

AquaChem 9.0 Re-Design Build 17.20.220.6 (February 2020)

Data Management:

- 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 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 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. Exceedances are automatically color-coded for quick reference.

Interactive Plots:

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

Functions and Analyses:

- 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

Recent History of Changes

Fixed in 17.299.206 (November 2017)

- When language settings use a comma separator instead of a decimal some plot legends appeared disproportionately large

- Error when using Excel Time Series report option after having connected to an HGA project
- Incorrect values being used for Trend Analysis after having connected to an HGA project
- Difficulties adjusting the axis labels for a Langelier Ludwig plot
- Trend Analysis R2 value not calculated correctly
- Outlier Test raw data tab allowed user to edit raw data before running test
- Unable to Assign Symbols to the first record in list
- After having connected to an HGA project the Exceedance report shows only the first sample
- Unable to export data for Stacked Bar plots
- Incorrect min and max values displayed in Lines dialog when calculating Linear Regression

Fixed in 14.297.1147 (December 2014)

- Updated to work with Hydro GeoAnalyst 2014.2
- Resolved problem where incorrect symbols were used on Durov and Piper plots (symbols did not correspond to correct sample)
- Fixed problem when opening older project from version 2011 or 2012
- Resolved issue with incorrect placement of Pie Charts on a Map Plot
- Fixed problem when using 1 Plot per Symbol option for Piper Plot

Fixed in 14.185.844 (July 2014)

- Updated to work with Hydro GeoAnalyst 2014.1
- Resolved problem where incorrect values were displayed on the Scatter plot if units are meq/L
- Fixed problem where many error messages would appear if using the View/Table View/Default option with more than 181 samples
- Fixed problem where many error messages would appear if using the View/Table View/Default if the parameters were not measured
- SEL and ACT columns should no longer appear in the Stations tab
- Resolved difficulties printing the Sample Summary Report
- Resolved problems with the way Stiff diagrams appear on a Map Plot
- Fixed several issues when running on Windows 8.1 operating system (ensure you are running program in compatibility mode).
- No longer need to close and reopen the project to get New Water Quality standard exceedances to become highlighted
- Fixed Summary Statistics Report errors
- Resolved problem where Correlation matrix would display incorrect values if the "Use only Selected Samples" option is selected

Added in 14.13.347 (December 2013)

- Generate Time Series by pushing data to Excel templates
- Updated WHO water quality standard

Fixed in 14.13.339 (December 2013)

- Difficulties saving changes to calculations

- Exceedences where not being highlighted correctly after modifying preferences
- Unable to add a sample when comparing duplicates
- Error when running a query on metadata
- AquaChem has stopped working message on some computers only when opening or closing projects or using Save As
- Unable to perform Trend Analysis on some specific projects
- Percent Non-Detects not calculated correctly in Data Summary Report
- Difficulties assigning proper units to parameters in projects created with customized template
- Difficulties saving a selection of stations
- Error when changing maximum date on time series plot
- Saving and reloading a plot configuration results in different data being shown in client specific project
- Unable to add a standard to the sample details window
- Unable to plot symbols in Piper plot due to corrupt project file
- Changes to units were not saved in the Parameter Details
- Google Earth option in Station Details unresponsive
- Using a station specific filter on the samples tab caused an error
- Difficulties updating symbols after the Station ID has been edited
- Y2 axis disappears from time series plot when saving the configuration
- Auto scale function not working correctly on Y2 axis
- Difficulties importing time series data
- Outlier Test not providing results
- Unable to run a Find Query using IS NULL or IS NOT NULL
- Columns in Plot Legend do not align correctly
- Difficulties entering formula weights when importing new parameters
- Summary Statistics showing incorrect number of samples
- Some tests in the Reliability Check were not being calculated
- Error encountered when added a QC Flag
- Y axis of time series plot is not updated after changing the unit it is displayed in
- 1 Plot per Symbol option for the Piper Plot is not saved in the Plot Configuration
- Difficulties opening older projects
- Calculated Parameters not appearing after opening older project
- Trend Analysis not providing an extrapolation or predicted value
- Unable to manually assign a symbol to a sample
- Some symbol settings were not being saved correctly
- Symbols in plots are different than in the Define Symbol settings
- Difficulties adding a new parameter
- Unable to change the frequency of labelled ticks in time series plot
- Difficulties encountered if Admin user installs and Restricted user runs program
- Open Database dialog appears twice

Added in v.2012.1.123 (June 2012)

- AquaChem can now run entirely on a Hydro GeoAnalyst SQL server database. From within Hydro GeoAnalyst you have the option to add the GeoChemistry Extension by selecting the AquaChem icon. This will include all necessary tables and information that previously was stored in the AquaChem project (.aqc) into the Hydro GeoAnalyst database. This is an even tighter integration of the two products than what was previously achieved through an ODBC link. Of course, you can continue to run

AquaChem projects based on an .aqc file (MS Access database) as in previous versions if you prefer.

