AquaChem

Geo-chemical Analysis Software

Featuring a fully customizable database of physical and chemical parameters and a comprehensive selection of analysis, calculation, modeling, and graphing tools, AquaChem is a truly unique groundwater software package.

AquaChem’s analysis tools cover a wide range of functions and calculations used for analyzing, interpreting and comparing water quality data. These tools include simple unit transformations, charge balances, statistics and sample mixing to more complex functions such as correlation matrices and geothermometer calculations.

These powerful analytical capabilities are complemented by a comprehensive selection of commonly used plotting techniques to represent the chemical characteristics of aqueous geochemical and water quality data.

**AquaChem Product Details Summary**

| Data Management | Built around a customizable MS Access database that can be configured to include more than 1000 alphanumerics per sample. Parameters are divided into the following parameter groups: station description parameters, sample description parameters, measured parameters, and modeled parameters. Each parameter group contains pre-defined parameters which can be used to create a customized data structure for your sampling and reporting requirements. Data may be imported and exported in various formats including MS Access, MS Excel and .TXT files. |
| Data Analysis | AquaChem uses the common measured values (cations and anions) for each sample to calculate additional geochemical values including water type, sum of Anions, sum of Cations, Ion Balance, TDS, hardness, Alkalinity, Common Ion Ratios, Sodium Adsorption Ratio, Magnesium Hazard, Oxygen saturation and Scaling Indexes such as Langlelier Index, Ryznar Stability Index, Puckorius Scaling Index and Larson-Skoid Index. Data Analysis features include: Compare Samples, Correlation Matrix, Water Quality samples, Mix Samples, Data Reliability check, Rock Source Deduction. |
### Statistical Calculations
AquaChem includes a comprehensive list of statistical features, optimized to work with your water quality data set. Statistical features included with this software are: Trend analysis (Mann Kendall, Sen's Test), Outlier Tests (Extreme value, Discordance, Rosner, Walsh test), Test For Normality (Studentized range test, Geary's, Shapiro, D'Agostino test).

### Water Quality Modeling
AquaChem provides a link to one of the popular public domain geochemical modeling programs, PHREEQC available from the USGS.

PHREEQC generated values (saturation indicies, activities) can be read back to the database and used for reporting, plotting or statistics.

### Plotting, Mapping & Reporting
One of AquaChem's most powerful features is its ability to efficiently manage, create, and graphically display a wide range of water quality data.

Includes a comprehensive selection of more than 23 industry-standard plots including: Piper, Schoeller, Scatter, Box & Wisker, time series, histogram, Stiff, Radial and Pie chart.

AquaChem offers a unique way to interact with graphics and allows for quick identification of points on plots.

AquaChem water quality analysis & reporting applications include:

- Reporting water quality data from groundwater sampling programs
- Analyzing water data to determine potential drinking water issues
- Managing & reporting analytical lab data obtained from supply wells, rivers, reservoirs, etc.
- Managing water quality data from sanitary landfills, contaminated sites, etc.
- Mapping & reporting guideline exceedances in water quality data
- Aqueous geochemical analysis of potable water supplies
- Identifying mineralization trends in water for mining exploration
- Calculating water hardness and scaling tendency for use in water Treatment
- Calculating mixed water compositions in an ASR project
- Assessment of suitability of a water for irrigation
- Modeling gas mole transfers to account for differences in water composition

![Highlighting data points and identifying records](image-url)
### Detailed Description of AquaChem Plots

