A User's Guide to RockWare®

Aq•QA®

Version 1.5

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A Guided Tour of Aq•QA®

About Aq•QA®

Imagine you could keep the results of your chemical analyses in a spreadsheet developed especially for the purpose. A spreadsheet that knows how to convert units, check your analyses for internal consistency, graph your data in the ways you want it graphed, and so on.

A spreadsheet like that exists, and it's called Aq•QA. Aq•QA was written by water chemists, for water chemists. Best of all, it is not only powerful but easy to learn, so you can start using it in minutes. Just copy the data from your existing ordinary spreadsheets, paste it into Aq•QA, and you're ready to go!

To see what Aq•QA can do for you, take the guided tour below.

Data Sheet

When you start Aq•QA, you see an empty Data Sheet. Click on **File → Open…**, move to directory "\My Documents\AqQA\Examples" and open file "Example1.aqq".

The example Data Sheet

is arranged with samples in columns, and analytes – the things you measure – in rows.

You can flip an Aq•QA Data Sheet so the samples are in rows and analytes in columns by selecting **View → Transpose Data Sheet**. Click on this tab again to return to the original view.

> **Tip:** Aq•QA by default labels analytes by name (Sodium, Potassium, Dissolved Solids, …), but by clicking on **View → Show Analyte Symbols** you can view them by chemical symbol (Na, K, TDS, …).

To include more samples or analytes in your Data Sheet, click on the "Add Sample" or "Add Analyte" button:
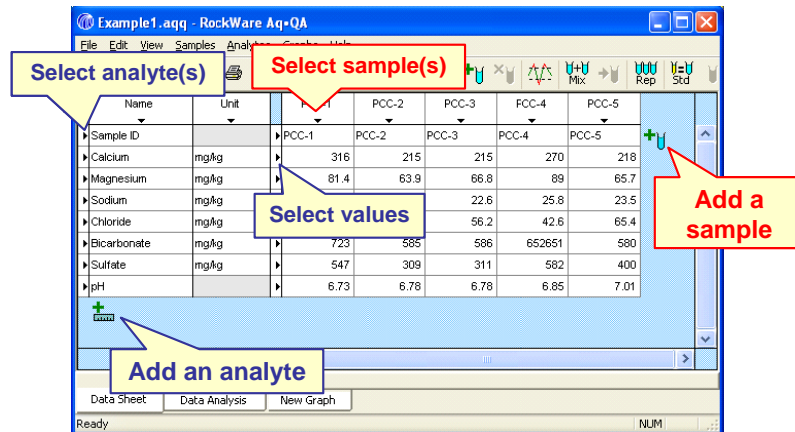
You select analytes or samples by clicking on "handles", marked in the Data Sheet by small triangles. You can select the values associated with an analyte using a separate set of handles, next to the "Unit" column. Give it a try!

> **Tip:** To rearrange rows or columns, select one or more, hold down the **Alt** key, and drag them to the desired location.

Entering Data

To see how to enter your own data into an Aq•QA Data Sheet, begin by selecting **File → New**. Add to the Data Sheet whatever analytes you need, and delete any you don't need.

> **Tip:** To delete analytes, select one or more and click on the ⬛ button. To delete samples you have selected, click on the ⬛ button.

When you click on the "Add Analyte" button, you can pick from among a number of predefined choices in various categories, such as "Inorganic Analytes", "Organic Analytes", and so on:

"Add Analytes" button …

… lets you choose analytes from various categories
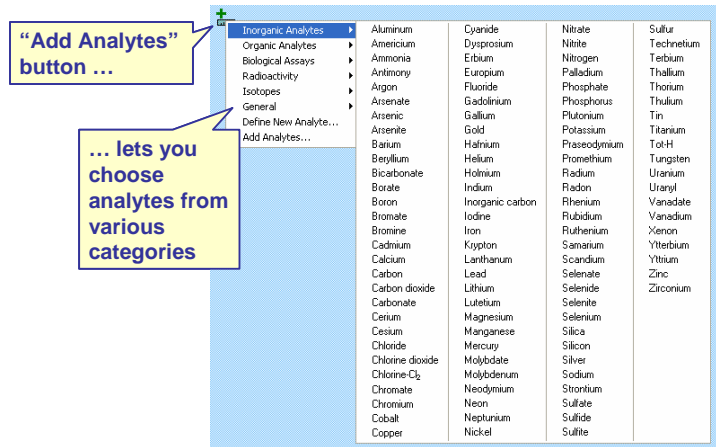
A number of commonly encountered data fields (Date, pH, Temperature, …) can be found in the "General" category.

Tip: If you don't find an analyte you need among the predefined choices, you can easily define your own by clicking on **Analytes → New Analyte…**.

To make your work easier, rearrange the analytes (select, hold down the **Alt** key, and drag) so they appear in the same order as in your data.

Tip: You can add a number of analytes in a single step by clicking on **Analytes → Add Analytes…**.

Set units for the various analytes, as necessary: right click in the unit field and choose the desired units from under **Change Units**, or select **Change Units** under **Analytes** on the menubar.

Right click to change units
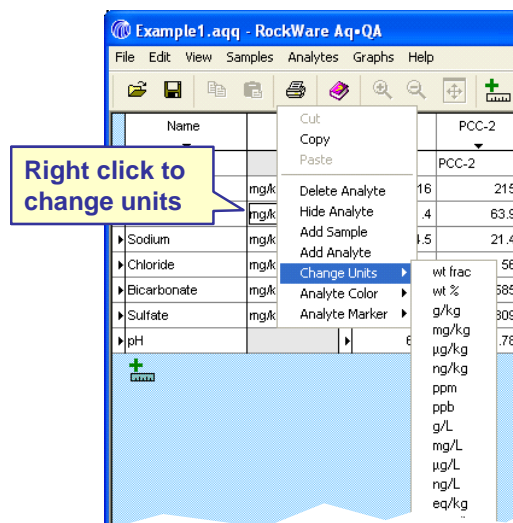
> **Tip:** You can change the units for more than one analyte in one step. Simply select any number of analytes and right-click on the unit field.

> **Tip:** Analyses are sometimes reported in elemental equivalents. For example, sulfate might be reported as "SO_4 (as S)", bicarbonate as "HCO_3 (as C)", and so on. In this case, right click on the unit of such an analyte and select **Convert to Elemental Equivalents**.

You can now enter your data into the Data Sheet as you would in an ordinary spreadsheet.

> **Tip:** If you have an analysis below the detection limit, you can enter a field such as "<0.01". Aq•QA knows what this means. If the analysis reports an analyte was not detected, enter a string such as "n/d" or "--". For missing data, enter a non-numeric string, or simply leave the entry blank.

You of course can type data into the Data Sheet by hand, or paste the values into cells one-by-one. But it's far easier to copy them from an ordinary spreadsheet or other document as a block and paste them all at once into the Aq•QA Data Sheet.

Making sure the analytes appear in the same order as in your spreadsheet, copy the data block, click on the top, leftmost cell in the Aq•QA Data Sheet, and select **Edit → Paste**, or touch **ctrl+V**.

> **Tip:** If there are more samples in a data block you are pasting than in your Aq•QA Data Sheet, Aq•QA will make room automatically.

> **Tip:** If the data arranged in your spreadsheet in columns fall in rows in your Aq•QA Data Sheet, or vice-versa, you can transpose the Data Sheet, or simply select **Edit → Paste Special → Paste Transposed**.

> **Tip:** You can flag data in an Aq•QA Data Sheet that fall outside regulatory guidelines. Select **Samples → Check Regulatory Limits**, or click on . Violations on the Data Sheet are flagged in red.

Working With Data

Once you have entered your chemical analyses in the Data Sheet, Aq•QA can tell you lots of useful information.

Click on **File → Open…** and load file "Example2.aqq" from directory "\My Documents\AqQA\Examples". To see Aq•QA's analysis of one of the samples in the Data Sheet, select the sample by clicking on its handle and then click on the Data Analysis tab. This moves you to the Data Analysis pane, which looks like
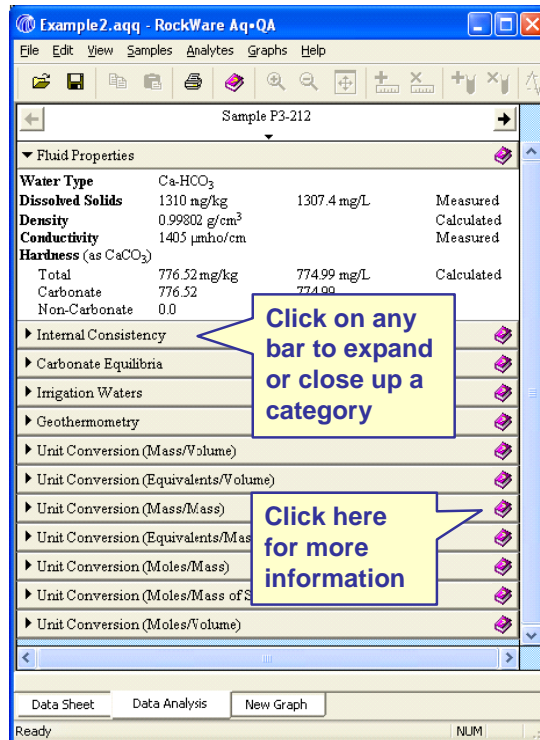
There are a number of categories in the Data Analysis pane. To open a category, click on the corresponding bar. A second click on the bar closes the category. Clicking on the ◆ symbol gives more information about the category.

> **Tip:** You can view the data analysis for the previous or next sample in your Data Sheet by clicking on the ← and → buttons to the left and right of the top bar in the Data Analysis pane.

The top category, **Fluid Properties**, identifies the water type, dissolved solids content, density, temperature-corrected conductivity, and hardness, as measured or calculated by Aq•QA.

The next category, **Internal Consistency**, reports the results of a number of Quality Assurance tests from the American Water Works Association "Standard Methods" reference. For example, Aq•QA checks that anions and cations balance electrically, that TDS and conductivity measurements are consistent with the reported fluid composition, and so on.

