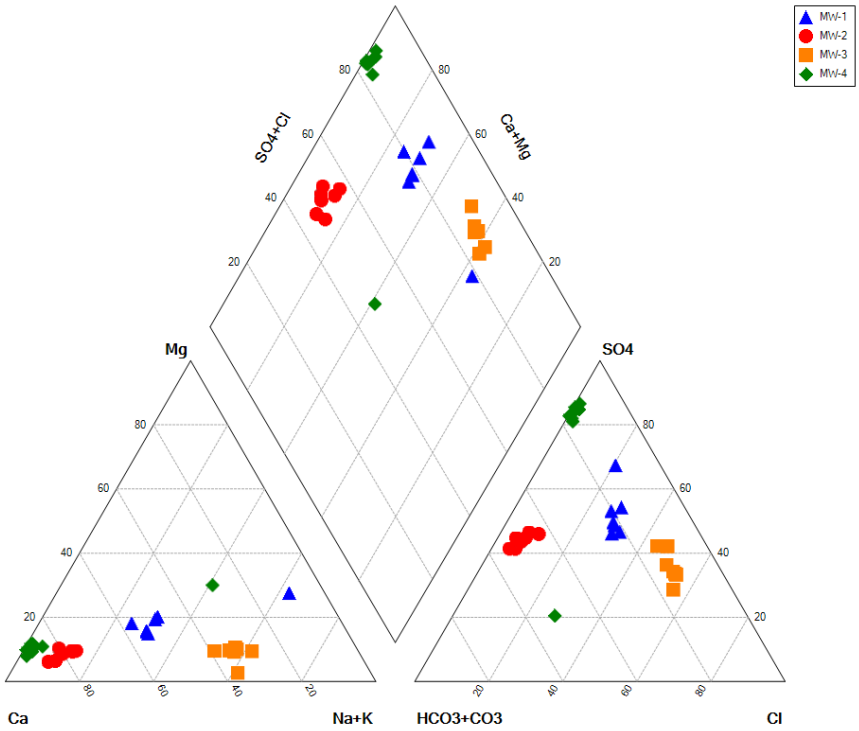
The Pie tab contains the following options:

- **Slice Option:** defines which labels will be shown for each slice:
  - *None*: no labels will be shown
  - *Series*: parameter labels
  - *Value*: parameter values
  - *Percentage*: slice percentage
- **Show Outline**: shows/hides the outline of the pie and category slices
- **Color**: color of the outline
- **Thickness**: thickness of the outline
- **Bar Colors**: color picker for each parameter in the pie



13.3.9 Piper Diagram

The Piper plot is useful for showing multiple samples and trends in major ions. An example of the Piper plot and the corresponding Piper Plot Options dialogue is shown in the figure below.

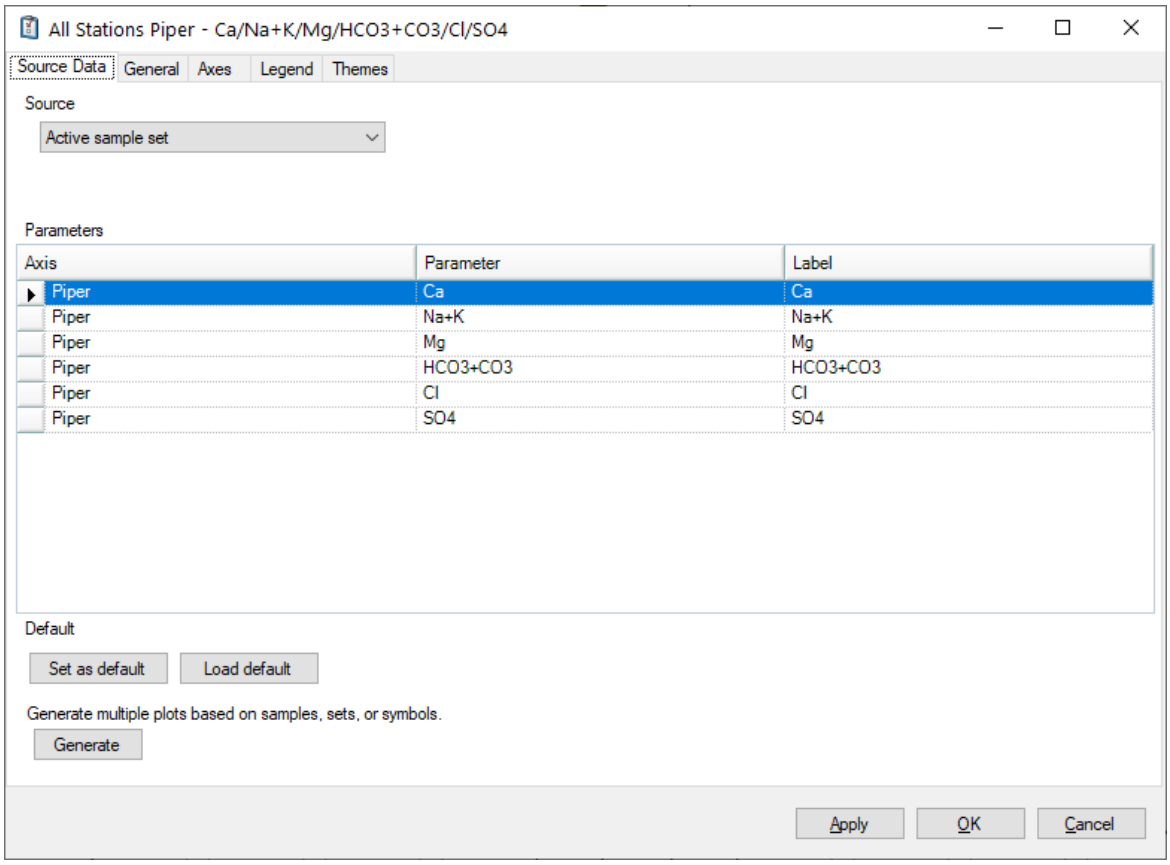


In a Piper plot, the major ions are plotted on separate cation (typically: Na+K, Ca, and Mg) and anion (typically: Cl, HCO_3+CO_3, and SO_4) ternary diagrams in terms of percent milliequivalents in two triangles along the base. The total cations in meq/l, and the total anions in meq/l, are set equal to 100%. The data points in the two triangles are then projected onto the diamond grid. The projection reveals certain useful properties of the total ion relationships. Every sample is represented by three data points; one in each triangle and one in the projection diamond grid.

The Piper plot allows comparisons of 6 parameters between a large number of samples. Like all trilinear plots, it does not portray absolute ion concentrations. The main purpose of Piper plots is to show clustering of samples and infer hydrochemical facies of samples or clusters of samples.

Source Data Tab

Data are specified in a Piper plot as follows:



Source

See common plot settings.

Parameters

Piper Plots have a total of six required parameters:

- three major **cations**, typically: sodium (Na) and potassium (K), magnesium (Mg), and calcium (Ca); and
- three major **anions**, typically: chloride (Cl), bicarbonate (HCO3) and carbonate (CO3), and sulfate (SO4)

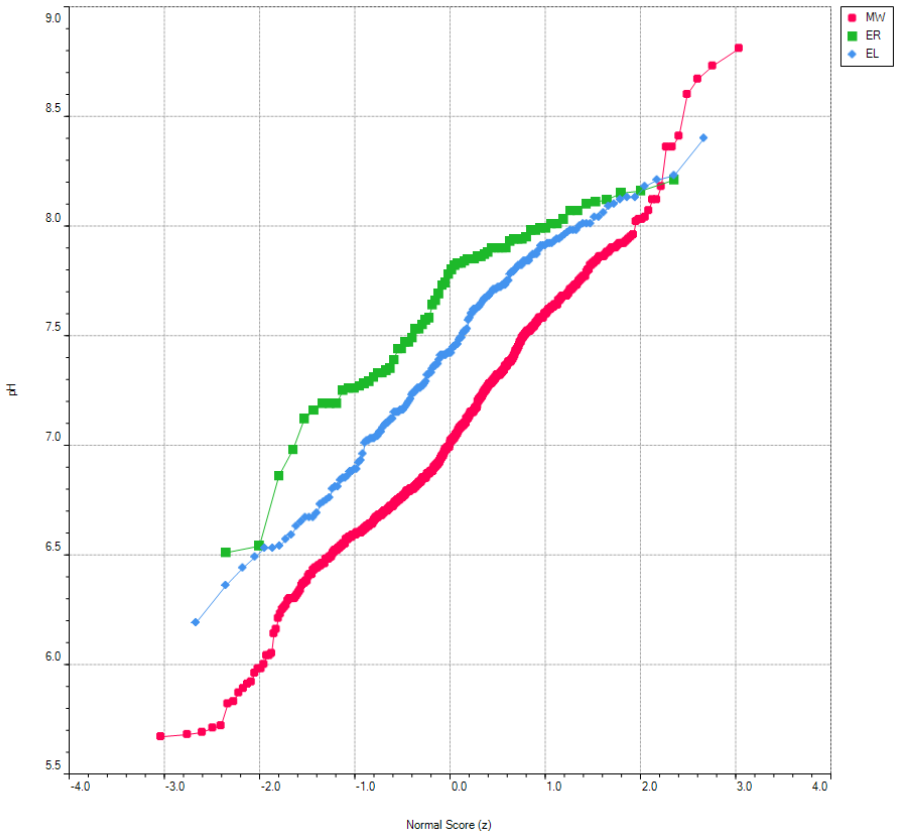
The cations specify the parameters that are presented in the lower left triangle. Default settings are the major cations Na+K, Ca, and Mg; however the parameters can be reordered or any other parameter can be selected (e.g. gas composition, trace elements etc.). The anions generally specify the parameters for the lower right triangle. Default settings are the major anions Cl, SO4, and HCO3+CO3 and, as with cations, anions can be reordered or substituted with other suitable parameters.

Each of the parameters also contain a matching Label field. This allows customization of the parameter labels on the plot diagram. For example, if you used Alkalinity as one of the input

(anion) parameters, you may wish to edit the label so that the parameter is displayed as `HCO3+CO3'.

13.3.10 Probability Plot

Probability plots involve plotting ranked data against quantiles of the normal distribution. They are particularly useful for spotting irregularities within the data when compared to a specific distribution model, particularly the Normal distribution, which plots as a straight-line on a Probability plot (where the slope is the standard deviation and the Y-intercept is the mean). An example based on the value of field-measured pH of samples in the Demo project is shown below:



To create a probability plot, the data are ranked in order of lowest value (1) to highest value (n, where is the number of values). The y-coordinate of the probability plot is the value of the data. The x-coordinate is based on the Normal Score (z), which AquaChem automatically determines using the uniform order statistic (U), as follows:

$$z = \Phi^{-1}(U_i)$$

where: z = Normal Score

Φ^{-1} = inverse function of the normal distribution

U_i = is the uniform order statistic given by:

$$U_i = \frac{(i-a)}{(n+1-2a)} \; for \; i = 1, 2, 3, \ldots, n-1, n$$

where: i = rank of i^{th} smallest value for the plot dataset

n = count of all values for the plot dataset

a = 0.3175

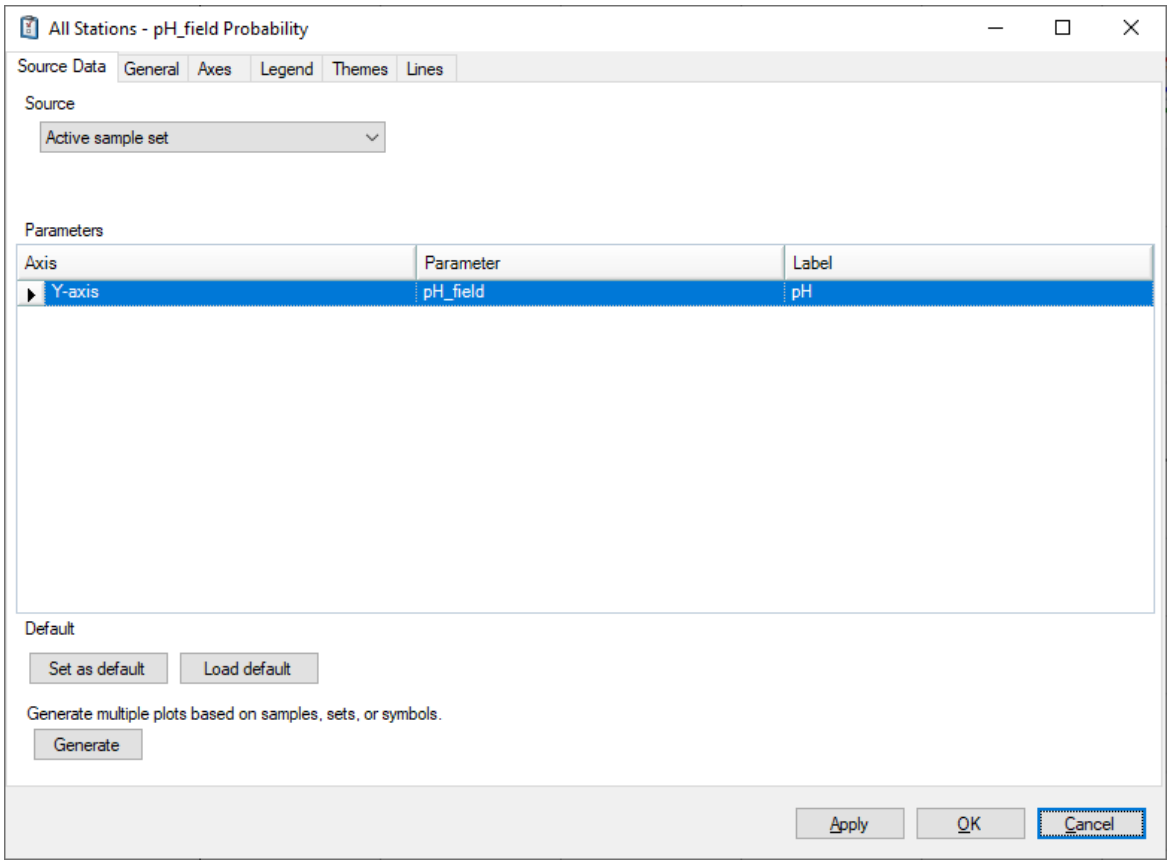
Using this plot, it is possible to observe whether and where departures from Normality are occurring - in the middle ranges of the data or in the extreme tails. Probability plots can also indicate:

- the presence of possible outlier values
- different subsets of the data that do not follow the basic pattern of the data, and
- the presence of significant positive or negative skewness.