<table>
<thead>
<tr>
<th>Plot Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>X-Y Scatter Plots</strong></td>
<td>A simple approach to the interpretation of geochemical data. Single plots of ion relationship and parameters that show significant data can be easily created and patterns are quickly identified and easily understood. Both normal scale and log scales are supported for the x and y axes and multiplication factors can be applied to either the x or y parameter. Parameter ratios and sums may also be included for either axis.</td>
</tr>
<tr>
<td><strong>Ludwig-Langelier Plots</strong></td>
<td>Similar to the projection areas of Piper and Durov diagrams. Suitable groupings of cations and anions are selected and plotted as percentages of milli-equivalents. All major elements can be displayed in one plot with the Ludwig-Langelier diagram. However, like the Piper and Durov diagrams, it displays relative ratios rather than absolute concentrations.</td>
</tr>
<tr>
<td><strong>Wilcox Diagram</strong></td>
<td>Can be used to quickly determine the viability of water for irrigation purposes based on conductivity and SAR values. The Wilcox plot is also known as the U.S. Department of Agriculture diagram. The Wilcox plot is a simple scatter plot of Sodium Hazard (SAR) on the Y-axis vs. Salinity Hazard (Cond) on the X-axis. The Conductivity (COND) is plotted by default in a log scale.</td>
</tr>
<tr>
<td><strong>Geothermometer Plots</strong></td>
<td>Geothermometer plots can be used to test the quality of geothermometer estimates for a given geological and hydrogeological condition.</td>
</tr>
<tr>
<td><strong>Meteoric Water Line</strong></td>
<td>The standard way to portray measurements of stable isotopes from water. Consists of a scatter diagram showing 18O on the x-axis and 2H on the y-axis. The meteoric water line is where most precipitations and groundwater fall. In cases where the measurements are shifted from this line, the type of shifting provides important information regarding to the process leading to the observed shift.</td>
</tr>
<tr>
<td><strong>Box and Whisker Plot - Time-Series</strong></td>
<td>Displays a statistical summary of any measured database parameter(s). It is composed by a central box showing the spread of the bulk of the data (interquantile range) and the whiskers, showing the length of the tails.</td>
</tr>
<tr>
<td><strong>Box and Whisker Plot - Multiple Parameters</strong></td>
<td>Displays a statistical summary of multiple measured database parameters, at a selected station location. The plot displays the following statistical analyses: Minimum measured value Q1: the first quartile (25th percentile), 25% of the data lie below this value Q2: the second quartile (Median), 50% of the data lie below this value; Q3: the third quartile (75th percentile), 25% of the data lie above this value Maximum measured value</td>
</tr>
</tbody>
</table>
| **Box and Whisker Plot - Multiple Stations** | Displays a statistical summary of any measured database parameter, at multiple station locations.  

The plot displays the following statistical analyses:  

- Minimum measured value  
- Q1: the first quartile (25th percentile), 25% of the data lie below this value  
- Q2: the second quartile (Median): 50% of the data lie below this value  
- Q3: the third quartile (75th percentile), 25% of the data lie above this value  
- Maximum measured value |
| **Frequency Histogram** | Most commonly used to check the number of populations within a given range of measured values.  

View a large number of samples without the diagram becoming too cluttered with data points.  

The Frequency Histogram can be used to plot all samples in the open database or selected sample groups. The range of values can be customized up to 10 or more groups and the individual samples can be identified at the associated value along the x-axis. |
| **Quantile Plot** | Identify the ranked data from lowest to highest on the background of lines that denote Q25, Median, and Q75. Quantile are used to determine if two data sets come from populations with a common distribution. |
| **Detection Summary** | Used to visualize the relative proportions of samples above the specified water quality parameters. The plot shows a summary bar for every specified parameter. |
| **Piper Diagrams** | Plots the major ions as percentages of milli-equivalents in two base triangles.  

This plot reveals useful properties and relationships for large sample groups. The main purpose of the Piper diagram is to show clustering of data points to indicate samples that have similar compositions.  

The Piper diagram can be used to plot all samples in the open database or selected sample groups. |
| **Durov Diagrams** | An alternative to the Piper diagram which plots the major ions as percentages of multi-equivalents in two base triangles. This plot reveals useful properties and relationships for large sample groups. The main purpose of the Durov diagram is to show clustering of data points to indicate samples that have similar compositions.  

The Durov diagram can be used to plot all samples in the open database or selected sample groups. Other options include individual multiplication factors for each selected ion to prevent data point accumulation along a base line. |
| Ternary Diagrams  | Used to identify trends and relationships between groups of samples. It is generally easier to understand than Piper or Durov diagrams since it involves fewer parameters and does not project data points onto a grid.  

The Ternary diagram plots the ions as percentages of their concentration value and is not limited to using only meq units.  