The **Carbonate Equilibria** category tells the speciation of carbonate in solution, carbonate concentration calculated from measured titration alkalinity and vice-versa, the fluid's calculated saturation state with respect to the calcium carbonate minerals calcite and aragonite, and the calculated partial pressure of carbon dioxide.

The **Irrigation Waters** category shows the irrigation properties of a sample, and the **Geothermometry** category shows the results of applying chemical geothermometers to the samples, assuming they are geothermal waters.

Finally, the sample's analysis is displayed in a broad range of units, from mg/kg to molal and molar.

> **Tip:** You can print results in the Data Analysis pane: open the categories you want printed and click on **File → Print…**

Graphing Data

Aq•QA can display the data in your Data Sheet on a number of the types of plots most commonly used by water chemists.

To try your hand at making a graph, make sure that you have file "Example2.aqq" open. If not, click on **File → Open…** and select the file from directory "\My Documents\AqQA\Examples".

On the Data Sheet, select the row for Iron. Hold down the **ctrl** key and select the row for Manganese. Click on New Graph and select **Time Series Plot**. The graph appears in Aq•QA as a new pane.

The result should look like:
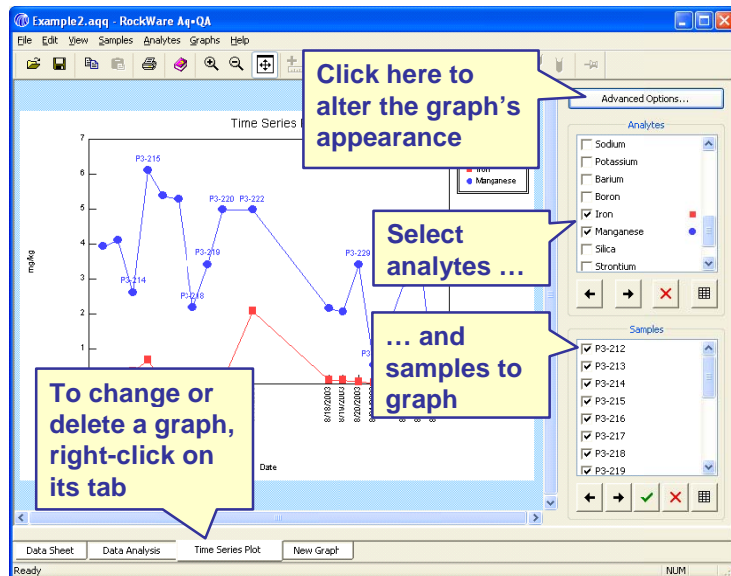
You can select the analytes and samples to appear in the graph on the control panel to the right of the plot. Right clicking on the pane's tab, along the bottom of the Aq•QA window, lets you change the plot to a different type, or delete it.

> **Tip:** You can alter the appearance of a graph by clicking on the **Advanced Options…** button on the graph pane.

You can copy the graph (**Edit → Copy**) and paste it into another program, such as an illustration program like Adobe[®] Illustrator[®] or Microsoft[®] PowePoint[®], or a word processing program like Microsoft[®] Word[®].

> **Tip:** Once you have pasted a graph into an illustration program, you can edit its appearance and content. To do so, select the graphic and ungroup the picture elements (you may need to ungroup them twice).

You can also send it to a printer by clicking on **File → Print**.

> **Tip:** In addition to copying a graph to the clipboard, you can save it in a file in one of several formats: as a Windows[®] EMF file, an Encapsulated PostScript[®] (EPS) file, or a bitmap. Select **File → Save Image As…** and select the format from the "Save as type" dropdown menu.

> **Tip:** Select a linear or logarithmic vertical axis for a Series or Time Series plot by unchecking or checking the box labeled "Log Scale" on the **Advanced Options… →** Series Plot dialog or Time Series Plot dialog.

Aq•QA can display your data on a broad variety of graphs and diagrams: simply choose a diagram type from the NewGraph pulldown.

In addition to Time Series plots, Aq•QA can produce the following types of diagrams:

Series Diagrams.
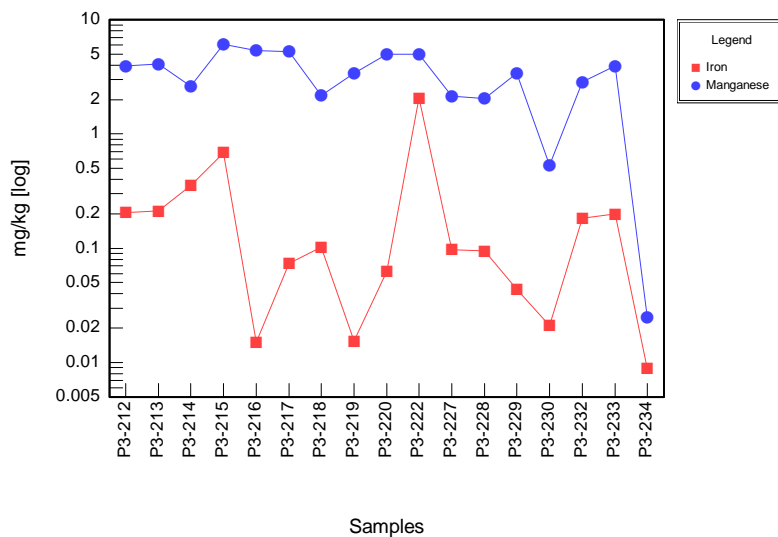
Cross Plots, in linear and logarithmic coordinates.
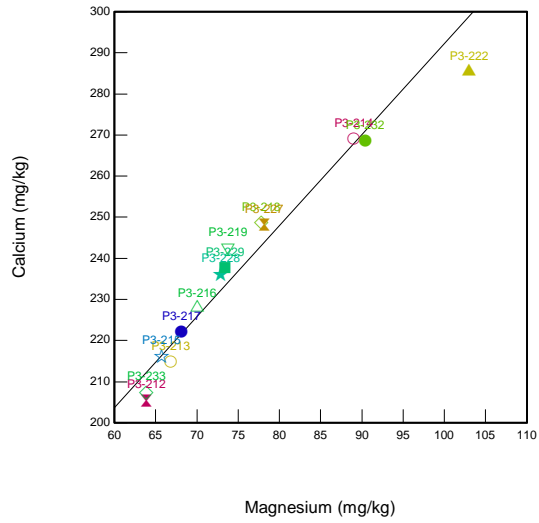
Ternary diagrams.
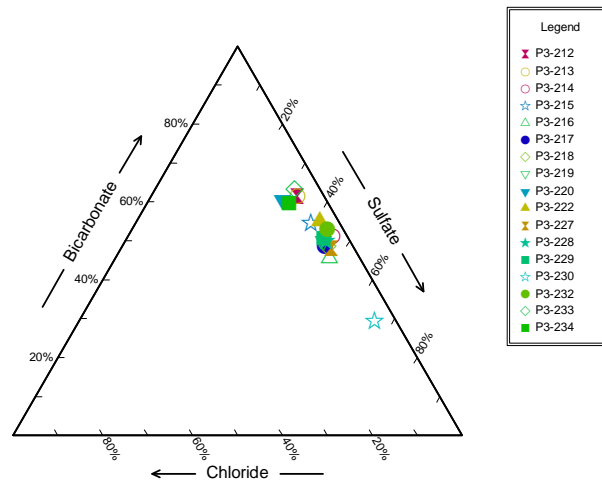
Piper diagrams.
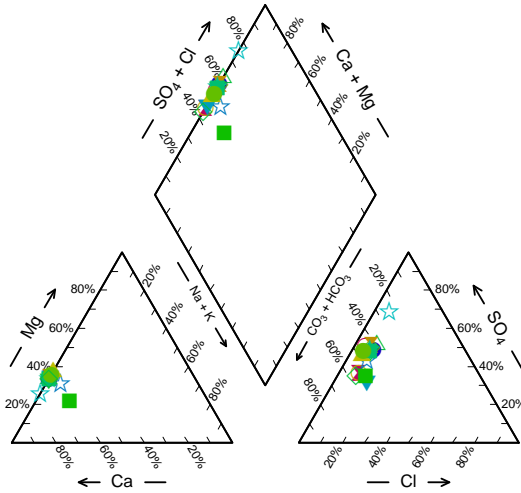
Durov diagrams.
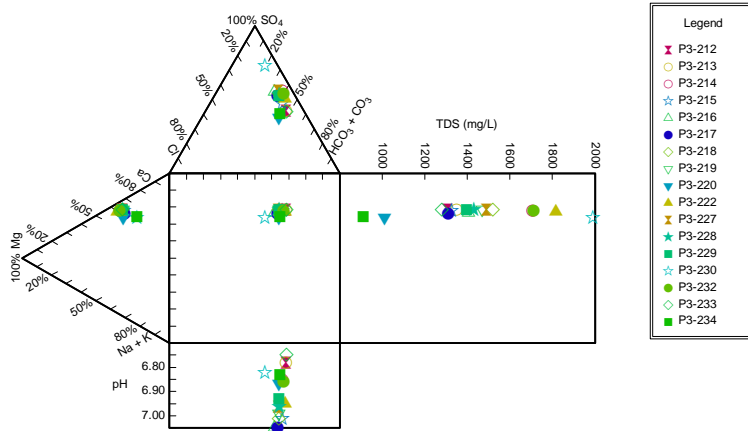
Schoeller diagrams.
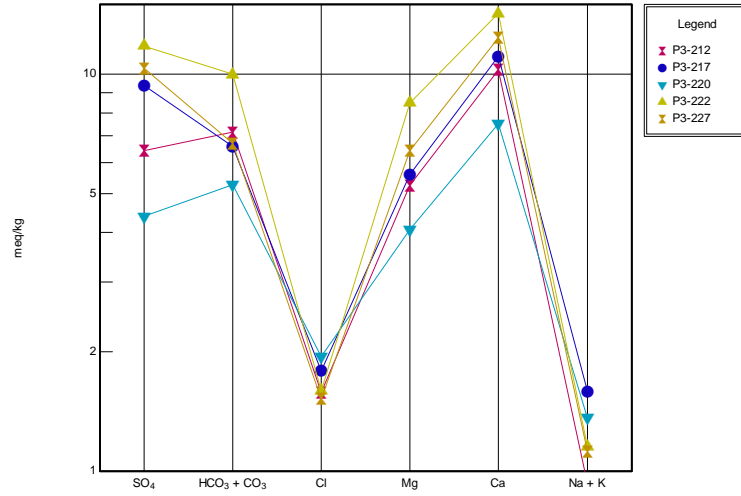
Stiff diagrams.
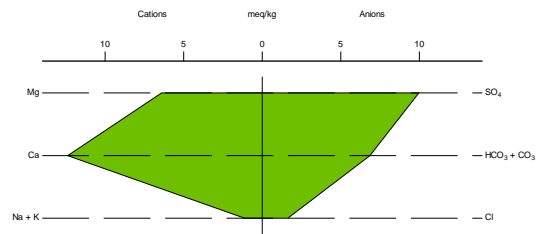
Radial diagrams.
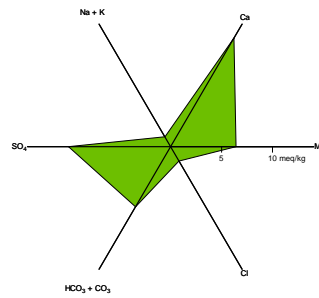
Ion balance diagrams.
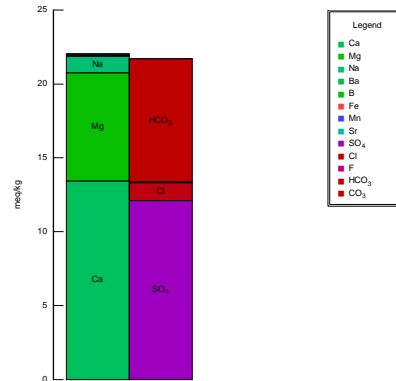
Pie charts.
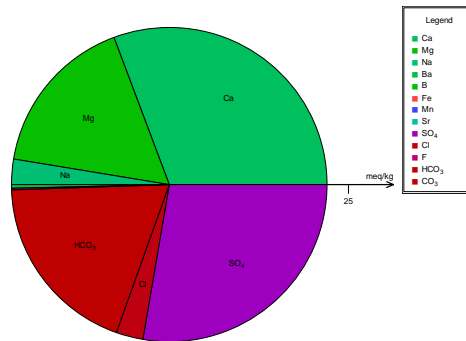
Replicates, Standards, and Mixing