A log-scale transformation on the y-axis may be used to test whether a dataset that shows non-normal behavior is log-normally distributed.

Source Data Tab

Data are specified in a Probability plot as follows:



Source

See common plot settings.

Parameters

Probability plots are limited to a single selectable parameter, plotted on the Y-axis. The x-axis data are plotted based on the Normal score (z), as defined above.

13.3.11 Quantile Plot

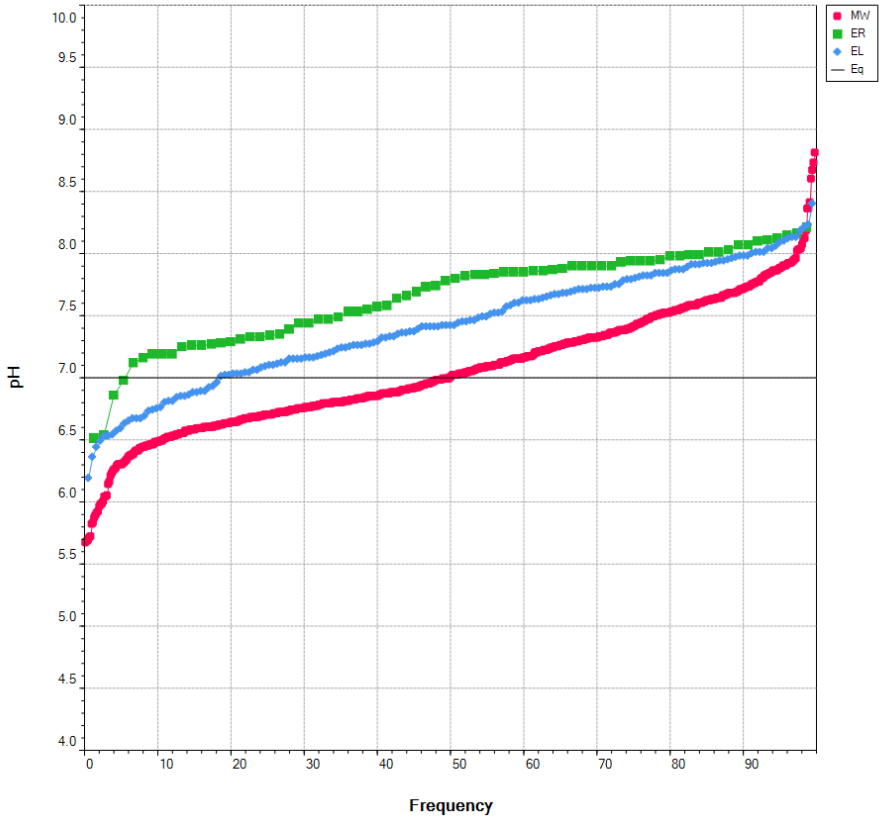
The Quantile chart (sometimes known as the cumulative frequency chart) plots the values of the ranked data from lowest to highest on the Y-axis and the cumulative frequency on the X-axis. The estimated cumulative frequency (X-coordinate) of the data is given by:

$$q_i = \frac{i}{(n+1)} \; for \; i = 1, 2, 3, \ldots, n-1, n$$

where: q_i is the cumulative frequency/quantile of the ranked dataset, $0 < q_i < 1$

i is the rank of the i^{th} sample
n is the number of samples

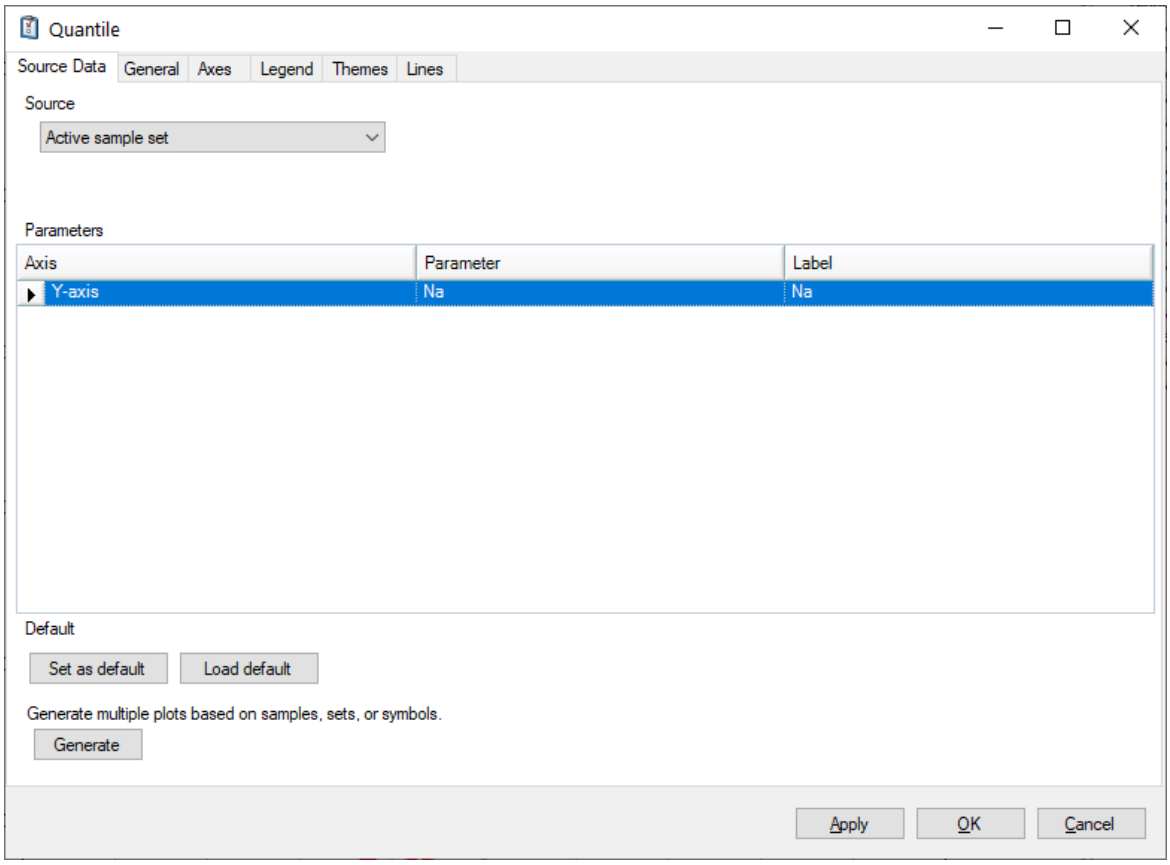
An example based on the sodium concentration of samples in the Demo project is shown below:



Using this plot, it is possible to observe the distribution of the data and estimate quantile values and ranges.

Source Data Tab

Data are specified in a Quantile plot as follows:



Source

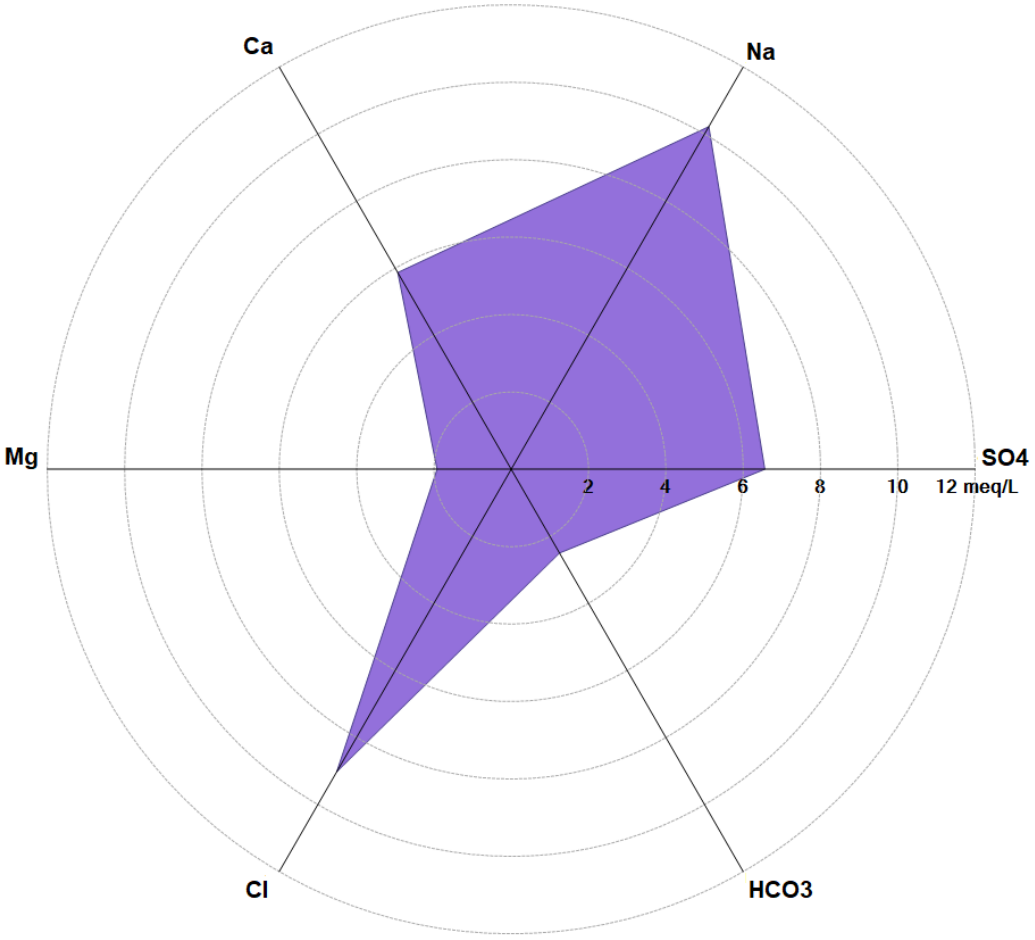
See common plot settings.

Parameters

Quantile plots are limited to a single selectable parameter, plotted on the Y-axis. The x-axis data are plotted based on the estimated cumulative frequency, as defined above.

13.3.12 Radial Plot

Radial plots (also known as radar plots) are used to compare multiple parameter values for a single sample and to compare the ratios of these values for many different samples. An example of the Radial plot is shown in the figure below.