The Ternary diagram can be used to plot all samples in the open database or selected sample groups. Other options include individual multiplication factors for each selected ion to prevent data point accumulation along a base line. |
|------------------|------------------------------------------------|
| Schoeller Plots  | Semi-logarithmic diagrams developed to represent major ion analyses in meq/l and to demonstrate different hydrochemical water types on the same diagram.  

This graph has the advantage of displaying and comparing actual sample concentrations.  

The Schoeller diagram can be used to plot all samples in the open database or selected sample groups only. |
| Giggenbach Triangle | This diagram is commonly used for geothermal exploration and allows estimation of the degree of equilibrium achieved with the host rock as well as the original subsurface temperature. |
| Time Series Plots - Multiple Stations | Displays the evolution of a physical or chemical parameter for multiple sampling locations, as a function of time.  

Plot is a standard technique for interpreting hydrochemical and hydrogeological processes in natural waters. Regulatory standards can be plotted as horizontal lines to visualize exceedances.  

Used to plot all samples in the open database or selected sample groups. |
| Time Series Plot - Multiple Parameters | Displays the evolution of multiple chemical or physical parameters for a given sampling point as a function of time.  

Standard technique for interpreting hydrochemical and hydrogeological processes in natural waters. |
| Time Series Plot - Bar Chart | Used to display a statistical summary over a specified time period as a bar chart.  

Options for the time period over which the data is to be aggregated include month or year.  

Summary values can be displayed as Minimum, Maximum, any Quantil, and Standard Deviation. |
| Radial Diagrams  | Plotted for individual samples as a method of graphically comparing the concentrations of measured parameters for several individual samples.  

Shape formed by the Radial diagram identifies samples that have similar compositions and are particularly useful when used as map symbols to show the geographic location of different water facies. |
Stiff Diagrams
Plotted for individual samples as a method of graphically comparing the concentration of selected anions and cations for several individual samples.

Shapes formed by the Stiff diagram identify samples that have similar compositions and are particularly useful when used as map symbols to show the geographic location of different water facies.

Pie Charts
Used to plot the concentrations ratio of the major ions (or any combination of parameters) for individual samples.

Used to graphically compare the concentration ratios of several measured parameters for several different samples.

Depth Profile Plot
Similar to a borehole log done in the field; the plot displays the change of a measured parameter over a measured sampling depth.

Can be used to plot all samples in the open database or selected sample groups.

Plotting over Georeferenced Raster Images
Sample locations can be displayed on an X-Y graph and detailed site maps can be imported from a variety of RASTER images such as JPG, BMP, TIF, etc. Overlaying your water quality plots over a georeferenced image will provide a familiar point of reference when you are analyzing sample data. In addition, the map plot can be used to display the location of different water types, or the symbols can be scaled in color or in size according to the concentration of a selected measured element.

Plotting over Vector Files
Sample locations can be displayed on an X-Y graph and a detailed site map can be imported from AutoCAD DXF or ESRI shape files to provide a familiar point of reference when you are analyzing sample data. In addition, the map plot can be used to display the location of different water types, or the symbols can be scaled in color or in size according to the concentration of a selected measured element.

PRINTING
AquaChem prints all reports and graphical displays to any printer or plotter supported by Windows 98/NT/2000/XP. The printing utility allows you to size and arrange the location of an unlimited number of open graphical displays on the page. The graphs can be arranged and printed on a blank page, or you can select from a set of built-in page layout templates that allow you to enter details about the project, the page title, and a description of the figures. Alternatively, AquaChem allows you to customize the page layouts or create your own template (including importing a bitmap of your company logo).
AquaChem is accompanied by a comprehensive user's manual containing easy-to-follow instructions and a step-by-step tutorial. Technical support is provided via phone, fax or e-mail.

**SYSTEM REQUIREMENTS**

Supported on Windows 2000 SP4, Windows XP Pro SP2, Windows Vista (Business, Ultimate & Enterprise), and Windows XP 64-bit
RAM - 512MB
Hard drive space: 50MB
A minimum screen resolution of 1024 X 768
A Microsoft compatible mouse