Aq•QA can check replicate analyses, compare analyses to a standard, and figure the compositions of sample mixtures.

Replicate analyses are splits of the same sample that have been analyzed more than once, whether by the same or different labs. The analyses, therefore, should agree to within a small margin of error.

To see how this feature works, load (**File → Open…**) file "Replicates.aqq" from directory "\My Documents\AqQA\Examples".

Select samples PCC-2, PCC-2a, and PCC-2b: click on the handle for PCC-2, then hold down the **shift** key and click on the handle for PCC-2b.

Now, click on the button on the toolbar.

A new display appears at the right side of the Aq•QA Data Sheet, or along the bottom if you have transposed it.

The display shows the coefficient of variation for each analyte, and whether this value falls within a certain tolerance. Small coefficients of variation indicate good agreement among the replicates. The tolerance, by default, is ±5, but you can set it to another value by clicking on **Samples → Set Replicate Tolerance…**.

A standard is a sample of well-known composition, one that was prepared synthetically, or whose composition has already been analyzed precisely. Enter the known composition as a sample in the Data Sheet and click on **Samples → Designate As Standard**, or the ⨄ button.

Then select an analysis of the standard on the Data Sheet and click on **Samples → Compare To Standard**, or the ⨄⨄ button. The display at the right or bottom of the Data Sheet shows the error in the analysis, relative to the standard. Set the tolerance for the comparison, by default ±10, clicking on **Samples → Set Standard Tolerance…**.

To find the composition of a mixture of two or more samples, select two or more samples and click on the ⨄+⨄ button on the toolbar. The composition of the mixed fluid appears to the right or bottom of the Data Sheet.

The Data Sheet

About the Data Sheet

The Aq•QA® Data Sheet is a special spreadsheet that holds your chemical data. The data is typically composed of the values measured for various analytes, for a number of samples.

You can enter data into a Data Sheet and manipulate it, as described below.

Creating a New Data Sheet

To create a new Aq•QA Data Sheet, select **File → New**, or touch **ctrl+N**. An empty Data Sheet, containing a number of analytes, but no data, appears.

The appearance of new Data Sheets is specified by a template. You can create your own template so new Data Sheets contain the analytes you need, in your choice of units, and ordered as you desire. For more information, see **Template for New Data Sheets** in the **Tapping AqQA's Power** chapter of this guide.

Opening an Existing Data Sheet

Aq•QA files end with the extension ".aqq". These files contain the data entered in the Data Sheet, as well as any graphs produced and the program's current configuration.

You can open an existing Data Sheet by clicking on **File → Open…** and selecting a ".aqq" file, either one that you have previously saved or an example file installed with the Aq•QA package. A number of example files are installed in the "Examples" directory within your "My Documents\AqQA" folder.

Layout of the Data Sheet

An Aq•QA Data Sheet contains the values measured for various analytes (Na^+, Ca^{2+}, HCO_3^-, and so on) for any number of samples that have been analyzed. Each piece of information about a sample is considered an analyte, even sample ID, location, sampling date, and so on.

By default, each analyte occupies a row in the Data Sheet, and the samples fall in columns. You can reverse this arrangement, so analytes fall in columns and the samples occupy rows, by clicking on **Edit →** **Transpose Data Sheet**. To flip the Data Sheet back to its original arrangement, click on this tab a second time.

You can rearrange the order of analytes or symbols on the Data Sheet, as described below under **Reordering Rows and Columns**.

Selecting Rows and Columns

To select a row or column, click on the marker to the left of a row, or the top of a column. The marker for a row or column appears as a small triangle. Analytes have two markers, one for selecting the entire analyte, and one for selecting only the analyte's data values.

You can select a range of rows or columns by holding down the left mouse button on the marker at the beginning of the range, then dragging the mouse to the marker at the end of the range. Alternatively, select the beginning of the range, then hold down the **shift** button and click on the marker for the end of the range.

To select a series of rows or columns that are not necessarily contiguous on the Data Sheet, select the first row or column, then hold down the **ctrl** key and select subsequent rows or columns.

By clicking on one of the small blue squares at the top or left of the Data Sheet, you can select either the entire sheet, or all of the data values on the sheet.

Reordering Rows and Columns

You can easily rearrange the rows and columns of samples and analytes in your Data Sheet. To do so, first select a row or column, or a range of rows and columns, as described under **Selecting Rows and Columns**. Then, holding down the **alt** key, press the left mouse button, drag the selection to its new position, and release the mouse button.

Adding Samples and Analytes

To include more samples or analytes in your Data Sheet, select on **Samples → Add Sample**, or **Analytes → Add Analyte**, or simply click on the or buttons on the toolbar. To add several analytes at once, select **Analytes → Add Analytes…**, which opens a dialog box for this purpose.

When you add an analyte, you choose from among the large number that Aq•QA knows about. These are arranged in categories: inorganics, organics, biological assays, radioactivity, isotopes, and a general category that includes things like pH, temperature, date, and sample location.

If you don't find the analyte you need, you can quickly define your own. Select **Analytes → New Analyte…**, or **New Analyte…** from the dropdown menu. For more information about defining analytes, see the **Analytes** chapter of the guide.

Deleting Samples and Analytes

To delete analytes or samples, select one or more and click on **Analytes → Delete**, or **Samples → Delete**. Alternatively, select an analyte and click on the button, or a sample and click on .

Using Analyte Symbols

Analytes are labeled with names such as Sodium, Calcium, and Bicarbonate. If you prefer, you can view them labeled with the corresponding chemical symbols, such as Na^+, Ca^{2+}, HCO_3^-. Simply click on **View → Show Analyte Symbols**. A second click on this tab returns to labeling analytes by name.

Data Cells

Each cell in the data sheet contains one of several types of information:

1. A numerical value, such as the concentration of a species.
2. A character string.
3. A date or a time.

Numerical values are, most commonly, simply a number. You can, however, indicate a lack of data with a character string, such as "n/d" or "Not analyzed", or just leaving the cell empty.

If an analysis falls below the detection limit for a species, enter the detection limit preceded by a "<". For example, "<0.01".

Character strings, such as you might enter for the "Sample ID", contain any combination of characters, and can be of any length.

You can enter dates in a variety of formats: "Sep 21, 2003", "9/21/03", "September 23", and so on. Aq•QA will interpret your input and cast it in your local format (e.g., mm/dd/yy in the U.S.). Similarly, enter time as "2:20 PM" or "14:20". Append seconds, if you wish: 2:20:30 PM".

To change the width of the data cells (i.e., the column width), drag the dividing line between columns to the left or right. This changes the width of all the data columns in the Data Sheet.

Entering Data

To enter data into an Aq•QA Data Sheet, you can of course type it in from the keyboard, or paste it into the cells in the Data Sheet, one by one.

It is generally more expedient, however, to copy all of the values as a block from a source file, such as a table in a word processing document, or a spreadsheet. To do so, set up your Aq•QA Data Sheet so that it contains the same analytes as the source file, in the same order (see **Adding Samples and Analytes** above, and **Reordering Rows and Columns**). You don't necessarily need to add samples: Aq•QA will add columns (or rows) to accommodate the data you paste.

Now, select the data block from the source document and copy it to the clipboard. Move to Aq•QA, click on the top, leftmost data cell, and select **Edit → Paste**. If the source data is arranged in the opposite sense as your Data Sheet (the samples are in rows instead of columns, or vice-versa), transpose the Data Sheet (**View → Transpose Data Sheet**), or select **Edit → Paste Special → Paste Transposed**.