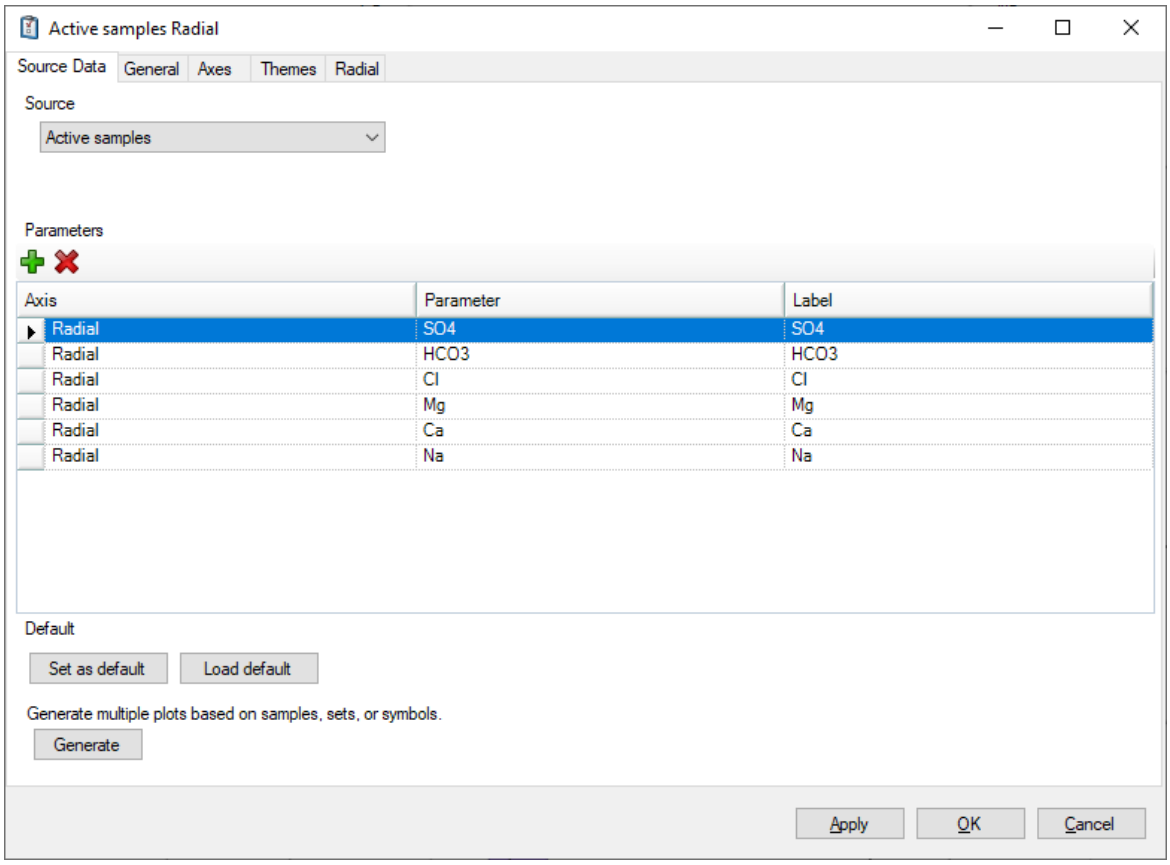


Radial plots can be used to evaluate the change in water quality at a single location over a period of time, or they can be used to evaluate the change in water quality as the water passes through different geologic formations or different subsurface conditions.

When a radial plot is based on multiple samples, the average parameter values of the applicable samples will be plotted. If one or more of the parameters in a given sample are missing, that particular sample will not be included in the average. If you want to create a series of individual plots for samples in a particular sample set or station group, you can use the generate multiple plots option.

Source Data Tab

Data are specified in a Radial plot as follows:



Source

See common plot settings.

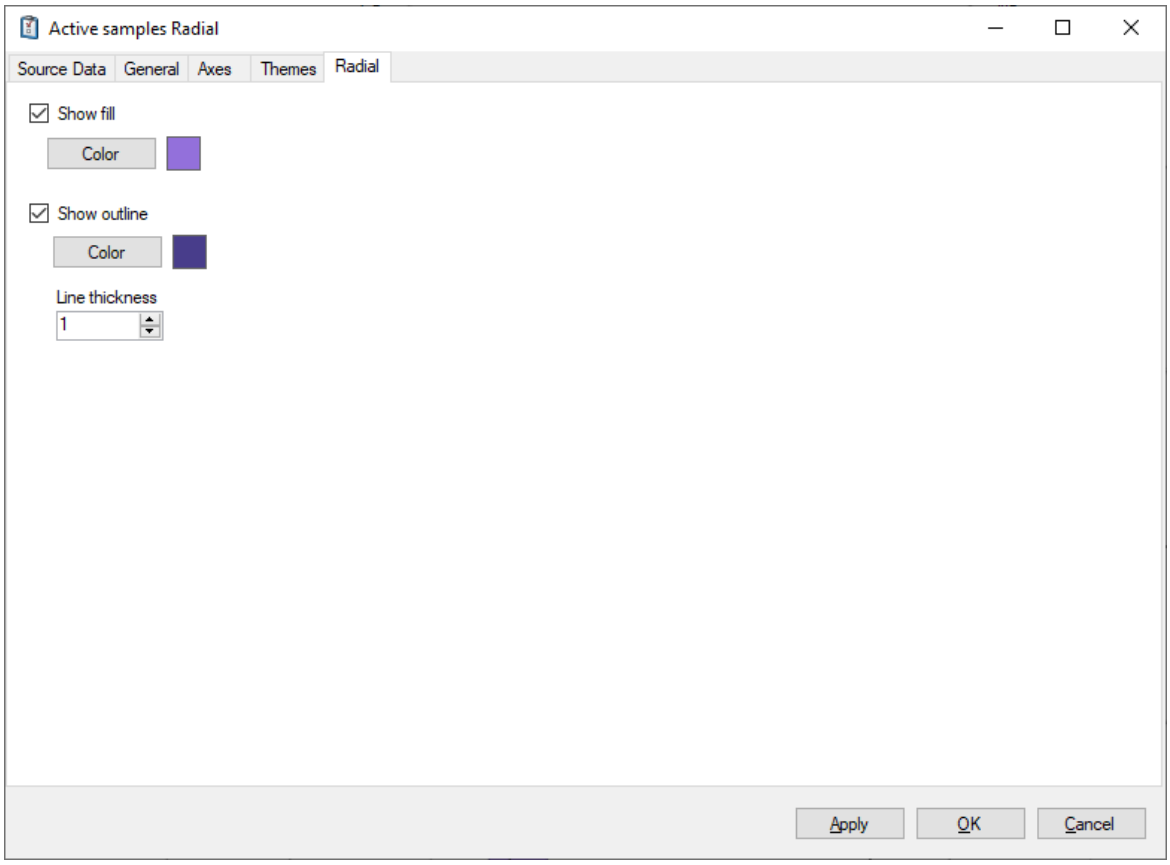
Parameters

Radial plots can have any number of numeric parameters as input.

Radial Plot Settings Tab

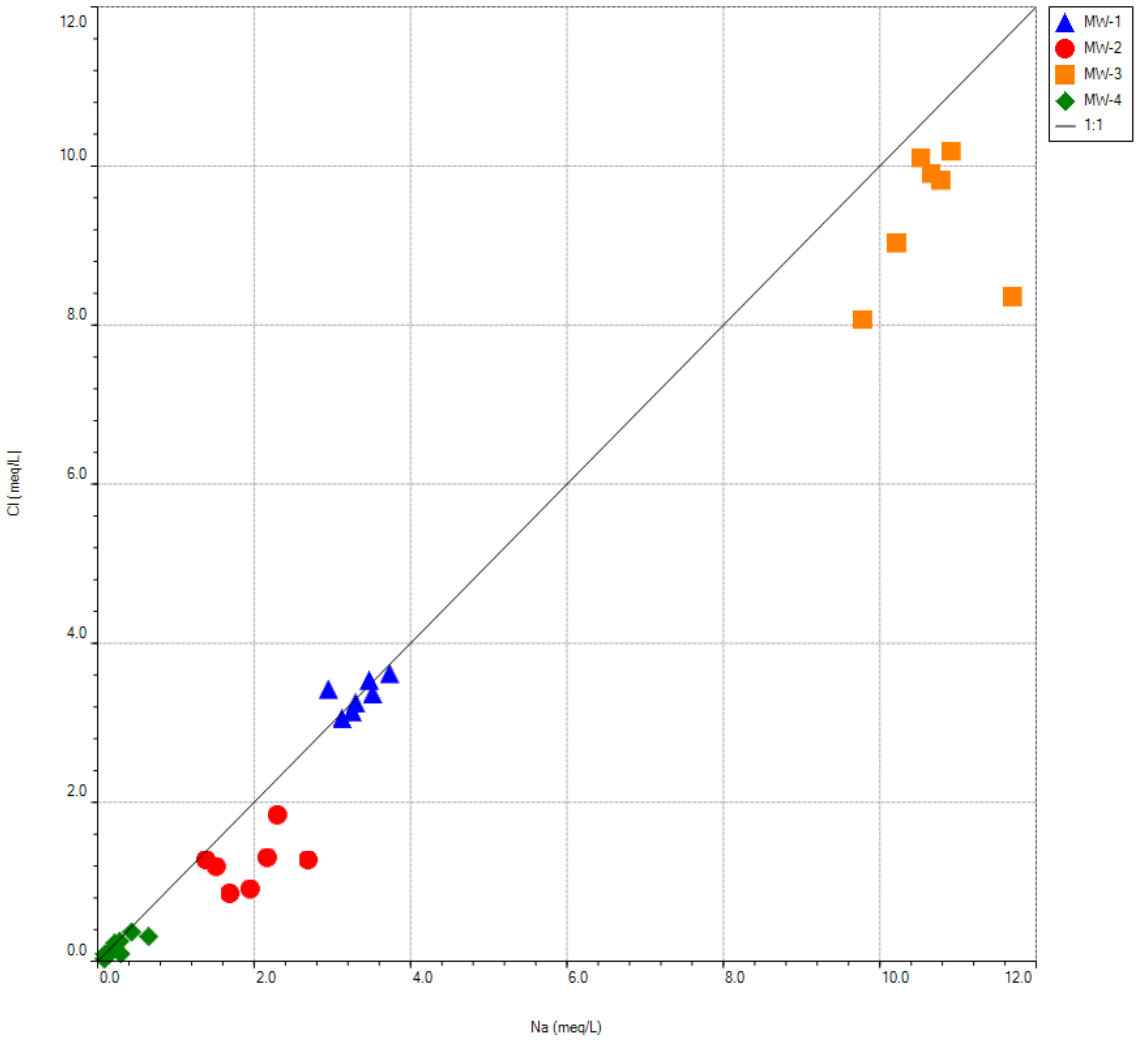
The Radial tab contains the following options:

- **Show fill:** if selected, the radial plot will include a fill color as defined below
- **Color**: color of the radial plot fill
- **Show outline:** if selected, the radial plot will include a line color as defined below
- **Color**: color of the outline
- **Thickness**: thickness of the outline



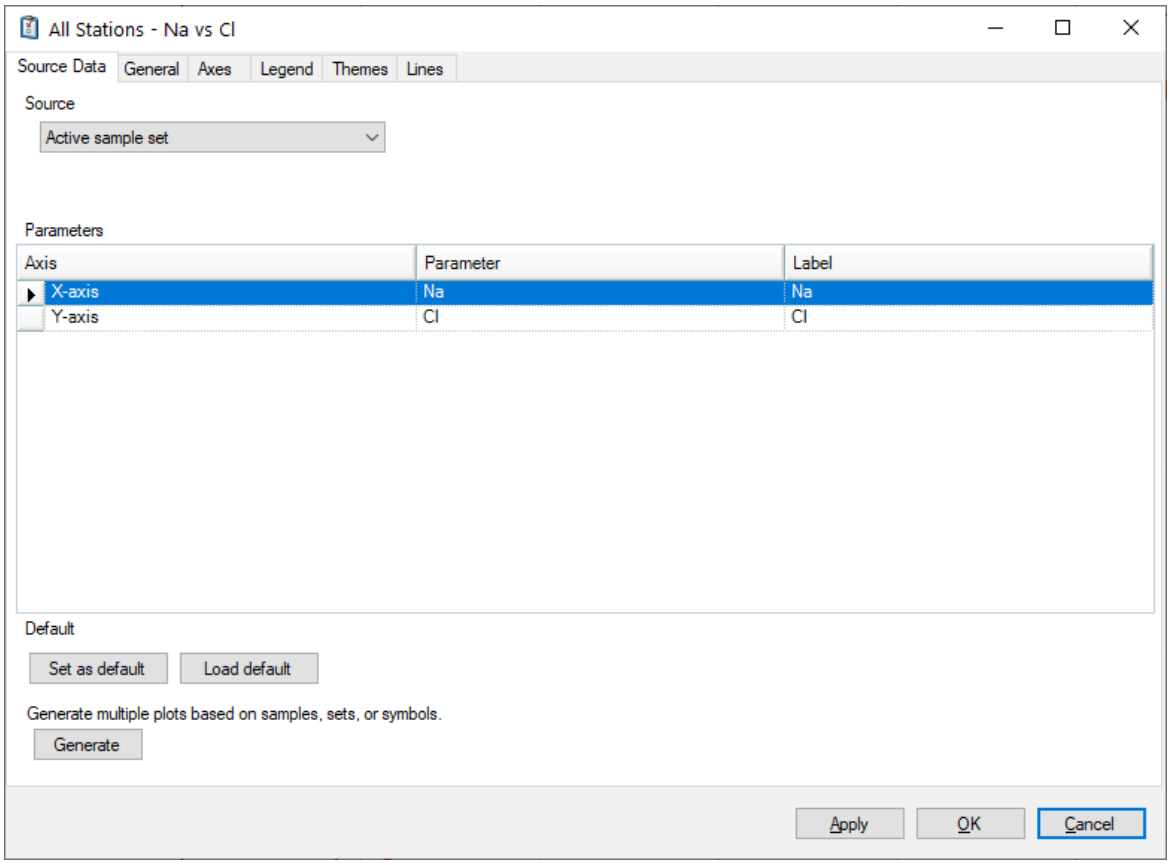
13.3.13 Scatter Plot

Scatter plots are the most simple and popular approach to interpreting hydrochemical data. Scatter plots can show effects such as correlation of parameters or clustering of samples in a very intuitive manner. An example of the Scatter plot and the corresponding Scatter Plot Options dialogue is shown in the figure below. Note a custom (1:1) line has be added to the plot.