Fixed in v.2012.1.123 (June 2012)

- Summary Statistics Report data did not line up with the report headers
- Conflict with the licensing component also used within Visual MODFLOW causing AquaChem to no longer launch successfully
- QA/QC Compare Duplicates option was not finding any duplicates
- Unable to display standards on a time-series plot
- Once you have created and saved 100 queries any subsequent queries you created, saved and tried to run from the Filter drop down list did not work
- Measured values not displaying in the Table View (Spreadsheet)
- Trend Analysis not showing all test results.
- Plots not showing in Print Preview
- Unable to save ranges for calculated values
- Inconsistencies in the calculation of LSI
- Incorrect display of data in Piper plot (in the projection)
- Difficulties with vertical lines for Salinity classification in Wilcox Plot when adjusting x-axis
- Time Series Plot do not display symbols properly
- Box and Whisker plot displays all samples instead of selected samples
- Error when saving a QA/QC result with an invalid filename
- Trend Analysis showing incorrect values for the estimated results
- Cations and Anions are reversed in the Stiff diagram
- Warning message and file name not saved when creating a New project
- Unable to Cancel creating a New Project
- Unable to add a new chemical to the Chemical Master Table
- Unable to save a new report template in the Report Designer
- Implemented an Auto-Notification of New Updates that are available
- Preferences dialog prompting to save even when no changes have been made
- Not all Parameters are being shown in the Summary Statistics
- Format changes to a report template not retained after closing AquaChem
- Active toolbars icons not consistent with menu options
- Error when selecting a solution in PHREEQC (Basic) dialog
- Error messages when converting old projects
- Unable to save project location as Southern Hemisphere (always reverts to Northern)
- Filter toolbar icons appear inactive when they are active
- Error messages if you try and plot inappropriate records in the Trend Analysis results

Fixed in v.7.0.61 (January 2012)

- Sum of Ions was not being calculated
- Durov Plot default settings placed anions and cations in the same ternary diagram
- Piper Plot default settings placed anions and cations on incorrect ternary diagram
- Aladdin dongles were not recognized by the software
- When opening some older projects, new plot options were not available
- Unable to calculate certain Saturation Indices
- Min and Max values for some parameters were displayed incorrectly in the Database Summary

- Calculated TDS being displayed in Box and Whisker Plots are several orders of magnitude higher than in the database
- Runtime Error when accessing the options for Schoeller plot through View/Options menu
- Box and Whisker plot will not display data when only one station is being viewed
- Unable to plot calculated parameters on a time series plot
- Aggregated options for Mann-Kendall test were not being applied to data set
- Unable to delete parameters from a Box and Whisker plot (red X always greyed out)
- Box and Whisker (multiple stations) plots showed incorrect (mixed up) values for some parameters
- Runtime error when selecting options for a Normality Test (due to no default Normality test being available)
- Number of exceedences and percent of exceedences were not being calculated on Table Views
- Difficulties importing Water Quality Standards after having deleted a standard
- Resolved run time error in Trend Analysis
- Resolved issue where incorrect data was being displayed on the Box and Whisker (Grouped by Station) plot
- Fixed aggregate options for the Mann-Kendal Trend Analysis

Added in v.7.0.39 (May 2011)

- we now provide a basic demo project as well as an advanced demo project, additionally we now provide basic and advanced database templates
- support for MS Office 2007 Excel and Access file formats (*.xlsx and *.accdb) for importing and exporting
- the options File/Preferences and File/Database have been consolidated into File/Preferences
- database summary now includes first sample date and last sample date
- option to use numbers as symbols
- additional align options within the Template Designer (for reports)
- option to allow re-ordering of plots so they can be reported in the correct order (this feature is available within the List of Plots options)
- option to include Lab pH in PHREEQC Basic if no field pH available instead of the default of 7
- parameter groupings are now available in the parameter list to aid user to find particular parameter quicker
- option to query for detects or non-detects for a particular parameter
- option to import page templates and plot layouts from other projects
- option to add a vertical line to plots (useful on Histograms to show a standard)
- option to make a lowest standard by combining multiple standards
- allow user to set a standard for a calculated parameter
- option to create a kml file on only one single station (on Station Details tab)
- new decay correction utility for radioactive analysis
- option to save calculated values into the database
- option to create Piper and Durov plots per station (instead of all stations on one plot)
- option to adjust stacked bar thickness
- option to associate duplicates in batch mode (Tools/Manage Duplicates)
- option to use significant digits or decimals in Table View
- option to plot calculated data in box and whisker plots