Changing Units

You can change the units of analytes on the Data Sheet at any time. To do so, select one or more analytes, then click on **Analytes → Change Units**. Alternatively, right click and choose a new unit from the options under **Change Units**. If you have entered numerical data for the analyte (or analytes), you will be given the option of converting the values to the new unit.

Some unit conversions require that the program be able to estimate values for the fluid's density, dissolved solids content, or both. If you have entered values for the Density or Dissolved Solids analytes, Aq•QA will use these values directly when converting units.

If you have not specified this data for a sample, Aq•QA will calculate working values for density and dissolved solids from the chemical analysis provided. It is best, therefore, to enter the complete analysis for a sample before converting units, so the Aq•QA can estimate density and dissolved solids as accurately as possible.

Aq•QA estimates density and dissolved solids using the methods described in the **Data Analysis** section of the User's Guide, assuming a temperature of 20°C, if none is specified. Aq•QA can estimate density over only the temperature range 0°C –100°C; outside this range, it assumes a value of 1.0 g/cm^3, which can be quite inaccurate and lead to erroneous unit conversions.

Using Elemental Equivalents

You may find that some of your analytical results are reported as elemental equivalents. For example, sulfate might be reported as "SO_4 (as S)", bicarbonate as "HCO_3 (as C)", and so on.

In this case, select the analyte or analytes in question and click on **Analytes → Convert to Elemental Equivalents**. Alternatively, select the analyte(s), then right click on your selection and choose **Convert to Elemental Equivalents**.

To return to the default setting, select **Analytes → Convert to Species**, or select the **Convert to Species** option when you right-click.

Notes and Comments

When you construct a Data Sheet, you may want to save certain notes and comments, such as a site's location, who conducted the sampling, what laboratory analyzed the samples, and so on.

To do so, select **File → Notes and Comments…** and type the information into the box that appears. This information will be saved with your Aq•QA document; you may access it and alter it at any time.

Flagging Data Outside Regulatory Limits

You can highlight on the Data Sheet concentrations in excess of an analyte's regulatory limit. Select **Samples → Check Regulatory Limits**. Concentrations above the limit now appear highlighted in a red font. Select the tab a second time to disable the option. Touching **ctrl+L** also toggles the option.

Aq•QA can maintain a regulatory limit for each analyte. The analyte library contains default limits based on U.S. water quality standards at the time of compilation, but you should of course verify these against standards as implemented locally. You can easily change the limit carried for an analyte, as described in the **Analytes** chapter of this guide.

Saving Data

Before you exit Aq•QA, you will probably want to save your workspace, which includes the data in your Data Sheet, any graphs you have created, and so on, in a .aqq file.

To save your workspace, select **File → Save**, or click on the button on the Aq•QA toolbar.

To save your workspace as a .aqq file under a different name, select **File → Save As…** and specify the file's new name.

You may also want to save the data in the Data Sheet as a file that can be read by other applications, such as Microsoft® Excel®. For information on saving data in this way, see the next section, **Exporting Data to Other Software**.

Exporting Data to Other Software

When Aq•QA saves a .aqq file, it does so in a special format that includes all of the information about your Aq•QA session, such as the current option settings and the plots you have created. In this way, you can resume working where you left off.

You may wish, however, to save the data in your Data Sheet in a format that you can read from programs such as Excel, or with a text editor. To do so, you create a text file in which the data cells are delimited with a special character, such as a comma or tab.

Select **File → Export Data…** and on the resulting dialog box choose a character (e.g., comma or tab) to serve as the column separator. On this box, you can also set details of how you want the data saved and what data you want included in the file.

Printing the Data Sheet

You can print the contents of the Data Sheet by selecting **File → Print…**. To control the appearance of the printed page, such how to scale the Data Sheet to the page, select **File → Print Setup…**.

You can check what the printed Data Sheet will look like before you print it be selecting **File → Print Preview**. If you wish to continue, select the **Print…** button. To return to the Data Sheet, select the **Close** button.

Analytes

About Analytes

Analytes are the various measurements or properties of a sample that Aq•QA® can store, use, and display. Analytes include sodium, TCE, temperature, and so on.

Analytes in Aq•QA fall into six categories.

1. Inorganic Analytes – calcium, sulfate, and so on.
2. Organic Analytes – tricholorethylene, vinyl chloride, etc.
3. Biological Assays – coliform bacteria, viruses, etc.
4. Radioactivity – α particles, β particles, etc.
5. Isotopes – ^{18}O, ^{13}C, and so on.
6. General – temperature, pH, etc.

Aq•QA comes with a set or "library" of predefined analytes, each of which has a set of properties that you can alter, if you wish. You can also readily define your own analytes to meet your needs.

Analyte Properties

Each analyte has associated with it a set of properties that define how Aq•QA treats it. Depending on category, the analyte properties may include:

- Name. A label, such as "Sodium" or "Dissolved Solids", for referring to the analyte.

- Symbol. An optional symbol, such as "Na" or "TDS", for referring to the analyte.

- Dimension. The type of unit, such as "concentration", "density", or "distance", used to measure the analyte.

- Display Unit. The unit, such as "mg/kg", "g/cm³", or "cm", used by default to represent the analyte.

- Mole Weight. The molecular weight of the analyte, if it is a chemical species.

- Equivalent Element. An element sometimes used to represent an analyte. The concentration of carbonate, for example, is

sometimes represented in terms of elemental carbon as "mg/kg as C"; sulfate in terms of sulfur as "mg/kg as S".

- Elemental Atoms Per Molecule. If the analyte is a species that has an equivalent element, this is the number of times the element appears in the species' formula.

- Ionic Charge. The electrical charge on the species, if the analyte is a species.

- Conductivity Factor μmho/cm per meq/L. The numerical factor used with the analyte's concentration to calculate electrical conductivity, according to Standard Method 2510-A.

- Minimum Acceptable Limit Value. A regulatory or other limit on the least acceptable value for the analyte.

- Minimum Acceptable Limit Units. The unit corresponding to this value.

- Maximum Acceptable Limit Value. A regulatory or other limit on the greatest acceptable value for the analyte.

- Maximum Acceptable Limit Units. The unit corresponding to this value.

- Regulation. The regulatory source, such as a USEPA MCL, or Maximum Contaminant Level, for above.

- Description. An optional note describing the analyte.

- Source. An optional note giving the data source.

- Aq•QA Uses As. If the program recognizes the analyte as having a special role in its calculations, that role is noted here.

- Significant Digits. The number of digits used to display a value for the analyte.

- Conserved. A flag indicating whether the analyte is conserved during mixing, used in Aq•QA's "mix" feature.

Changing the Properties of an Analyte

You can change the properties of any analyte on your Data Sheet. You might, for example, want to change the acceptable limit for lead to a new value.

To change an analyte's properties, click on **Analytes → Analyte Properties** and select the analyte category corresponding to the analyte in question. Alter any or all of the properties for the analyte, then click on the **Data Sheet** pane to return to your data.

When you change properties in this way, you alter them only within the current Aq•QA document. To alter properties in future documents, see **Editing the Analyte Library**.

Creating a New Analyte

You can create your own analyte to reflect, for example, a species not included in the analyte library. Click on **Analytes → New Analyte…** and in the dialog box that appears select the appropriate category ("Inorganic Analytes", "Organic Analytes", etc.). If no other category seems applicable, choose "General".

Fill in the properties requested on the dialog box and click "OK". The new analyte appears in your Data Sheet, along with Aq•QA's pre-defined analytes.

You can change the analyte's properties, as well as define those not included in the dialog box, at any time by clicking on **Analytes → Analyte Properties**.

Analyte Libraries

Aq•QA comes with a library of analytes known to it, and analytes' properties. The analyte library, named "library.aqq", is installed in the Aq•QA installation directory (e.g., "\ProgramData\RockWare\AqQA").

You can easily define your own library, generally by modifying or adding to the analytes in library.aqq, as discussed in the next section, **Editing the Analyte Library**. You can save your custom library under any name, in any directory.

To tell Aq•QA to use a custom library instead of the default, select on **File → Preferences** and click on the **Browse** button next to the **Import Standard Analytes From** field. From now on, when you add analytes to your Data Sheet, or create a new Aq•QA file, Aq•QA will take analytes and their properties from your custom library.

Editing the Analyte Library

To create a custom analyte library, open the library as you would any Aq•QA file, by clicking on **File → Open…**. It's a good idea to save a copy of the default library that comes with Aq•QA under a different name, and modify the copy. As described in the previous section, **Analyte Libraries**, use the **File → Preferences** dialog to tell Aq•QA to use the custom instead of default library.

Once you have opened the custom library, select the category (inorganics, organics, and so on) you would like to edit from **Analytes → Analyte Properties**. Edit the analytes as you would any Aq•QA Data Sheet. You can add analytes, delete them, and alter analyte properties.

Continue by editing the analytes in the other categories, as desired. When you are done editing the library, save it as you would any other Aq•QA file, by clicking on **File → Save** or **File → Save As…**.

Updating Aq•QA Files

Once you have changed analyte properties in the analyte library, or added analytes to the library, your changes will appear in the new Aq•QA documents you create, provided you have set Aq•QA to use the new library (on the **File → Preferences** dialog).

Your exisiting .aqq files, however, will be unaffected by changes to the library, unless you update them. For example, if you change the regulatory limit for an analyte in the standard library, the new limit will be reflected in new .aqq files you create, but not exisiting files, unless you update them.

If you have modified any of the analyte definitions in the default template ("default.aqq") or any templates you have created (see **Template for New Data Sheets**), furthermore, you will need to update these files.

To update an Aq•QA document, open it (**File → Open…**) and click on **Analytes → Update Analytes…**. The resulting dialog box allows you to reconcile analyte properties in the current document with an analyte library, or with the analyte properties in any other Aq•QA document.

The dialog box will list the analyte properties that differ between your document and the library. To accept the updates, click on **Select All**, or select only those you wish to apply, and then **Apply Selected**. Click on **Done** to return to working with the revised Aq•QA document.