Source Data Tab

Data are specified in a Scatter plot plot as follows:



Source

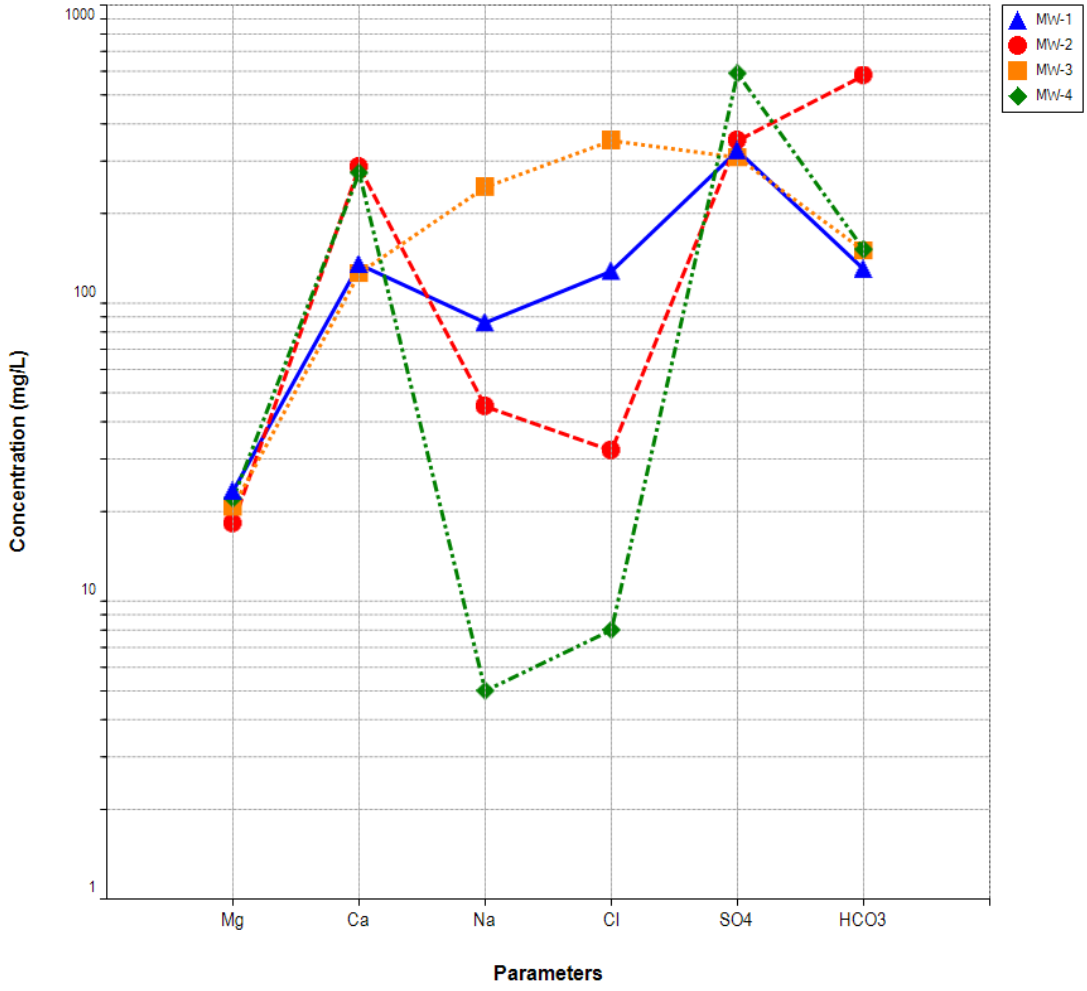
See common plot settings.

Parameters

Scatter plots consist of two input parameters, an X-axis parameter and Y-axis parameter. Both X- and Y-axis parameters must contain numerical inputs.

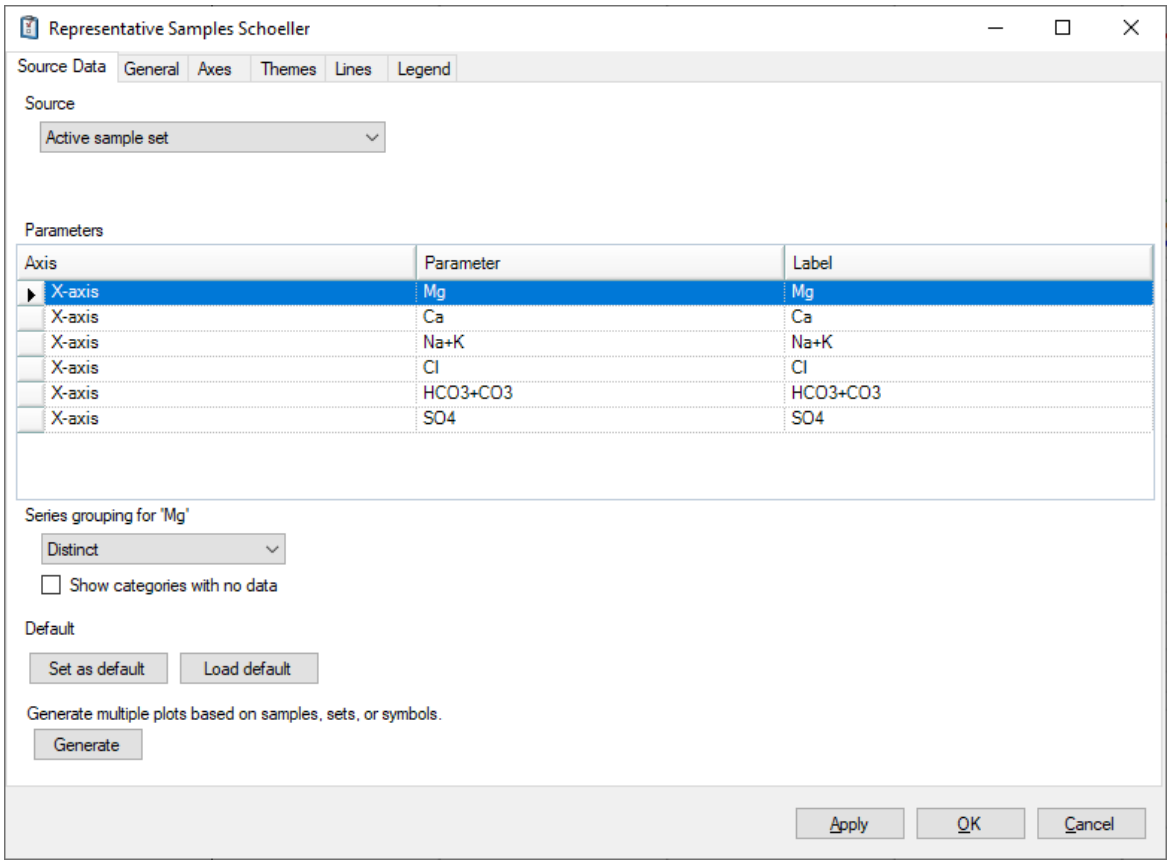
13.3.14 Schoeller Plot

Schoeller (1962) developed semi-logarithmic plots to represent major ion analyses in milliequivalents per liter (meq/L) and to demonstrate different hydrochemical water types on the same plot. Altough multiple analyses (i.e. samples) can be plotted on a Schoeller plot, the number is practically limited to a small number as the graph can be difficult to interpret as more data series will increase clutter on the plot. However, the plot has the advantage that, unlike trilinear plots, actual parameter concentrations are displayed. An example of the Schoeller plot is shown in the figure below.



Source Data Tab

Data are specified in a Schoeller plot as follows:



Source

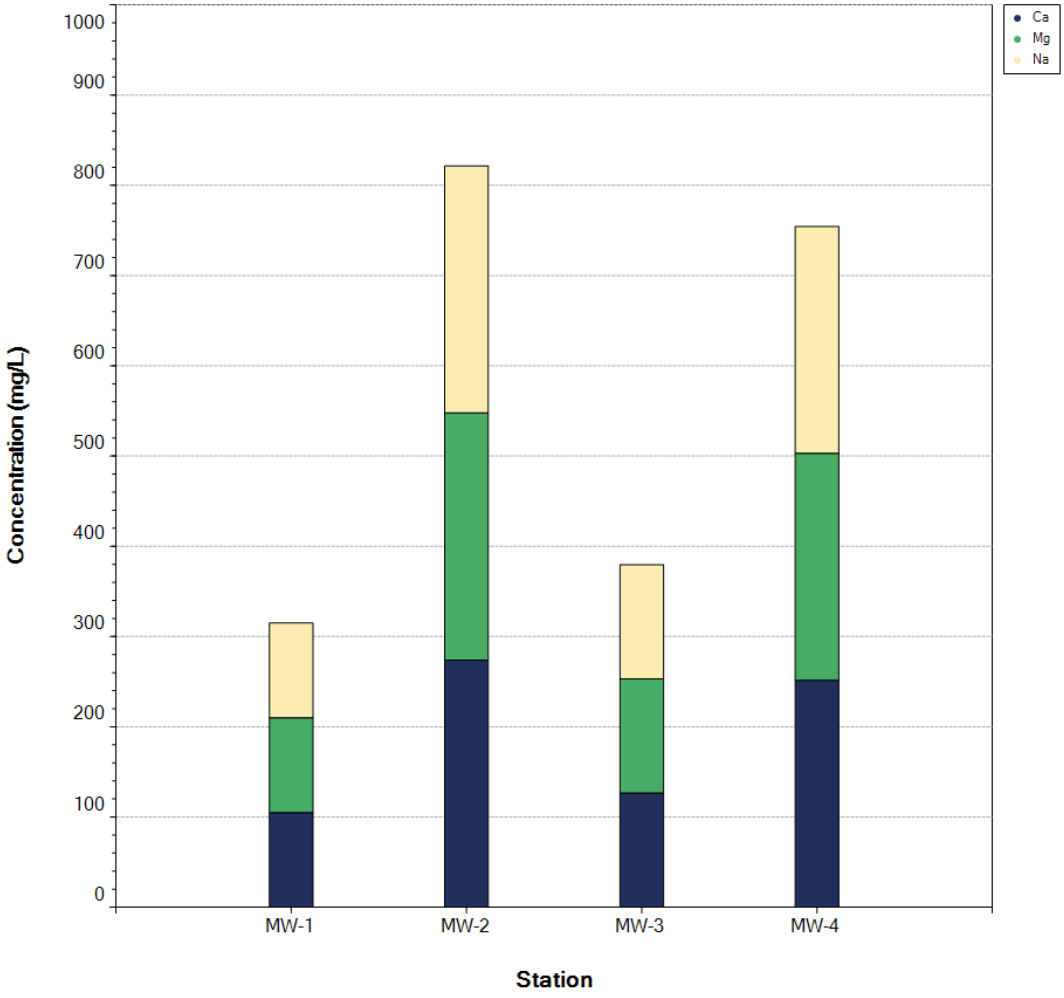
See common plot settings.

Parameters

Schoeller plots consist of two input parameters, an X-axis parameter and Y-axis parameter. Both X- and Y-axis parameters must contain numerical inputs.