Fixed in v.7.0.39 (May 2011)

- often a blank page at the end of reports spanning multiple pages
- in Report Designer, if you have selected the option to order by stations and then select the refresh button the report becomes blank
- error message if you export to kml and there is null data
- difficulties running PHREEQC on Windows Vista and Windows 7 operating systems
- list of plots option for turning legend on/off was not working
- table view option for showing MDL was not working
- option to show Non-Detects symbol in Legend was not saved in scene configuration
- Normality test was not running
- Non-Detects do not show up properly on Time Series (Multiple Stations) plots
- run time error if you use the up and down arrows to rearrange order of plots in the Report Template Designer (this feature has been added to the List of Plots dialog options)
- Advance PHREEQC option will not launch PHREEQCi
- program freezes while comparing duplicates
- PHREEQC does not run on 64bit machines
- calculated values (number of samples, number of non-detects) when grouped by symbol were not being calculated correctly
- unnecessary warning message when selecting edit/replace option
- min and max values in datasets with all non-detects were showing MDL/2 instead of the actual MDL in the Statistics Summary and in the Table View
- while importing time series data if you map the date to a non-date field in your source file you will receive an error and program closes
- long plot names are cut off in the print preview (you can now resize the list of plot names)
- received a run-timer error and program closed if you entered text into the legend field for Time Series (Statistics Summary) plot

Added in v.6.0.83 (March 2010)

Data Management

- The query utility has been enhanced to find exceedances in just one step, by selecting the desired parameter and standard
- The query utility now includes a SQL Editor which allows you to query the AquaChem database using SQL statements
- The import utility has been enhanced to allow the import of USGS water quality data in National Water Information System (NWIS) format
- Geographic station coordinates can now be converted to UTM coordinates, and vice versa
- The table view settings now have additional options. For example, non detects or non measured parameters may be substituted by a code, e.g., ND, N/A. Also an additional row in the header may display all method detection limits
- The meta data for each parameter now includes a user defined code. This may be useful if your organization has its own parameter codes or numbering system, and you want to include this information in the AquaChem database

- The number of total samples, and the number and percentage of selected samples are now displayed in the sample list header after manual interaction or query based selection

Data Analysis

- Parameters can now be compared with hardness dependent standards according to EPA Freshwater Standards
- Parameter results can be compared to percentages of water quality standards, e.g., 50% EPA standards
- A new tool called „Aggregate Samples” allows you to create a new sample based on a number of selected samples, which are aggregated using various algorithms such as, minimum, maximum, quantile, geometric mean etc

Statistical Calculations

- Various statistical tests, including trend, outlier and tests for normality, have been updated and can run in batch mode for a selection of stations and parameters
- The database parameter settings now include parameter statistics; Minimum (Min), Maximum (Max), Average (Avg) and Count
- Statistics now include the geometric mean.
- Statistics now include the Probability(x). For example, you may calculate the probability that the water standard (or any other concentration of interested) exceeds in additional samples you will take in the future
- Statistics now include the Percentile Exceedance flag. The flag returns a true or false value for your data population, depending whether a defined percentile exceeds a specified value. Regulatory requirements often request that a defined proportion of the data remains below the water standard. This can be verified easily using this function

Plotting, Mapping & Reporting

- Added the ability to export station data in *.KML file format for use in geobrowser software, e.g., Google Earth
- Improved the Durov plot to show two additional parameters, e.g., pH, EC, TDS, on the same plot
- Added the ability to create several time series plot for multiple stations in a single step
- Added the ability to create Box and Whisker plots for multiple stations in a single step
- Added Stacked Bar chart option, which allows anions/cations to be plotted side by side to provide an estimate of ion balance
- Included a new Box plot variation called „Group Box and Whisker” plot. This plot can be used to compare station box and whisker plot belonging to different domains, e.g., different watersheds or upgradient versions down-gradient, etc. The domains and their color code are included in the plot legend
- Added a „List of Plots” utility which allows you to change several plots simultaneously. For example, you may generate time series plots for a several stations, then use the list of plots utility to adjust the axis extents, change fonts and symbols, etc.
- Added „Geometric Markers” as an alternative to „True Type Fonts”
- Added the ability to plot a secondary Y-Axis on time series plots and to assign any given parameter to either axis
- The data summary utility now allows you to document the entire database or a portion of the database. A report will be generated based on the active samples providing the

number of stations, number samples per station, number and basic statistics of measurements for each chemical parameter a matrix showing on how many measurements there are for each parameter and station combination