Data Analysis

About Data Analysis

The Data Analysis pane displays useful information about a water sample from the Data Sheet. The sheet contains a number of categories of information, with horizontal bars for each category labeled "Fluid Properties", "Internal Consistency", and so on.

To see the information under a given category, click on the bar. Clicking on the bar a second time closes the category, and clicking on the button displays helpful information about the category.

The label for the sample in question is shown at the top of the pane. Also there are two arrow buttons that allow you to scan forward and backward through the samples on the Data Sheet.

In performing the calculations on this pane, Aq•QA® assumes conditions of 20°C, unless a temperature has been entered for the sample on the Data Sheet. If no density is reported, Aq•QA will estimate an appropriate value, as described below. Aq•QA can estimate density over only the temperature range 0°C –100°C; outside this range, it assumes a value of 1.0 g/cm^3, which can be quite erroneous. Finally, if no value is reported for dissolved solids, Aq•QA calculates one from the sample's chemical analysis, as described below.

In this chapter, an "AWWA Standard Method" refers to a method described in the cited section of the AWWA "Standard Methods" volume. The complete reference to this volume is:

Clesceri, L.S., A.E. Grrenberg, and A.D. Eaton, 1998, Standard Methods for the Examination of Water and Wastewater, 20th ed., American Public Health Association (Washington), American Water Works Association (Denver), and Water Environment Federation (Alexandria, VA).

Fluid Properties

The Fluid Properties category of the Data Analysis pane reports various properties of the water sample.

Water Type

The water type – e.g., Ca-HCO$_3$ or Na-SO$_4$ – is determined by finding the predominant inorganic cation and anion, figured on the basis of electrical equivalents.

In determining water type, Aq•QA accounts whenever possible for the carbonate speciation in solution, using the sum in electrical equivalents of the CO_3^{2-} and HCO_3^- concentrations to represent carbonate. If carbonate is the dominant anion by this criterion, Aq•QA states the water type in terms of whichever of the two species is present in larger equivalent concentration (e.g., Ca-HCO$_3$ or Na-CO$_3$).

Aq•QA also calculates, where pH is given, the free ion concentrations of H^+ and OH^-, and accounts for these species when assigning a water type. An acidic solution might be typed H-SO$_4$, for example, or an alkaline water, Ca-OH.

Dissolved Solids

The program displays the water's calculated dissolved solids content, along with the measured value, if supplied on the Data Sheet. Aq•QA calculates dissolved solids by summing the inorganic analytes, following by Standard Method 1030-E, except that it accounts for all of the inorganic analytes on the Data Sheet, and it accounts for carbonate specied as described in the next paragraph.

The contribution of carbonate to dissolved solids is taken as the sum of the masses of analytes bicarbonate, carbonate, and carbon dioxide (HCO_3, CO_3, and CO_2). If none of these analytes is specified, Aq•QA accounts for carbonate in one of the following ways: (1) from an analyses of total carbon, (2) from the carbonate concentration calculating from a specified alkalinity and pH, as described below under **Carbonate Speciation**, or (3) from a specified alkalinity in the absence of pH, according to $0.6 \times$ alkalinity.

Density

The program displays the water's calculated density, in g/cm^3, along with the measured value, if supplied on the Data Sheet. Density is calculated from salinity (dissolved solids expressed as permil salts) according to Standard Method 2520-C. Aq•QA calculates density only over the temperature range of 0°C–100°C.

Electrical Conductivity

The water's calculated electrical conductivity, in μmhos/cm, is displayed along with the measured value, if supplied on the Data Sheet. The temperature-corrected conductivity is calculated according to Standard Method 2510-A, accounting for ionic strength effects.

Wherever possible, Aq•QA figures when calculating conductivity the speciation of carbonate to produce HCO_3^- and CO_3^{2-}. Aq•QA also accounts for the contributions of the species H^+ and OH^-, whenever pH is specified.

Hardness

The program reports three values calculated for hardness: total hardness, carbonate hardness, and non-carbonate hardness. Each value is given in mg/L as an equivalent amont of $CaCO_3$.

Total hardness is calculated from the Ca^{2+} and Mg^{2+} content of the water from the equation

$$\text{Hardness [mg/L as } CaCO_3] = 2.497\ [Ca^{2+}, mg/L] + 4.118\ [Mg^{2+}, mg/L]$$

as prescribed by Standard Method 2340-B.

Carbonate hardness is the $Ca^{2+} + Mg^{2+}$ that can be balanced by the amount of carbonate (i.e., $HCO_3^- + CO_3^{2-} + CO_2$) in solution. Ca^{2+} and Mg^{2+} precipitate as a carbonate mineral such as calcite, $CaCO_3$ (i.e., $Ca^{2+} + HCO_3^- \rightarrow CaCO_3 + H^+$), so one mole of carbonate balances one mole of $Ca^{2+} + Mg^{2+}$. The carbonate hardness cannot exceed the total hardness, even if there's more carbonate than $Ca^{2+} + Mg^{2+}$ in solution.

The non-carbonate hardness is total hardness less carbonate hardness.

Internal Consistency

The Internal Consistency category of the Data Analysis pane shows the results of seven quality assurance/quality control tests applied to the analysis of the water sample. A green "OK" identifies each test that was completed successfully. A red message such as "Not within ± 5%" is applied to unsuccessful results. In other cases, as noted, there is not enough information for the sample on the Data Sheet.

The first six of the seven tests are described in 1030-E of the AWWA "Standard Methods" volume. Of the AWWA tests, the first three are considered of primary importance; the latter three may not be reliable for all water types. The final test checks for mass balance among organic analytes. The tests are:

Anion-Cation Balance

This test checks that the analysis honors the requirement that a water maintain electroneutrality. To make this test, the program figures the sum of the concentrations of the cations, expressed in meq/L, and the same value for the anions. This test is successful when the difference between the sums, or the percentage of the cation sum plus the anion sum that the difference represents, satisfies:

Anion sum, meq/L	Acceptable difference
0–3	± 0.2 meq/L
3–10	±2%
10–800	±5%

Wherever possible, Aq•QA figures when calculating the anion sum the speciation of carbonate to produce HCO_3^- and CO_3^{2-}. Aq•QA also

accounts for the contributions of the species H^+ and OH^- to the ion sums, whenever pH is specified.

Measured TDS Matches Calculated TDS

The ratio of the measured dissolved solids to the value calculated by Standard Method 1030-E, accounting for all inorganic analytes on the Data Sheet, should fall in the range 1.0 to 1.2.

Measured Conductivity Matches Calculated Value

The ratio of the measured electrical conductivity to the temperature-corrected value calculated by Standard Method 2510-A should fall in the range 0.9 to 1.1.

Measured Conductivity and Ion Sums

The ion sums for cations and anions multiplied by 100 should both fall within ±10% of the measured electrical conductivity. This test is considered by many to be less reliable and significant than the first three tests in this section.

Calculated TDS to Conductivity Ratio

The ratio of calculated dissolved solids (mg/L) to measured electrical conductivity (µmhos/cm) should normally fall in the range 0.55 to 0.7. In the presence of poorly dissociated calcium or sulfate ions, the ratio may be as high as 0.8. This test is considered by many to be less reliable and significant than the first three tests in this section.

Measured TDS to Conductivity Ratio

The ratio of measured dissolved solids (mg/L) to measured electrical conductivity (µmhos/cm) should fall in the range 0.55 to 0.7. This test is considered by many to be less reliable and significant than the first three tests in this section.

Organic Carbon Cannot Exceed Sum of Organics

This test compares a measured DOC (dissolved organic carbon, mg/L) value to the sum of the concentrations (mg/L, as C) of specific organic analytes. The DOC should not be more than 5% less than the sum. It may, however be greater, since all the organic species in solution have not necessarily been analyzed.

Carbonate Equilibria

The Carbonate Equilibria category shows the speciation among carbonate ions in solution, and various factors that depend on the speciation. For details of how these calculations are performed, see **Appendix: Carbonate Equilibria**.

Dissolved carbonate is distributed among the carbonate and bicarbonate ions (CO_3^{2-} and HCO_3^-) and aqueous carbon dioxide ($CO_2(aq)$). In order for Aq•QA to figure the species distribution, the following conditions must be met for the sample:

1. The pH must be specified.

2. At least one measure of carbonate concentration must be specified. This may be (A) the concentration of one of the inorganic analytes bicarbonate, carbonate, or carbon dioxide, (B) the carbon concentration [C], or (C) the titration alkalinity.

3. Temperature, which is set to 25°C if not specified, must fall in the range 0°C –300°C. (Note that in the range 100°C–300°C, it is necessary to specify fluid density directly, to avoid possibly significant calculation errors when converting units.)

If these conditions are met, the following information will appear:

Speciation

The program reports the predicted distribution of carbonate among the three carbonate species: HCO_3^-, CO_3^{2-}, and CO_2.

Total Carbonate From Titration Alkalinity

If the titration alkalinity is given on the Data Sheet, the program reports the calculated total carbonate concentration.

Titration Alkalinity From Total Carbonate

If the carbonate concentration is given on the Data Sheet, the program reports the calculated titration alkalinity, in mg/kg as $CaCO_3$.

Mineral Saturation

If the calcium concentration is given on the Data Sheet, the program reports the saturation indices calculated for the $CaCO_3$ minerals calcite and aragonite. The saturation indices tell whether the minerals are supersaturated ($SI > 0$), saturated ($SI = 0$), or undersaturated ($SI < 0$).

Partial Pressure of CO_2

The program shows the partial pressure of CO_2 in the water, in atm.

Irrigation Waters

The following parameters are used to judge the suitability of a water for irrigating crops. Unless noted, concentrations (e.g., [Na]) are in units of meq/L. The program reports a value only in cases in which all of the necessary concentrations are given.

Salinity hazard

This parameter is determined according to the following table. The program uses measured conductivity, if available, else measured dissolved solids, else calculated dissolved solids.