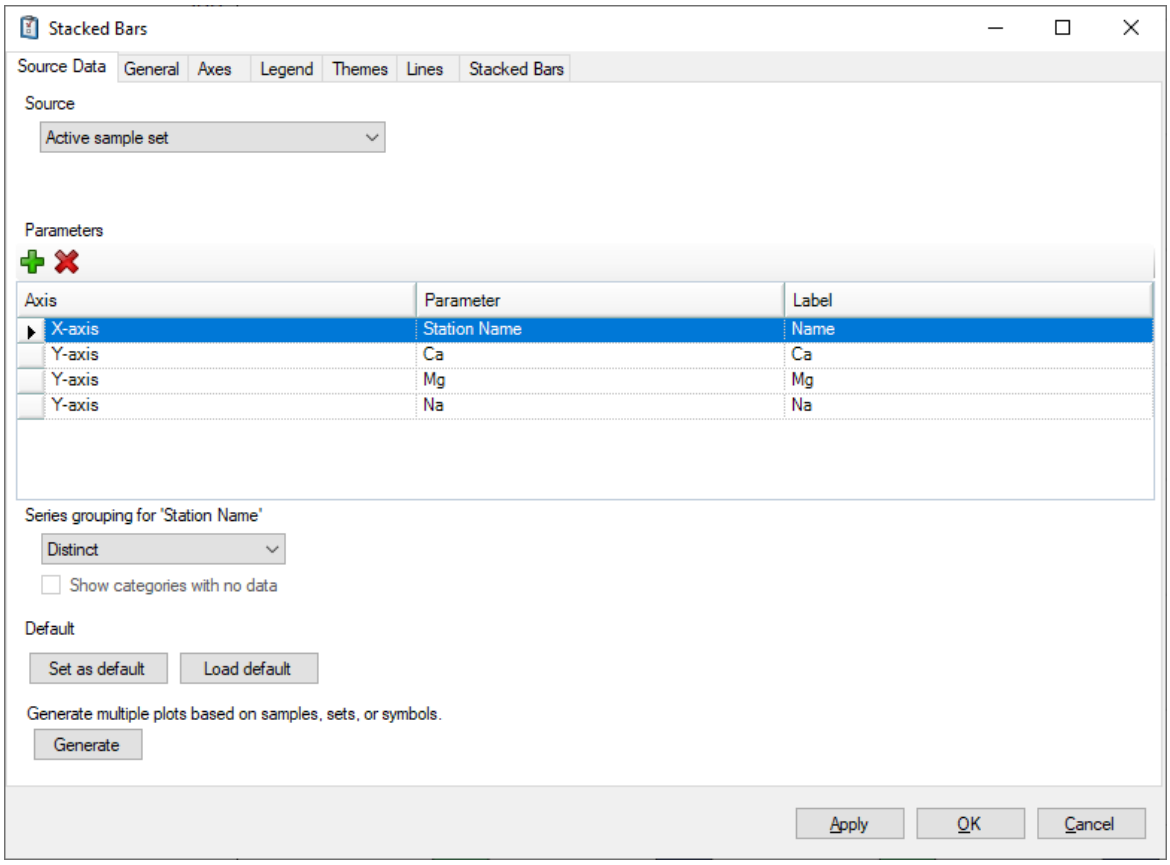
13.3.15 Stacked Bars Plot

The Stacked Bars plot allows you to select multiple numerical parameters of a similar category (e.g. cations) to plot for a specified category (e.g. Station, Sample ID, Sample Date, Site, etc.). Each parameter is represented by a bars that are stacked and scaled proportionately to their value.separately. The height of the resulting bar shows the combined result of the groups. However, stacked bar charts are not suited to data sets where some groups have negative values.



Source Data Tab

Data are specified in a Stacked Bar plot as follows:



Source

See common plot settings.

Parameters

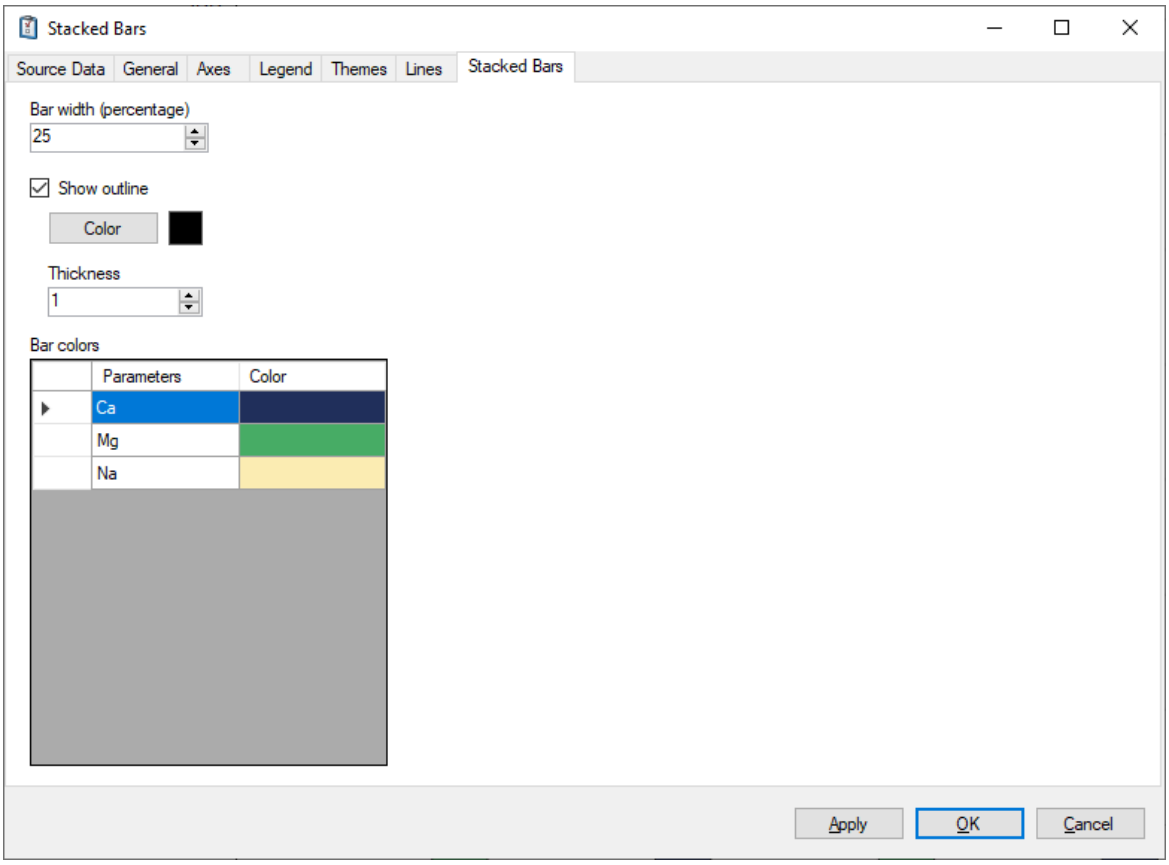
Stacked Bar plots consist of the following input parameters:

- **X-axis**: one category parameter
- **Y-axis**: one or more numerical parameter values.

Stacked Bar Settings Tab

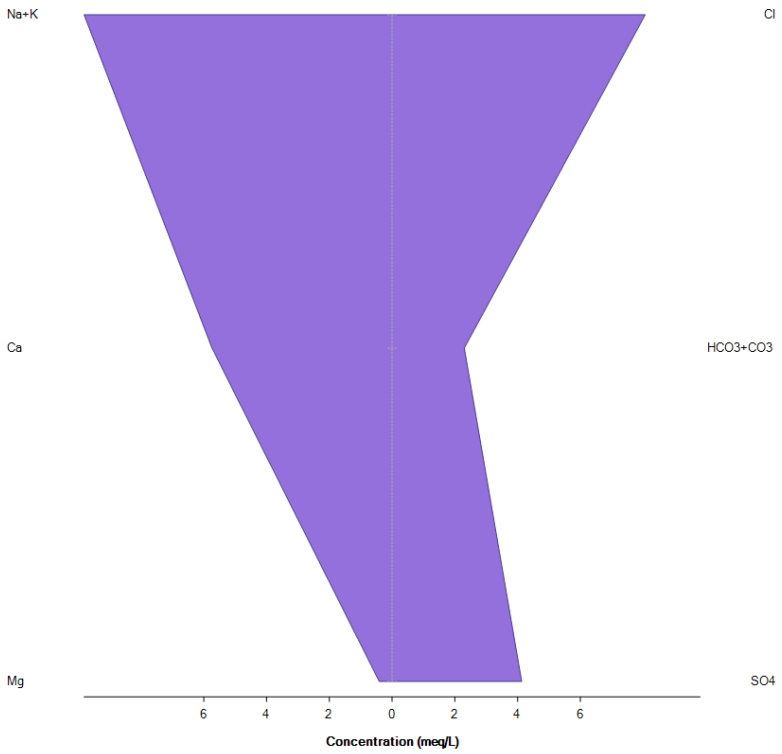
The Stacked Bar tab contains the following options:

- **Bar width:** width of the bar as a percentage of the category (i.e. a value of 100 will produce bars with no gaps)
- **Show Outline**: if selected, the bars will include an outline
- **Color**: color of the radial plot fill
- **Thickness**: thickness of the outline
- **Bar Colors**: color picker for each stacked bar parameter in the plot



13.3.16 Stiff Plot

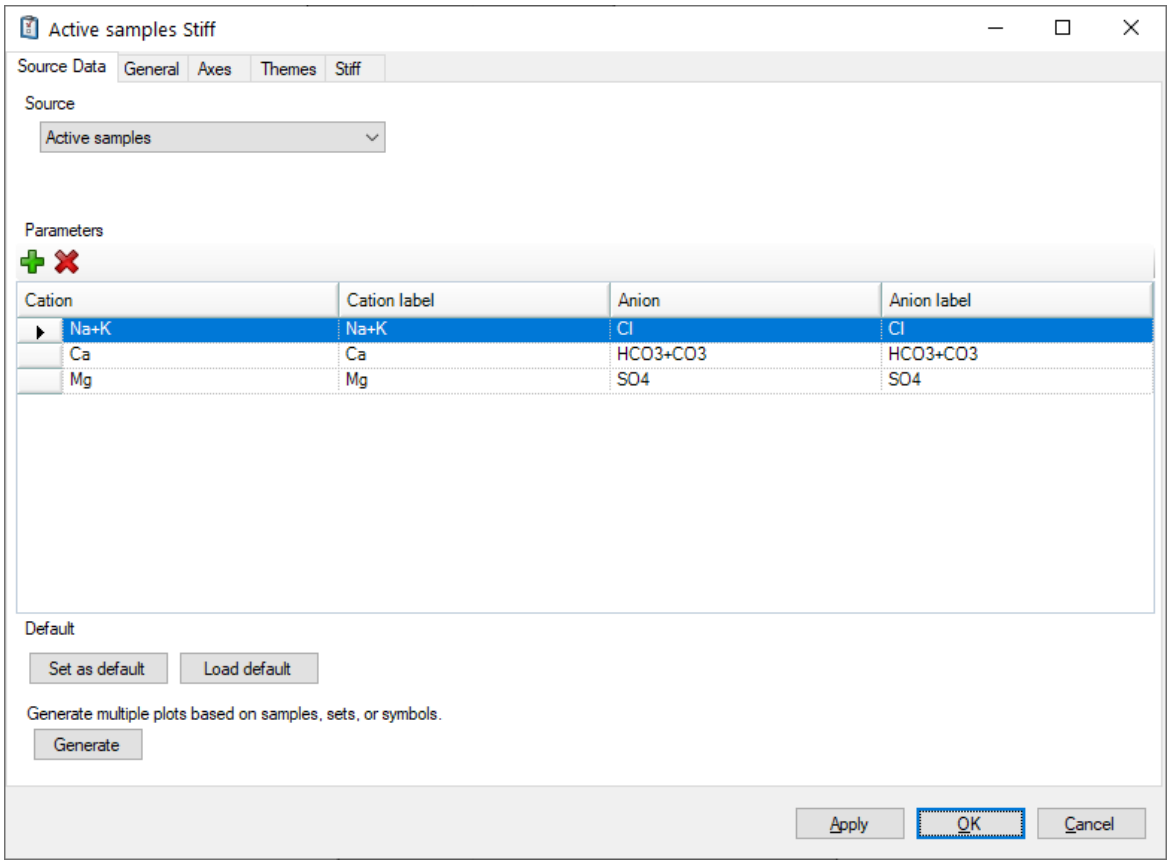
The Stiff plot belongs to the group of pattern plots (see Hem 1985, p. 175). It is constructed by plotting the milliequivalents per liter of (typically three) matched pairs of cations and anions. Stiff plots can be used to evaluate the change in water quality at a single location over a period of time, or they can be used to evaluate the change in water quality as the water passes through different geologic formations or different subsurface conditions. An example of the Stiff plot is shown in the figure below.



If multiple samples are selected, the Stiff plot will be based on the average concentrations of parameters specified in the source data. If you want to generate individual plots for many samples or stations, you can use the generate multiple plot options.

Source Data Tab

Data are specified in a Stiff plot as follows:



Source

See common plot settings.