- The symbols in a plot legend can now be arranged to appear in multiple columns
- Added the ability to import and show non chemical data as time series within a time series plot. This allows you to compare chemistry data with other data such as water levels, precipitation, etc.,

Fixed in v.5.1.170 (June 2008)

- AquaChem now gives you an option to use an alternative water type calculation that categorizes water samples into 4 redox categories: A (Strongly Oxidized), B (Weakly Oxidized), C (Weakly Reduced) and D (Strongly Reduced).
- A problem was solved for users that want to include Total Inorganic Carbon (TIC) in PHREEQC simulations. The problem occurred for samples where both TIC and alkalinity was specified.
- Non-detect signs cannot be imported if they are in a separate column in the source file
- Box and whisker plot configurations with several stations cannot be saved
- For Stiff Map plots, maximum concentration settings do not save in the plot options
- For Multiple Parameter time series plots, plot titles are not updated when a new station is selected in the plot options

Fixed in v.5.1.168 (April 2008)

- Improved performance when linking larger HGA WQ databases
- No longer receive an error message and software shut down when selecting the calculator icon in the Unit Calculator options
- When opening a project that was created in v.4.0, unable to close and reopen the project
- Assigning symbols to samples does not work properly when AquaChem is linked to HGA. All symbols are reverted to 1 (default) when closing and reopening AquaChem
- If identical symbol names are used in different symbol groups, Box and Whisker plots will appear blank
- Some non-mandatory parameters cannot be deleted
- The +/- sign in some geothermometer formulas cannot be changed
- The formula weight of formulas containing H₂O, e.g. CaSO₄·(H₂O)₂, is calculated incorrectly
- When creating a ternary plot and changing the parameters and labels, if the plot is saved as default, the parameter values are not saved
- When executing a query, only data up to row 500 is selected
- Plot legends do not update automatically after changing symbol groups
- Performance has been improved for larger databases
- Non-detect values do not work correctly under all language settings where the comma is set as the decimal separator
- The subtraction function does not work, e.g., T_{Field} - T_{Lab}
- Statistics summary option window disappears when clicking on a different window

Added in v.5.1.151 (January 2008)

- Support for Windows Vista (Business, Ultimate & Enterprise)
- Support for Windows XP 64-bit computers

- AquaChem can now be linked to a Hydro GeoAnalyst, database. It still uses the MS Access database format, but replaces the core tables (station, sample and analysis) with tables linked in the HGA/HGB/HGL database. Choose from two linking modes:
 - Express: For databases using the SWS Environmental template (v4.0, metric or imperial) database tables and parameters are automatically linked, with minimal user intervention
 - Customized: For databases with a customized data structure, tables and parameters are manually linked
- Enhanced water quality standards & guidelines structure:
 - Intervals can be defined for standard values, e.g., pH 6.5 - 8.8
 - Values can be checked against a mix of active levels, e.g., ODWS and PQWO, or USEPA and WHO
 - Parameters that do not exist as a database parameter can now be defined as a standard
- Generate PHT3D input interface has been completely revised:
 - Easily retrieve thermodynamic database settings from vmod.xml file (VMOD installation required) and element concentration settings from your existing VMOD project file
 - Preview generated input data for solutions, mineral composition and exchanger composition before exporting to importable text files
 - Create input files for initial concentration import or time-dependent recharge concentration import
- Sample filter list now includes the following custom filters: all ions, cations, anions and elements listed in standards list
- Non-detect values can now be shown as N.D or any other user specified code in the spreadsheet view
- Non-analysed values can now be shown as NA or any other user specified code, instead of an empty cell, in the spreadsheet view
- You can now change the name of the columns in the station and sample list. In the previous version, the column titles were identical to the field names in the database tables
- File \ Database \ Parameters menu item now includes a new update button for measured parameters. Parameters can be completed with information stored in the chemicals master table, if a matching formula or CAS number is found.
- Summary statistics now allow displaying standards for every parameter, if available
- Imported guidelines can now be viewed in the lookup table section (Tools\Lookup Tables\Water Standards)
- For statistical tests, the result grid can be copied to the clipboard by right-clicking and selecting Copy from the pop-up menu
- When manually selecting stations, samples or executing queries, the "Count Selected" menu item returns the number and percentage of selected records
- When working with sample or station record list that has been queried, pressing Ctrl+S selects the first highlighted record in the list. Every additional CTRL+S key stroke will advance to the next highlighted record