	Conductivity (μmhos/cm)	Dissolved solids (mg/L)
Low salinity, no detrimental effects expected	<250	<200
Medium salinity, detrimental effects to sensitive crops	250 – 750	200 – 500
High salinity, adverse effects on many crops	750 – 2250	500 – 1500
Very high salinity, suitable only for salt tolerant plants	2250 – 5000	1500 – 3000

Sodium Adsorption Ratio

The sodium adsorption ratio (SAR) is calculated according to

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

where [] represents concentration in units of meq/L.

Exchangeable Sodium Ratio

The exchangable sodium ratio (ESR) is calculated according to

$$ESR = \frac{[\text{Na}^+]}{[\text{Ca}^{2+}]+[\text{Mg}^{2+}]}$$

where [] represents concentration in units of meq/L.

Magnesium Hazard

The magnesium hazard (MH) is calculated according to

$$MH = \frac{[\text{Mg}^{2+}]}{[\text{Ca}^{2+}]+[\text{Mg}^{2+}]}\times 100$$

where [] represents concentration in units of meq/L.

Residual Sodium Carbonate

Residual sodium carbonate (RSC) is calculated according to

$$RSC = ([\text{CO}_3^{2-}] + [\text{HCO}_3^-]) - ([\text{Ca}^{2+}] + [\text{Mg}^{2+}])$$

where [] represents concentration in units of meq/L.

Reference

Lloyd, J.W. and J.A. Heathcote, 1985, Natural Inorganic Hydrochemistry in Relation to Groundwater, Oxford Press, Oxford, 296 pp.

Geothermometry

A geothermometer is a technique of estimating from a hydrothermal water's composition the temperature at which the water last equilibrated with its environment. The techniques can be applied only to geothermal or hydrothermal waters; you should not attempt to apply them to normal ground or surface water.

A number of geothermometers are implemented in Aq•QA. Each reflects differing assumptions about which minerals were in equilibrium with the water in question. Hence, the geothermometers invariably predict different temperatures. You should, therefore, not expect all of the temperatures to agree. Instead, choose one or more geothermometers appropriate for the conditions of interest.

Each geothermometer has a temperature range of applicability; predicted temperatures falling outside this range are noted. If, for example, the maximum temperature is 250°C and the predicted value is 300°C, Aq•QA reports ">250°C". The program, furthermore, can predict a temperature only in cases in which all of the necessary concentrations are given.

In each case below, the geothermometer predicts temperature in °C from concentrations reported in mg/kg. In other words, $[SiO_2]$ is mg/kg silica in the fluid, and $[Na/K]$ is the ratio of the Na concentration in mg/kg to the K concentration in mg/kg.

Quartz (no steam loss)[1]	$T = \dfrac{1309}{5.19 - \log[SiO_2]} - 273.15$	$0 \le T \le 250°C$
Quartz (max. steam loss)[1]	$T = \dfrac{1522}{5.75 - \log[SiO_2]} - 273.15$	$0 \le T \le 250°C$
Chalcedony[1]	$T = \dfrac{1032}{4.69 - \log[SiO_2]} - 273.15$	$0 \le T \le 250°C$
α-Cristobalite[1]	$T = \dfrac{1000}{4.78 - \log[SiO_2]} - 273.15$	$0 \le T \le 250°C$
β-Cristobalite[1]	$T = \dfrac{781}{4.51 - \log[SiO_2]} - 273.15$	$0 \le T \le 250°C$
Amorphous silica[1]	$T = \dfrac{731}{4.52 - \log[SiO_2]} - 273.15$	$0 \le T \le 250°C$

Na-K[1]	$T = \dfrac{1217}{1.483 + \log[\text{Na/K}]} - 273.15$	T > 150°C

$$T = \dfrac{1647}{2.47 + \log[\text{Na/K}] + \beta\left[\log(\sqrt{\text{Ca}}/\text{Na}) + 2.06\right]}$$

Na-K-Ca[1]	-273.15	$0 \le T \le 300°C$

$\beta = 4/3$ initially. If calculated T>100°C, or if $[\log(\text{Ca}^{1/2}/\text{Na})+2.06] < 0$, recalculate using $\beta = 1/3$.

Na-K-Ca-Mg[2]	$T_{\text{Na-K-Ca}} + \Delta T_{\text{Mg}}$, as described separately[2]	$0 \le T \le 350°C$
Mg-Li[2]	$T = \dfrac{2200}{5.47 + \log[\sqrt{\text{Mg}}/\text{Li}]} - 273.15$	$0 \le T \le 350°C$
Na-Li[2]	$T = \dfrac{1590}{0.779 + \log[\text{Na/Li}]} - 273.15$	$0 \le T \le 350°C$

References:

[1]Fournier, R.O., 1981, Application of water geochemistry to geothermal exploration and reservoir engineering. In L. Rybach and L.J.P. Muffler, eds., *Geothermal Systems, Principles and Case Histories*, Wiley, New York, p. 109-143.

[2]Kharaka, Y.K. and R.H. Mariner, 1989, Chemical geothermometers and their application to formation waters from sedimentary basins. In N.D Naeser and T.H. McCulloh, eds., *Thermal History of Sedimentary Basins*, Springer-Verlag, New York, p. 99-117.

Unit Conversion

The final sections in the Data Analysis pane contain the chemical analysis in question, converted into a variety of concentration units and presented in a tabular format.

These sections contain the following groups of units:

Mass/Volume	g/L, mg/L, µg/L, ng/L
Equivalents/Volume	eq/L, meq/L, µeq/L, neq/L
Mass/Mass	wt. %, g/kg, mg/kg, µg/kg, ng/kg
Equivalents/Mass	eq/kg, meq/kg, µeq/kg, neq/kg
Moles/Mass	mol/kg, mmol/kg, µmol/kg, nmol/kg
Moles/Mass of Solvent	molal, mmolal, µmolal, nmolal
Moles/Volume	molar, mmolar, µmolar, nmolar

In the unit conversion, the following is observed:

1. The solution mass is the solvent mass plus the mass of the solute.

2. The number of kg solution is the kg of solvent divided by $(1 - 10^{-6} \times TDS)$, where TDS is total dissolved solids in mg/kg.

3. The number of kg solvent is the kg solution multiplied by $(1 - 10^{-6} \times TDS)$.

4. Volume is mass divided by density, so L equals kg divided by density, where density is in g/cm^3.

5. An "equivalent" is the product of the number of moles of a dissolved species and the absolute value of the species' electrical charge. An uncharged species invariably has an equivalent concentration of zero.

Certain conversions, therefore, require knowledge of the sample's density, TDS, or both. Aq•QA uses density and TDS values entered on the Data Sheet, if possible.

If the density is not available, Aq•QA calculates a value from the solution salinity, according to Standard Method 2520-C. If the TDS is not available, the program calculates it by summing the dissolved masses of the various inorganic analytes. It is, therefore, important to enter a complete chemical analysis, so that density and TDS can be calculated correctly.

Replicates, Standards, and Mixing

About Replicates, Standards, and Mixing

Aq•QA$^®$ can help you evaluate the quality of your chemical analysis by checking replicate analyses, and analyses of known standards. It can also find the composition of a mixture of two or more of the samples on your Data Sheet.

Comparing Replicate Analyses

Replicate analyses are made on splits of the same sample. The splits are analyzed more than once, whether by the same or different labs. Since each replicate analysis is made on the same fluid, the analyses should agree to within a small margin of error.

To check agreement among replicate samples, go to the Data Sheet and select two or more samples. (To do so, click on the marker for the first sample, then hold down the **ctrl** key and click on the markers for the remaining samples.)

Select **Samples → Compare Replicates**, or click on the ![icon] button on the toolbar. A new display appears at the right side of the Data Sheet, or along the bottom if you have transposed it.

The display shows the coefficient of variation for each analyte, and whether this value falls within a certain tolerance. Small coefficients of variation indicate good agreement among the replicates.

Analytes with a coefficient of variation that does not fall within the tolerance are flagged by a red X. The tolerance, by default, is ±5, but you can change it by clicking on **Samples → Set Replicate Tolerance…** (or right-clicking on the replicate display and selecting this option) and entering a different value.

To disable the replicate display at the right or bottom of the Data Sheet, re-select **Samples → Compare Replicates**, or click again on the ![icon] button. To maintain the display, select **Samples → Freeze Mix and Compare**, or click on the ![icon] button.

Checking Against Standards

A standard is a sample of well-known composition, one that was prepared synthetically or whose composition has already been analyzed precisely. A chemical analysis of the standard, then, should agree with the known composition to within a small margin of error.

To check the analysis of a standard, enter both the standard's known composition and the results of analyzing the standard in the Data Sheet. Select the known composition and click on **Samples → Designate As Standard**, or the ⋃ button. A check mark will appear on the Data Sheet next to the standard's label.

Select the standard's analysis and click on **Samples → Compare To Standard**, or the button. The display at the right or bottom of the Data Sheet shows the error in the analysis, relative to the standard. If you select more than one sample to compare to the standard, the program shows the average error.

Analytes with errors that do not fall within a specified tolerance are flagged by a red X. The tolerance, by default, is ±10, but you can change it by clicking on **Samples → Set Tolerance…** (or right-clicking on the standard display and selecting this option) and entering a different value.

To disable the display, re-select **Samples → Compare To Standard**, or click again on the button. To maintain the display, select **Samples → Freeze Mix and Compare**, or click on the button.

Fluid Mixing

To calculate the composition of a mixture of samples, select on the Data Sheet the samples you want to mix. Click on **Samples → Mix**, or the button on the toolbar. The composition of the mixed fluid is shown in a new display at the right or bottom of the Data Sheet.

The mixed composition contains each analyte which is conservative during mixing. Ion compositions such as Na^+ and SO_4^{2-}, for example, are conservative, but pH is not. In other words, mixing a pH 5 water with a pH 7 water does not yield a mixture of pH 6.

To save the mixed fluid as a new sample on the Data Sheet, click on **Samples → Save Mixture**, or on the button. To disable the display, re-select **Samples → Mix**, or click again on the button. To maintain the display, select **Samples → Freeze Mix and Compare**, or click on the button.

Graphing Data

About Graphing Data

To make a graph in Aq•QA, you follow these steps:

- On the Data Sheet, select the data you want to appear on the plot. (Don't worry, you can change your choices later.) For example, you might select the row of data for an analyte, or just the data in that row for certain samples.