Parameters

Stiff Plots have cations and anions as required parameters:

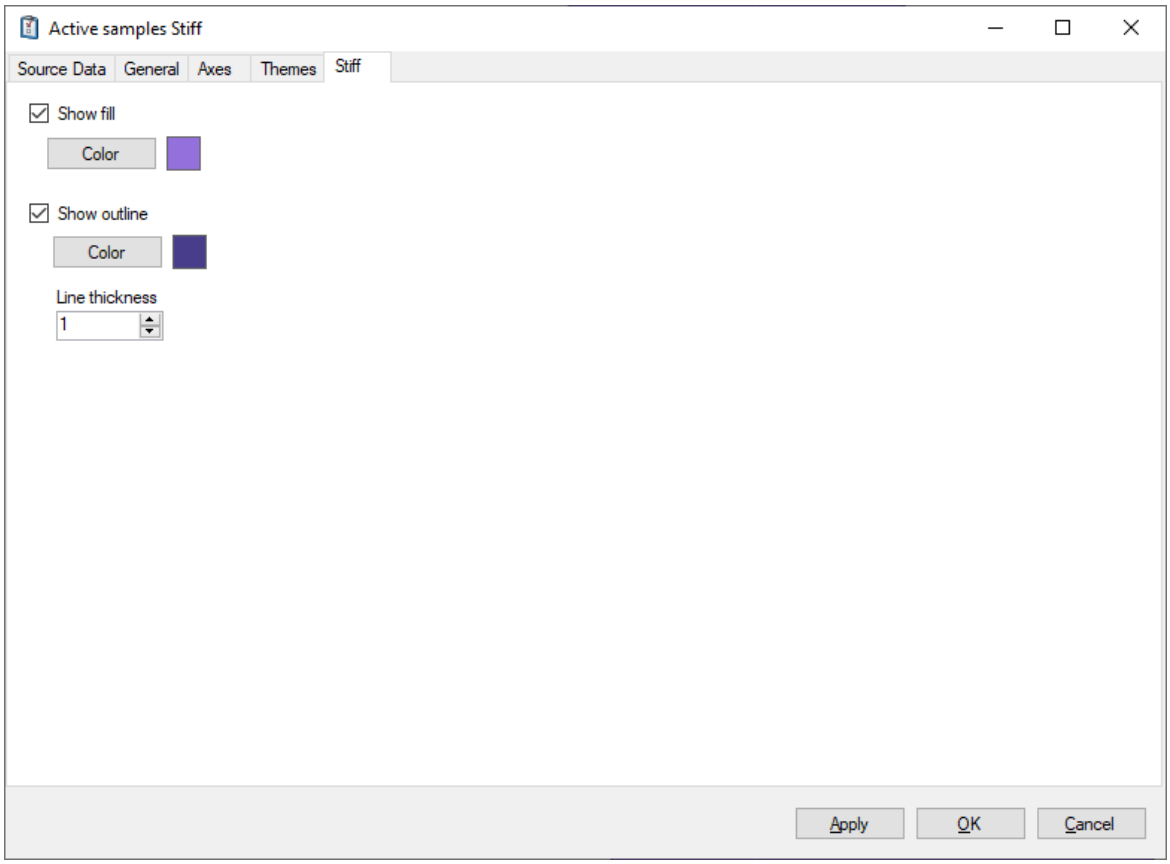
- **Cations**, typically: sodium (Na) and potassium (K), magnesium (Mg), and calcium (Ca); and
- **Anions**, typically: chloride (Cl), bicarbonate (HCO3) and carbonate (CO3), and sulfate (SO4)

The number of cations must match the number of anions (typically three of each), noting that cations/anions may be composed of more than one parameter (e.g. Na+K or HCO3+CO3). Multiple parameters can be selected by holding the <CRTL> key when selecting parameters in the parameter picker.

Stiff Plot Settings Tab

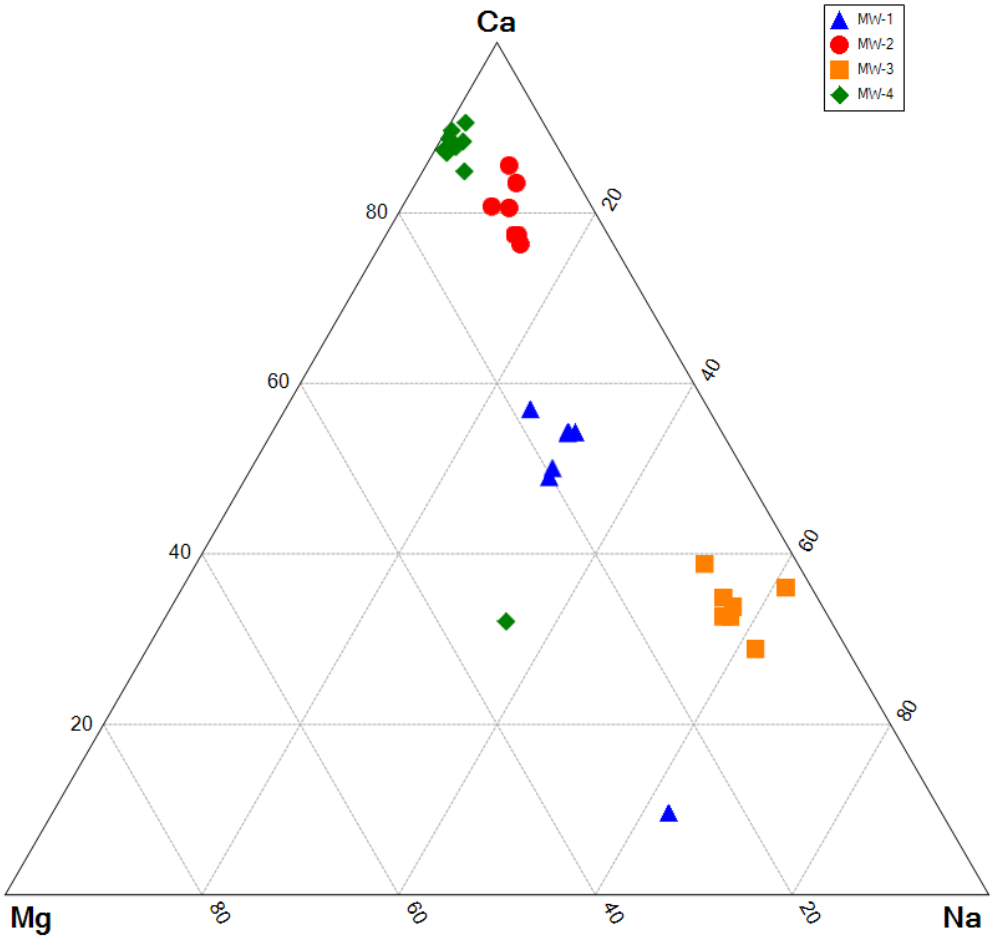
The Stiff Plot tab contains the following options:

- **Show Fill**: if selected, the Stiff plot will be filled
- **Color**: color of the Stiff plot fill
- **Show Outline**: if selected, the Stiff plot will include an outline
- **Color**: color of the outline
- **Thickness**: thickness of the outline



13.3.17 Ternary Plot

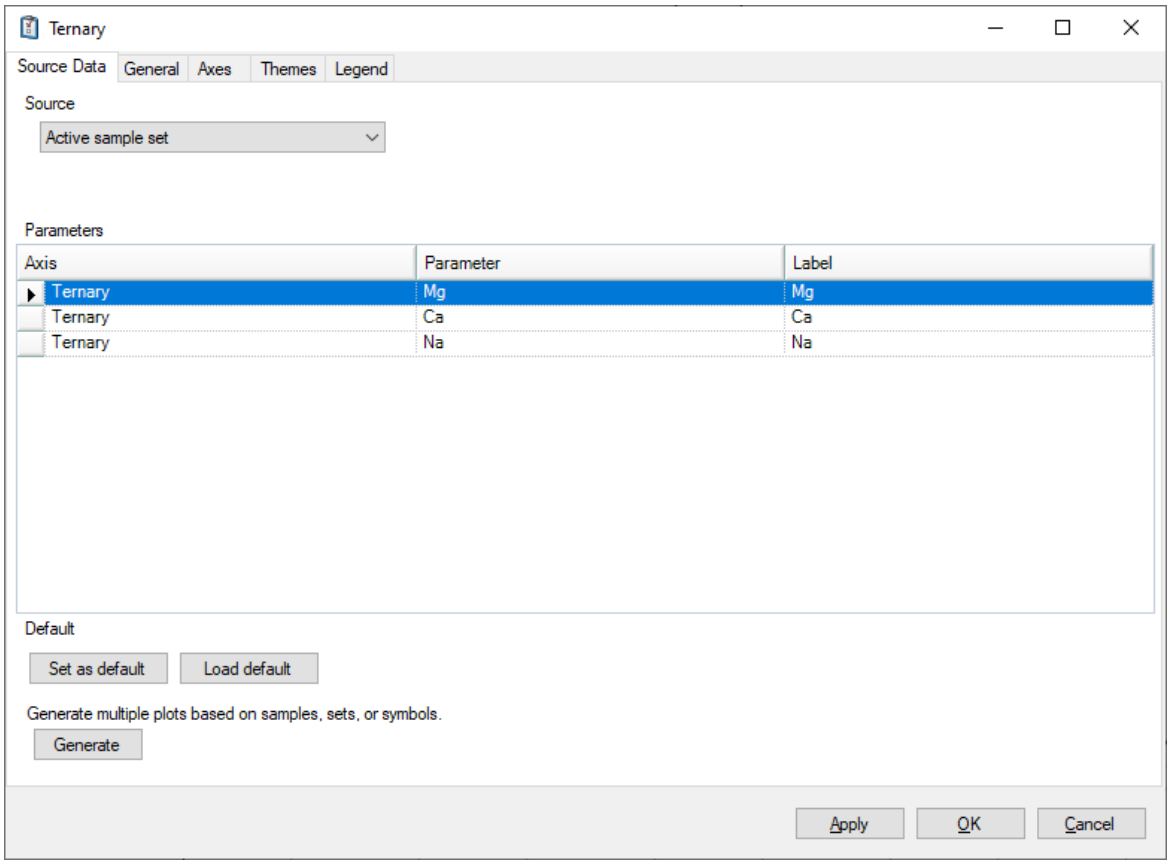
Ternary plots are used to determine the relationship between the concentrations of three different parameters in multiple samples. An example of the Ternary plot is shown in the figure below.



Like Piper and Durov plots, the Ternary plot displays relative concentrations of each parameter with respect to the sum of the concentrations of each parameter. Each vertex of the Ternary plot represents a relative concentration of 100% for the parameter at the respective vertex, while the base represents a relative concentration of 0% for the parameter plotted at the opposite vertex.

Source Data Tab

Data are specified in a Ternary plot as follows:



Source

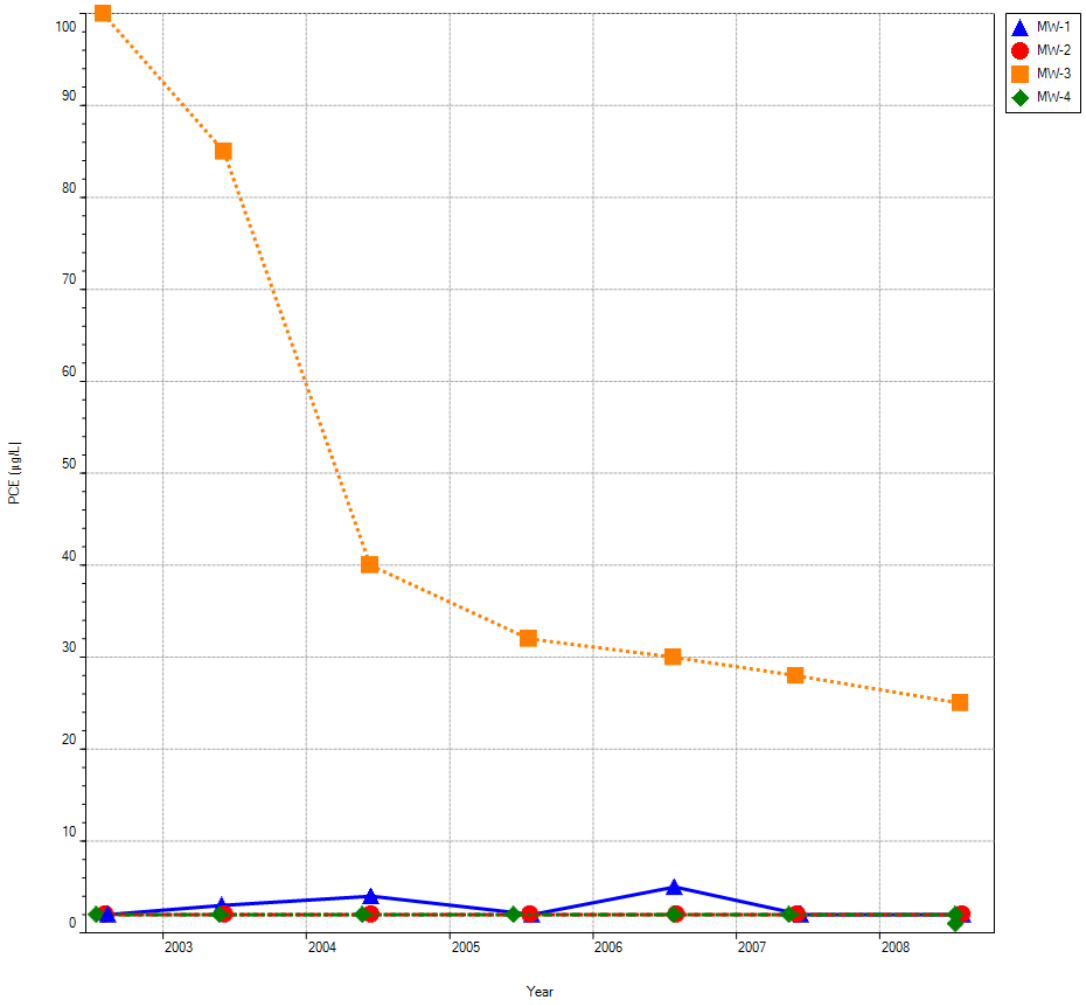
See common plot settings.