- When exporting data to image or excel files, AquaChem prompts you to open the file in its associated program (e.g. Excel). The respective program must be installed on the local computer and the extension of the created filename must be associated with this program
- The progress is now shown during the import process and new parameters can be added on-the-fly when importing one value per row style format.
- When changing the color for a symbol, the associated line is changed to the same color automatically
- Most grids can now be copied to the clipboard by pressing CTRL+C, including statistical tests

Fixed in v.5.1.151 (January 2008)

- In some cases, columns were duplicated after saving a spreadsheet configuration
- In the symbol group screen, not all symbols were shown in the symbol list
- Find within distance feature did not work correctly. The search has been fixed.
- Statistical results were wrong when dataset included only one value
- Exchange capacity estimation error in the PHREEQC Aquifer material calculator. Previous results were 100 times off due to an incorrect percentage calculation

Fixed in v.5.1.37 (September 2006)

- PHT3D Export
 - Al was not appearing in the list of exported species
 - Mineral concentrations now uses mol per L of bulk volume instead of L porewater
- Calculation error in aquifer conversion, all entries are now in percent
- Sum of Cations calculation did not include H⁺
- Sum of Anions was incorrect when displayed in a table view
- Mann-Kendall analysis, problems with calculation of probability value
- Problems with the Find Station at a distance calculation

AquaChem is backwards compatible, and is able to open any projects from versions 5.0 and later. It is recommended that you ALWAYS create a backup copy of any project files before you open them in the new version.

NOTE: AquaChem no longer supports opening projects from version 4 or earlier due to the differences in the data structure. We recommend you export your data from your older version of AquaChem and then use the current release to create a new project and import the data.

Known Issues

Although every reasonable effort has been made to fix any known problems with the software, there are some issues with the software we were not able to fix before the program was released. These issues are documented below:

Version 2014.2 (Build 17.299.206 and earlier)

- Puckorius Scaling Index is not currently being calculated.

- Values in the Corrosion and Scaling dialog are not always being calculated correctly. We recommend using the AquaChem function option – or adding the calculation you need to the calculated tab in the Sample Details dialog.
- As a Standard (Restricted) User you may encounter difficulties opening or editing a sample record. The work around for this issue is to have someone with Admin right log in and run the program – then log back in as a Standard use and you should be able to open and edit samples.
- On newer operating systems you may encounter difficulties opening a Sample Details dialog box. The work around is to right click on desktop icon and select properties – on the compatibility tab select to run in compatibility mode for windows 7 and then ok. Then right click on the desktop icon again and select run as admin.
- Newly added ranges are not available for Reliability Reports.
- Difficulties may be encountered with using non English regional and language settings – please ensure you are using a decimal delimiter (not comma)
- Changing the background colour in the main interface (option under Preferences / General) is not applied until you close and re-open AquaChem.

Limitations

Version 9.0 (Build 17.0219.0)

- Certain features, including support for PHREEQC, lab QA/QC utilities/reports, trend analyses, and support for shapefiles and KMLs, have not yet been developed in AquaChem 9.0; these will be re-introduced over the next versions of AquaChem based on feedback from users like you.
- The AquaChem link to HGA will not be continued as we will introduce a new premium edition of HGA that includes all the functionality of AquaChem 9.0 later this year.

Version 2014.2 (Build 17.299.206 and earlier)

- Currently annotations made on plots are not retained once the plot is closed (i.e. you cannot reload an annotation using a saved plot configuration).
- When linking AquaChem to an HGA project – user defined fields in the HGA project database will not be available in AquaChem.
- Please be aware that there is a new prerequisite for running AquaChem (version 2011.1 and higher). If you do not have MS Access 2010 or higher installed on your computer you will need to install the MS Access 2010 Runtime Engine (available on Microsoft website: <https://www.microsoft.com/en-us/download/details.aspx?id=10910>)