- Click on the New Graph tab, along the bottom of the Aq•QA window and select a plot type.

- Alter the content and appearance of the plot by changing the settings in the control panel along the right side of the Aq•QA plot pane, or by clicking on the **Advanced Settings…** button.

You can delete the current plot by selecting **Graphs → Delete Graph**, or by right clicking on the plot pane's tab, along the bottom of the Aq•QA window. To change the plot to another type, select **Graphs → Change Graph Type**, or right-click on the pane's tab.

Many of the graphs Aq•QA produces account for the calculated speciation of carbonate among carbon dioxide, bicarbonate ion, and carbonate ion. If you, for example, report alkalinity and pH, the program will figure the concentrations of the various ions and produce a graph reflecting them. The Piper, Durov, Schoeller, Bar Chart, Radial, and Stiff diagrams work this way.

For each of these diagrams except the Piper and Durov plots, you can choose instead to plot the carbonate concentrations as they are entered on the Data Sheet. To do so, click on the **Advanced Settings…** button, then on the tab corresponding to the diagram type, and de-select the "Show carbonate speciation" option.

Time Series Plots

Time Series plots are much like Series plots, except that the horizontal axis shows the sampling date or time. You click on New Graph and select **Time Series Plot**, which produces a graph like:
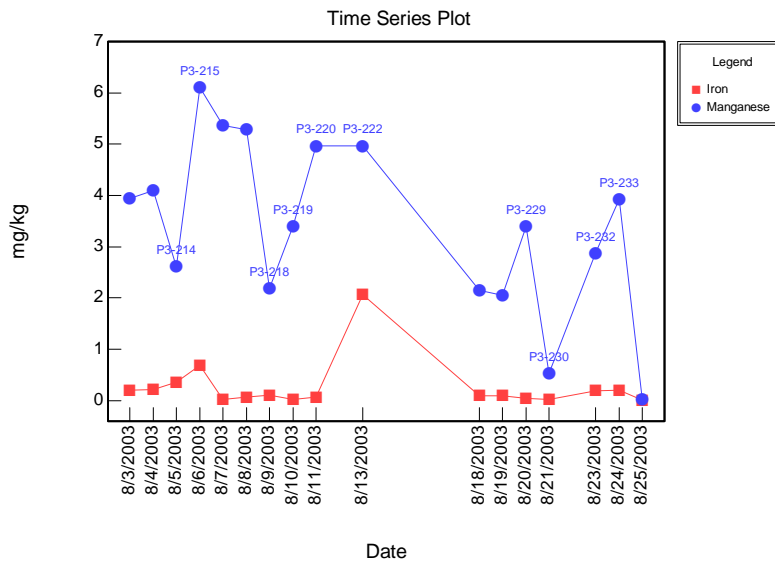
Time Series Plot

To make this type of plot, you must include in your Data Sheet either the Date or Time analyte, or both.

Series Plots

Series plots show one or more analytes on the vertical axis, and the samples in the Data Sheet along the horizontal. You can select the analytes to appear in the plot in the control panel along the right side of the Aq•QA window, as well as the samples to include.
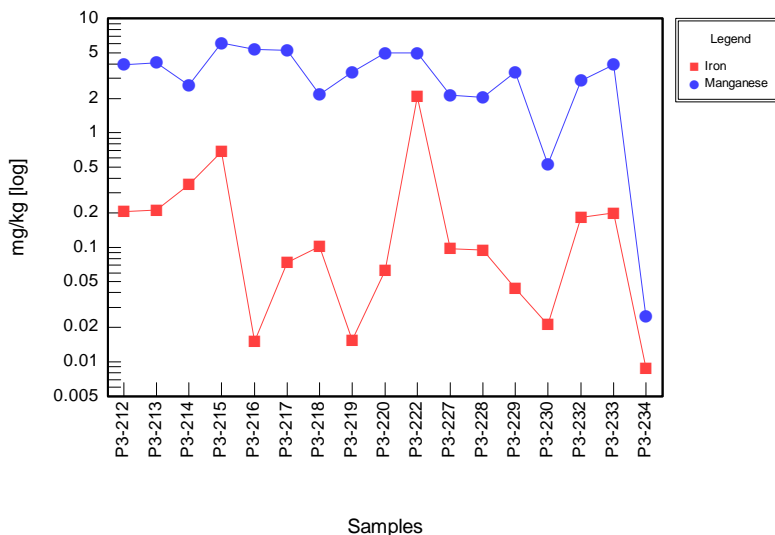
Note that you can include any number of analytes, provided they have the same type of unit. For example, you can plot any combination of analytes expressed in terms of concentration, but you can't include pH.

You can set a log scale on the vertical axis by clicking on **Advanced Settings…** and selecting that option on the ⌜Series Plot⌟ pane.

Cross Plots

To make a cross plot, click on ⌜New Graph⌟ and select **Cross Plot**. The graph will look like:
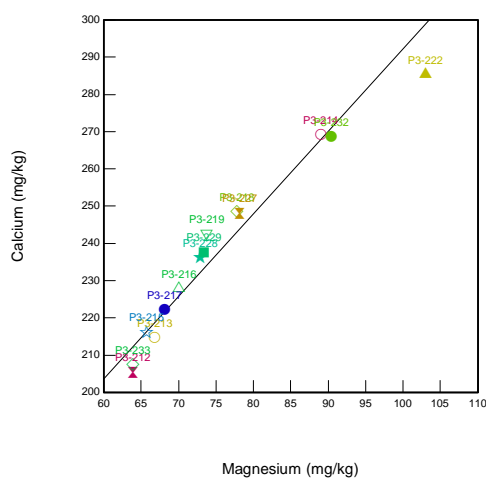
You can select the analytes to appear on the axes, as well as the samples to include in the plot on the Data Sheet, before making the plot, or along the right side of the plot pane.

Clicking on **Advanced Options…** on the control panel, you can set the axes to linear and logarithmic scales, and choose to superimpose a regression line on the plot.
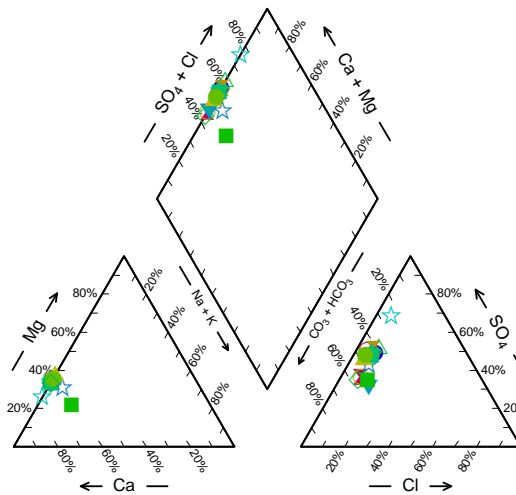
Ternary Diagrams

Ternary (or trilinear) diagrams show sample composition in terms of three analytes. For example:
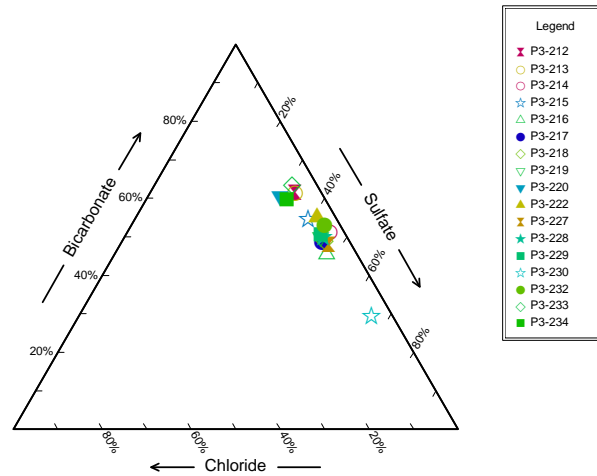
Set the three axes and samples to include on the Data Sheet, or in the control panel along the right of the pane. You also set the units on the control panel.
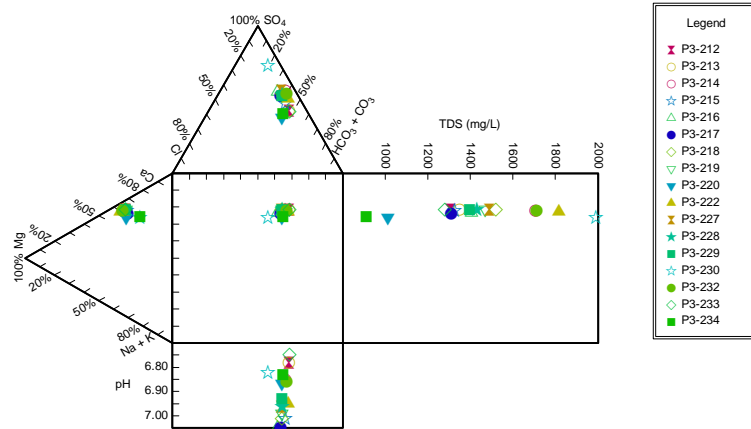
Piper Diagrams

Piper diagrams show the major ion compositions of any number of samples:

Select the samples to include on the Data Sheet, or on the control panel to the right of the plot pane. Click on the ✓ button on the control panel to include all of the samples from the Data Sheet.

Durov Diagrams

Durov diagrams represent the major ion composition, pH, and TDS content of any number of samples:

Select the samples to include on the Data Sheet, or on the control panel to the right of the plot pane. You control the pH and TDS ranges on the plot by clicking on Advanced Options… and moving to the [Durov Diagram] pane.