Parameters

Ternary plots have three required parameters.

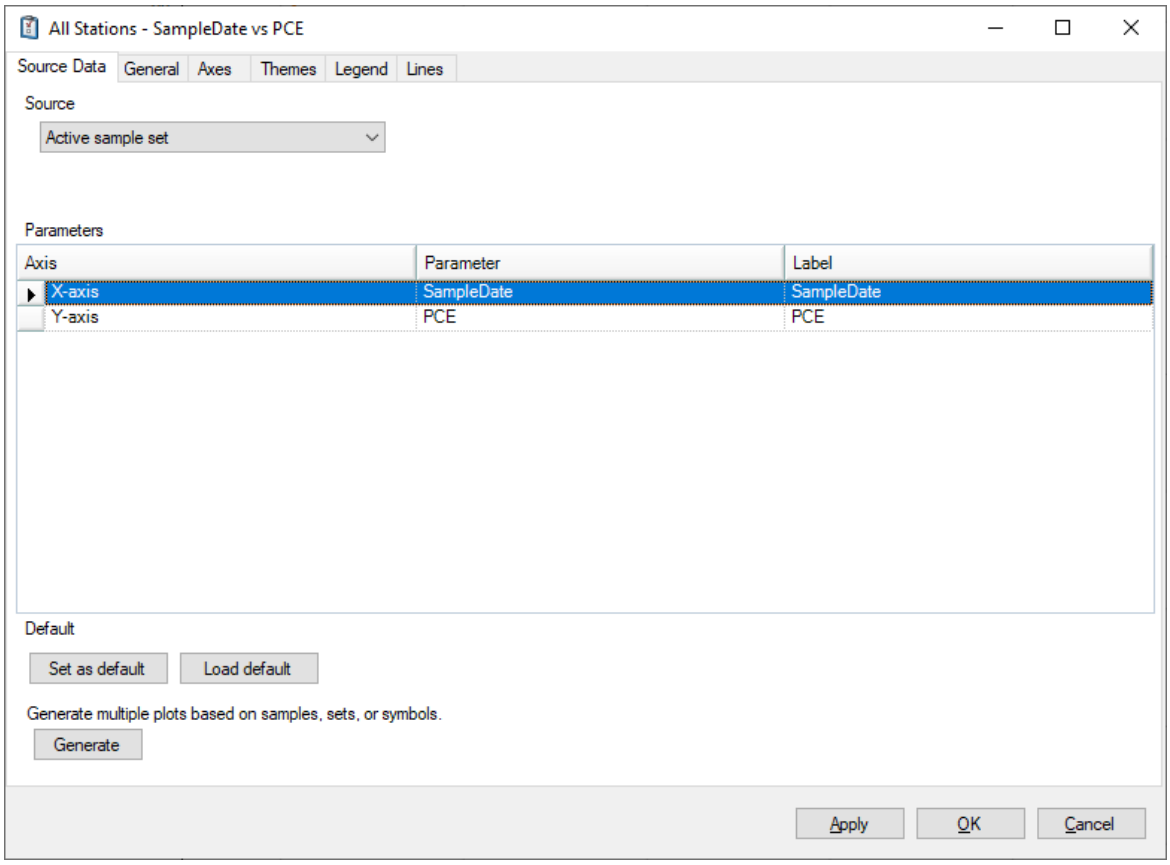
13.3.18 Time Series Plot

The Time Series plot shows the evolution of a chemical or physical parameter for a given sampling point as a function of time. This plot is a standard technique for interpreting hydrochemical and hydrogeological processes and in particular temporal trends in natural waters.



Source Data Tab

Data are specified in a Time Series plot plot as follows:



Source

See common plot settings.

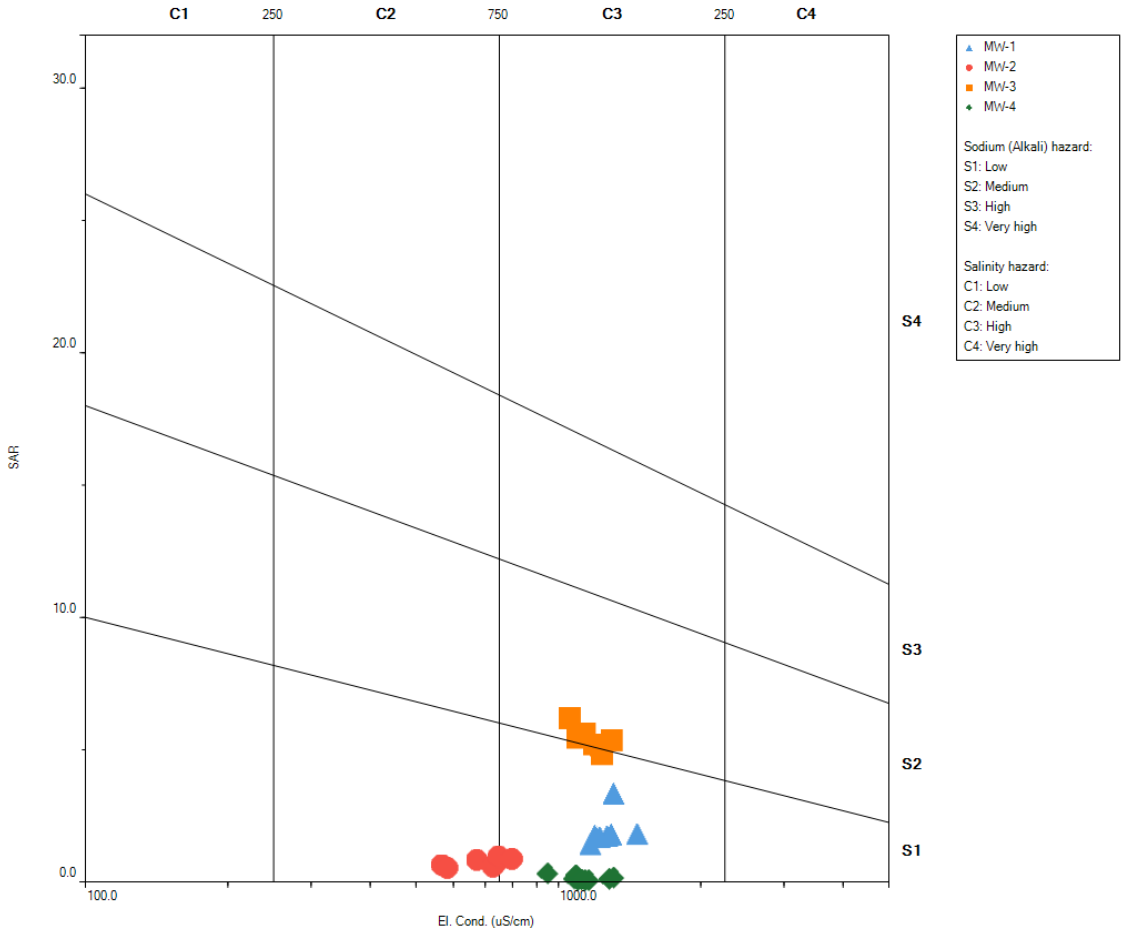
Parameters

Time series plots consist of two input parameters:

- **X-axis parameter:** a time/date data source, typically the sample date from the Sample List table
- **Y-axis parameter**: a numerical input, typically a concentration

13.3.19 Wilcox Plot

A Wilcox plot can be used to quickly determine the viability of water for irrigation purposes (Wilcox, 1955). The Wilcox plot is also known as the U.S. Department of Agriculture diagram (Richards, 1954). An example of the Wilcox plot is shown in the figure below.



The Wilcox plot is a semi-log scatter plot of the "sodium hazard" (sodium adsorption ration [SAR]) on the Y-axis versus the "salinity hazard" (electrical conductivity) on the X-axis. The conductivity is plotted by default in a log scale. The Wilcox plot contains the following zones:

Salinity Hazard Zones: based on electrical conductivity (us/cm)

- C1: Low (0-249)
- C2: Medium (250-749)
- C3: High (750-2249)
- C4: Very High (2250-5000)

Sodium Hazard Zones: based on Sodium Adsorption Ratio lines:

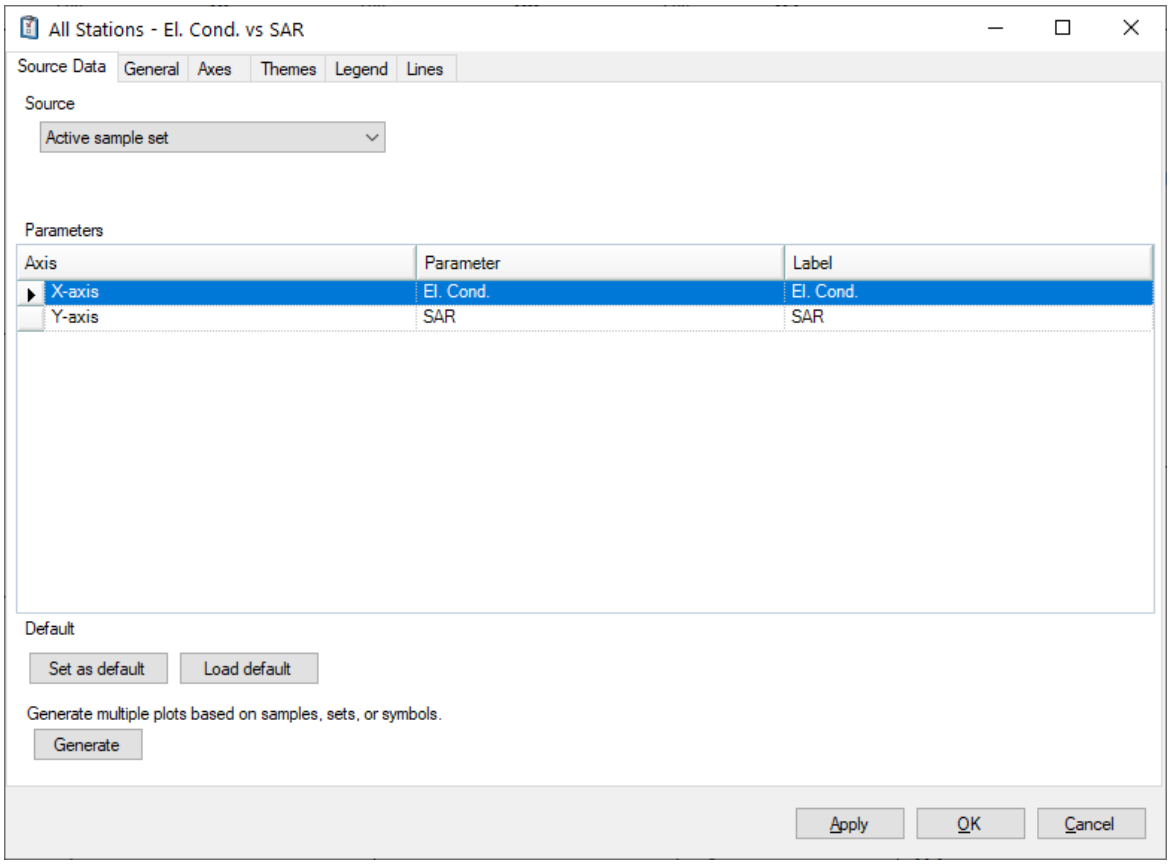
- S1: Low
- S2: Medium
- S3: High
- S4: Very High

The locations of the SAR lines are determined by the following equations:

- S1/2: Line equation: y= -1.5816E-3 x + 10.15816
- S2/3: Line equation: y= -2.2959E-3 x + 18.22959
- S3/4: Line equation: y= -3.0102E-3 x + 26.30102

Source Data Tab

Data are specified in a Wilcox plot as follows:



Parameters

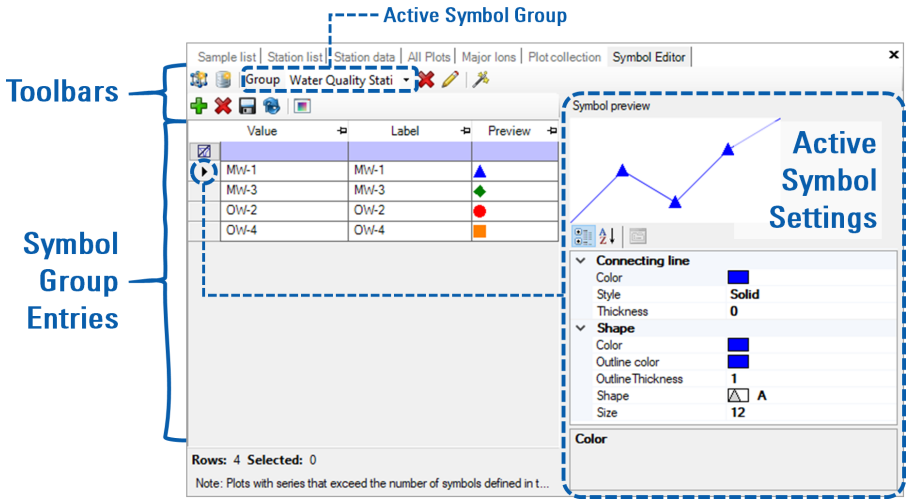
Wilcox plots have a total of two required parameters:

- X-Axis: typically the Electrical Conductivity parameter
- Y-Axis: typically the calculated Sodium Adsorption Ratio (SAR)

Note: the Sodium Hazard lines are added as custom lines and the default values of the slope and intercept of each line may be customized as desired.

13.4 Symbol Editor

The symbol editor allows you to define symbols assigned to Sample List and used in Plots. The symbol editor module is shown below:

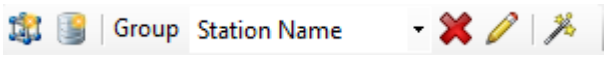


Toolbars

The Symbol Editor includes two toolbars:

Symbol Group Toolbar

The symbol group toolbar provides tools to manage symbol groups in the project:



New Parameter-Based Symbol Group: Creates a new parameter-based symbol group

New Symbol Group: Creates a new symbol group with a defined number of symbols

Group Selection Dropdown: a dropdown selection list of symbol groups in the project

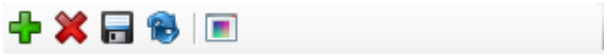
Delete: deletes the current symbol group

Rename: rename the current symbol group

Apply: applies the currently selected symbol group to the project and updates symbols in the sample list and active plot collections

Symbol Toolbar

The symbol toolbar provides tools to work with individual symbols:



Add Symbol: Adds a new symbol to the group

Delete Symbol: deletes the currently selected symbol(s)

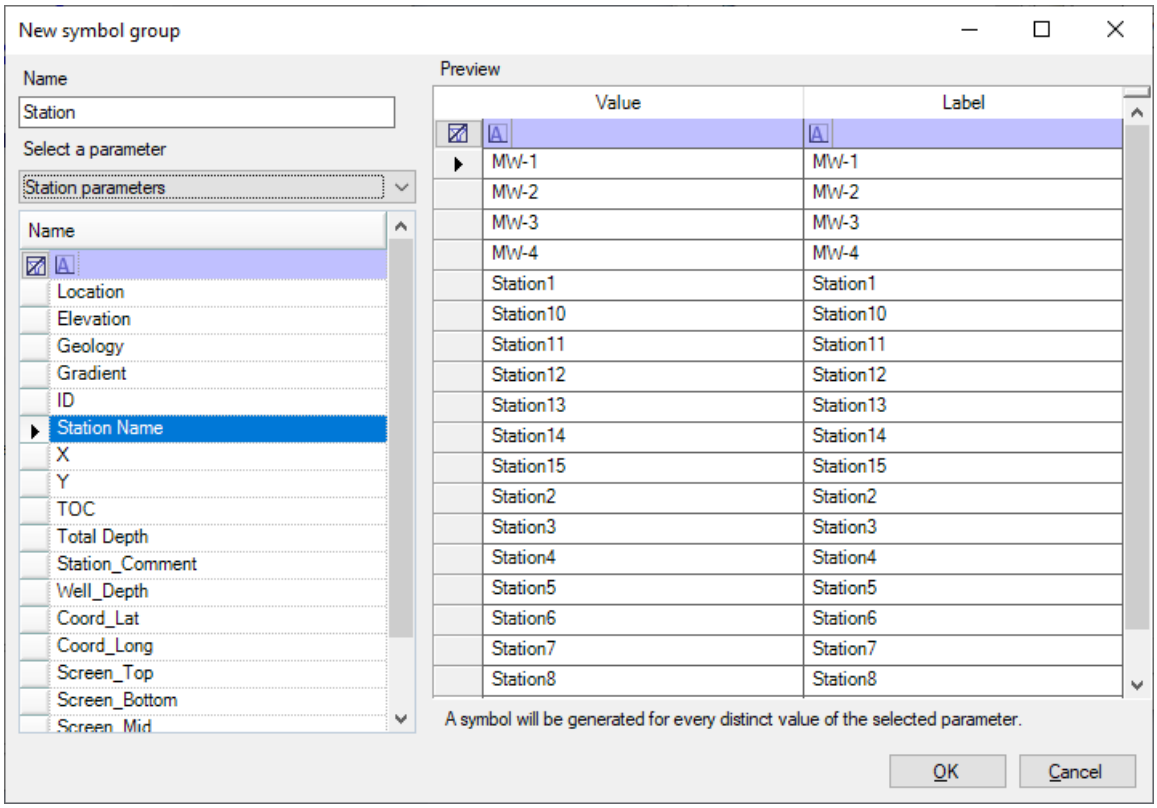
Save Changes: saves changes to the active symbol group

Refresh: reloads the symbols in the active symbol group from the database

Group Colors: loads the group settings window

Creating a New Parameter-Based Symbol Group

When you create a new symbol group, the "New symbol group" window be displayed:



To generate new symbols, simply select a parameter using the parameter picker on the left. You may filter the parameters using the dropdown list. In the example shown above, the Station parameters are shown and symbols will be based on the Station Name. A unique symbol will be generated for each value shown on the preview on the right side of the window.

Editing Individual Symbols

The following settings are available for individual symbols.

Connecting Line

The following settings are available for formatting individual symbols:

- **Color:** the color of the line connecting symbols for the same series
- **Style:** the connecting line style (Solid, Dash, Dot, DashDot, DashDotDot)
- **Thickness:** the thickness of the connecting line

Misc

The following settings are available for formatting individual symbols:

- **Label:** the text to be displayed in the legend

Range

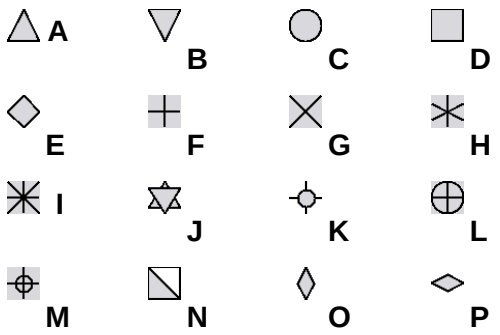
The following settings are available for formatting individual symbols:

- **From:** the value used to define the symbol; the lower bound if the source field is numeric and ranges of values are used
- **To:** the upper bound value used to define the symbol

Shape

The following settings are available for formatting individual symbols:

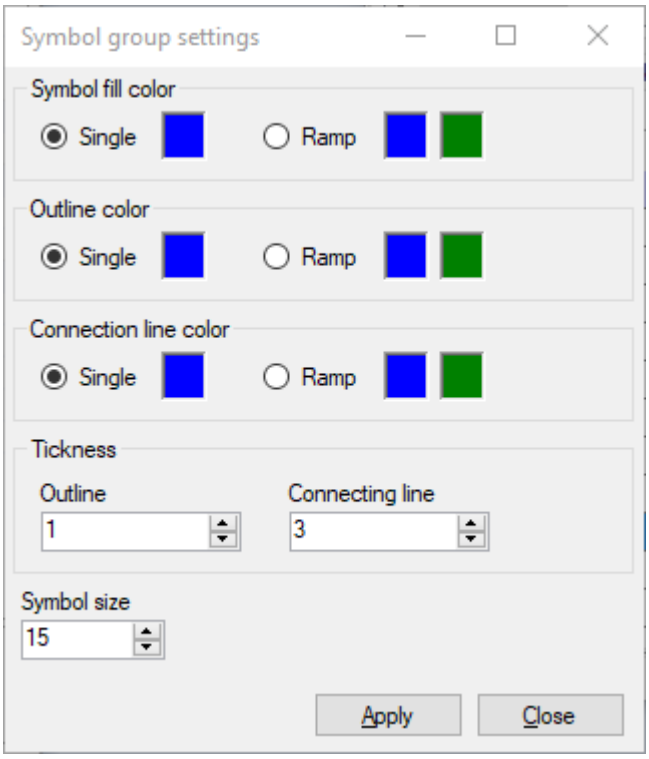
- **Color:** the fill color of the symbol (shown in grey below)
- **Outline color:** the color of the outline of the symbol (shown in black below)
- **Outline thickness:** thickness of the symbol outline
- **Shape:** one of the following 16 symbol shapes:



- **Size:** the size of the symbol

Symbol Group Settings

The symbol group settings controls allow you to edit symbol colors for ***all*** symbols in the active symbol group.



The following settings are available for editing all of the symbols in the current group. For each of the following settings:

- **Symbol fill color:** the fill color of symbols in the group
- **Outline color:** the symbol outline color
- **Connection line color:** the color of the connection line

You can select either a single color or a two-color ramp. Other settings are available for line thickness:

- **Thickness:** symbol outline thickness
- **Connecting Line:** the symbol outline color

and for the **symbol size**.

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Chapter 15 Appendix A: Troubleshooting and FAQ

The following list provides answers to some of the most common problems encountered by users of AquaChem. Please review this list of frequently asked questions before contacting Technical Support for assistance with your project.

Q1: My sample symbols do not show up on the plot.

A1. Check that you have assigned symbols to that sample(s) using the Symbol Editor.

A2. Ensure that you have entered data for each parameter required by that plot.

Q2: My symbols show up on the plot using a different color or symbol other than what I expected.

A1. Check that you have defined a symbol for the sample(s) using the Symbol Editor. The "unexpected" symbol you are seeing may be the default symbol. Samples with undefined symbols may be shown using the default symbol.

A2. Check which samples are selected in the Sample Picker. Selected symbols will be shown based on the Active Symbol style settings. Samples which are selected in the sample picker or sample list will be shown using a light blue color ( ) by default.

Q3: After I enter a value for a measured parameter, the 0 after the decimal place is cut off (for example, 7.20 in entered, however AquaChem displays this as 7.2).

A. This can be corrected by modifying the parameter format. Open the Parameter Editor, select the appropriate measured parameter using the parameter picker, and modify the "Display format" to set the number of decimal places to the desired value.

Q4. The station group I created from a sample set includes samples which do not meet the criteria for that sample set. Why are those extra samples included?

A. Station groups created based on a dynamic sample set contain *all* of the samples from stations associated with that sample set. Therefore, the sample set associated with a station group will typically contain more samples than what you find in the actual sample set itself. This may be useful in evaluating trends at stations meeting some criteria such as exceedances.

Q5. Why do I see a "Modeled" data tab in the Sample Results pane of the Sample List in some samples and not for others?

A. The modeled tab is only present in the Sample Results pane for samples imported from AquaChem 2014 projects that include PHREEQC results. New samples created in or imported into AquaChem version 9 will not include the Modeled tab. Support for PHREEQC

in newer versions of AquaChem is under development and will be available in an upcoming release.

Q6. Why does the calculated data tab display an error when I access it?

A1. Parameters required for the calculation have not been mapped. Select *Project* > *Properties* from the main menu and review the Parameters tab. If a required parameter has not been mapped then AquaChem doesn't know what values to use in the calculation.

A2. No result is available for one or more of the input parameters required for the calculation. If you do not collect the data required for a particular calculation, you can simply hide that calculated value from the *Calculated* data tab by clicking the *Properties*  button in the toolbar and hiding the calculation(s) that you don't need.

Q7. Is it possible to create two unique Piper plots showing two different sample groups?

A. Yes! In AquaChem you can define multiple Piper plots (or any other plot type) in one or more plot collections and define the source data for each plot based on one or more different data sources (e.g. Station Groups or Sample Sets).

Q8. My samples do not appear in the sample list.

A. Make sure that you activate a sample set that contains the missing data. If you just imported sample data, you may have to refresh your view(s) by clicking the refresh [] button. If you have activated a static or dynamic sample set that does not capture newly imported samples then they will not be displayed in the Sample List. To display all samples double-click the 'All Stations' sample group in the Project Tree. This will display all samples from the entire project within the Sample List.

Q9. I cannot install packages in R-Console.

A. If you cannot install packages in R using the *install.packages()* command; please follow the Installing R instructions. Conversely, you can try installing R in a local folder that does not require administrative privileges and pointing AquaChem to this installation location using the R-Console settings.

Q10. My R script is not showing anything in the Output window.

A. The R-Console output window has been streamlined to only output results using the *print()* command to improve script runtimes and reduce output clutter.

Q11. My R script works in RStudio or RGui but not in AquaChem.

A. Be sure to add a "+" at the beginning of each continued line. R-Console in AquaChem interprets R on a line-by-line basis and unlike RStudio and RGui, you must explicitly continue multi-line commands. Please refer to the differences between standard R and the version of R used in the R-Console in AquaChem.

Q12. Can I run AquaChem 10.0 and AquaChem 2014 on the same computer?

Yes. Both versions of AquaChem will run on the same computer provided the system requirements are met for each.

Index

- A -

- C -

- D -

- E -

- F -

- H -

- I -

- L -

- M -

- N -

- P -

- R -

- S -

- T -

- V -

- W -