Schoeller Diagrams

Schoeller diagrams represent the compositions of any number of samples in diagrams that look like:
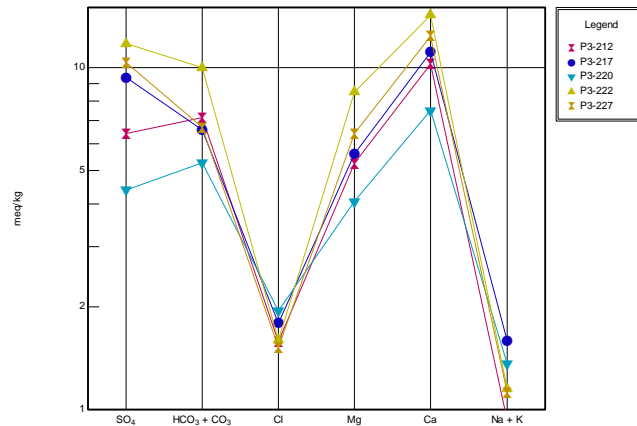
Select the samples to include on the Data Sheet, or on the control panel to the right of the plot pane. You set the units and value range for the vertical axis by clicking on **Advanced Options…** and moving to the [Schoeller Diagram] pane.

Stiff Diagrams

Stiff diagrams show the composition of a single sample, in terms of common cation and anions, with concentration represented in electrical equivalents. Select a sample on the Data Sheet, then select **Stiff Diagram** on the [New Graph] pulldown menu. A Stiff diagram looks like:
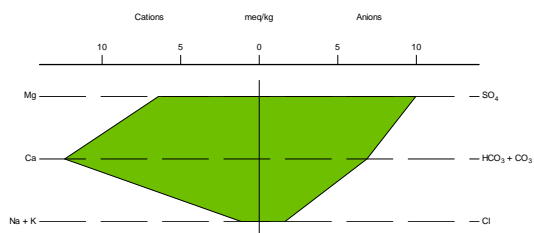
You can cycle through the samples on the Data Sheet by clicking on the ➜ and ⬅ buttons.

Radial Plots

Radial plots are similar to Stiff diagrams, except that composition is plotted along axes arrayed like spokes on a wheel. They look like:
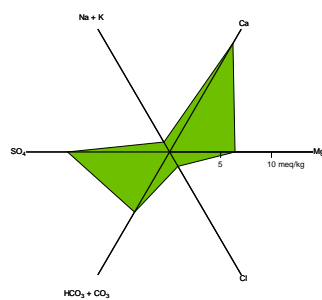
Ion Balance Diagrams

Ion balance diagrams show the cationic and anionic composition of a sample, in terms of electrical equivalents. You select a sample on the Data Sheet and make a graph by clicking on [New Graph] and choosing **Ion Balance Diagram**. The diagrams look like:
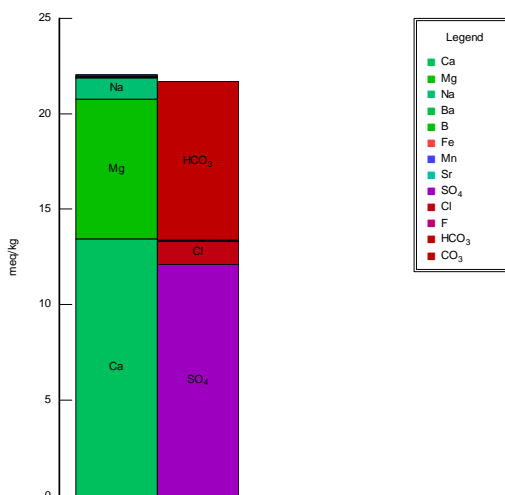
Unlike the ion balance calculations on the Data Analysis pane, Aq•QA ion balance diagrams do not include the effects of carbonate speciation, nor do they account for the free concentrations of the ions H^+ and OH^-.

Pie Charts

Pie charts are similar to ion balance diagrams, except that ion concentrations are represented in terms of electrical equivalents as wedges that fit together into a circle. Example:
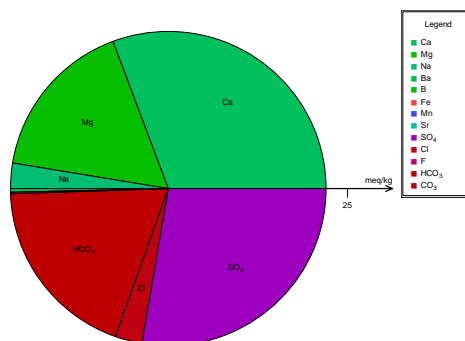
Unlike the ion balance calculations on the Data Analysis pane, Aq•QA pie charts do not include the effects of carbonate speciation, nor do they account for the free concentrations of the ions H^+ and OH^-.

Copying a Graph to Another Document

To copy a graph to another document, move to the Aq•QA pane containing the graph in question and select **Edit → Copy**, or touch **ctrl**+**C**. This will copy the graphic image to the clipboard. Now move to the target application and paste the image into your document.

You will be able to edit the graphic elements of the image as you would any vector graphic. To do so, select the graphic in your illustration program and then select the ungroup option. You may need to ungroup the graphic twice.

You can also copy the image to the clipboard as a bitmap, instead of as vector graphics, by selecting **Edit → Copy As Bitmap**. You will be able to edit the image as a bitmap, using programs such as Microsoft® Paint or Adobe® Photoshop®.

Saving Graphs

You can save any graph you make in Aq•QA as a graphic image that you can later edit in an illustration program, or import into other documents. Once you have created a graph you wish to save, make sure you are on the Aq•QA pane containing the graph and click on **File → Save Image As…**.

On the resulting dialog, you can save the graphic image as either a Windows® Enhanced Metafile, a Windows® bitmap, or an Encapsulated PostScript (EPS) file. Enhanced Metafiles are convenient formats for importing to Microsoft® Office® files, such as PowerPoint® presentations and Word® documents. EPS files can be opened directly for editing in Adobe® Illustrator®.

To edit an Aq•QA graphic in an illustration program, you select it and then ungroup its graphic elements. You may need to ungroup the object twice.

Tapping Aq•QA®'s Power

About Tapping Aq•QA®'s Power

As you become proficient with Aq•QA®, you will want to take advantage of more of its capabilities. The sections below explain how to do so.

Template for New Data Sheets

When you create a new Aq•QA document by selecting **File → New**, the initial, empty Aq•QA Data Sheet that appears is a "template". A template is simply a .aqq file, generally containing a list of analytes, but no data.

When you install the Aq•QA software, the default template is included in directory your installation directory (for example, in directory "\Program Files\AqQA"). The default template is named "default.aqq".

You may want to create your own template, or several, for the Aq•QA documents you create. For example, you may want to set a special list of analytes, in a certain order, with specific units.

To do so, create a new Aq•QA Data Sheet (**File → New**) and configure it as you wish. Save the file in a convenient location (**File → Save As…**).

Open the Preferences dialog by selecting **File → Preferences…** . In the box labeled **Template for New Data Sheets**, click on the **Browse…** button, and select the .aqq file you have just saved.

If you maintain several templates, you can change among them in this manner.

Exporting the Data Sheet

You may wish to export the contents of the data sheet to another program, such as Microsoft® Excel®. To do so, select **File → Export Data…** . From this dialog, you can choose to save the data as a tab delimited or comma delimited text file, which you can open in Excel.

Subscripts, Superscripts, and Greek Characters

You can include superscripts, subscripts, and Greek letters in character strings in your Aq•QA document. To set a character as superscript, for example, highlight it, right-click, and select **Superscript**.

You set subscripts, unscripted characters (neither subscript not superscript), greek, and roman characters in the same fashion.

Analyte Symbols

Aq•QA by default labels analytes by name, using strings such as "Sodium", "Potassium", "Dissolved Solids", and so on. You can also view analytes by their familiar chemical symbols: "Na", "K", "TDS", etc.

To change between viewing analytes by name or symbol, toggle the **View → Show Analyte Symbols** switch.

Colors and Markers

Each analyte can have associated with it a color and a marker, as can each sample. The color and data marker are used when creating graphs. By default, Aq•QA chooses the color and marker automatically, but you can associate specific choices with a given analyte or sample.

To assign a color and marker to an analyte, select it (or more than one), then choose a color from **Analytes → Analyte Color**, and a marker from **Analytes → Analyte Marker**. Alternatively, select one or more analytes and right-click to choose the color and marker.

Similarly, assign a color and marker to one or more samples by clicking on **Samples → Sample Color**, and a marker from **Samples → Sample Marker**, or by right-clicking.

Calculated Ions

Aq•QA can in its graphs display the concentrations of several "calculated ions" such a $Na^+ + K^+$, the sum of the sodium and potassium ions, and $HCO_3^- + CO_3^{2-}$, the sum of the bicarbonate and carbonate ions. By selecting **Graphs → Calculated Ion Settings…**, you can change the label, color, and symbol associated with each of these analytes.

Hiding Analytes and Samples

If your Data Sheet contains a large number of samples or analytes, you may wish to temporarily exclude some of your data from being displayed.

To hide one or more samples, select the samples to hide and select **Samples → Hide**. To restore the display, select **Samples → Show All**.

Similarly, to hide or re-display analytes in the Data Sheet, select
Analytes → Hide and **Analytes → Show All**.

Selecting Display Fonts

You can change the fonts and font sizes in the Data Sheet and Data
Analysis panes to suit your needs. Open the Preferences dialog (select
File → Preferences…). In the boxes labeled **Data Sheet** and **Data
Analysis**, you can select the font and point size for each pane.

Searching the Data Sheet

To search the Data Sheet for a character string, select **Edit → Find…**
and enter the string in the dialog box that appears. You can then search
forward or backward for the next occurrence of the string by selecting
Edit → Find Next or **Edit → Find Previous**.

Arrow Key Behavior During Editing

When you are editing a field in the Data Sheet, the left and right arrow
keys on your keyboard can function in one of two ways: they can move
to the preceding or next character in the field, or the can move to the
preceding or next field in the Data Sheet.

You can set the behavior you prefer by opening the Preferences dialog
(select **File → Preferences…**). In the box labeled **Data Sheet**, select the
option you prefer. You can toggle between options at any time by
touching **Shift+F2**.

Sorting Samples and Analytes

You can use Aq•QA's sort function to arrange the rows and columns in
your Data Sheet. To sort the samples, select **Samples → Sort…** and
choose an option under **Sort by:**. Depending on the option you select,
you can sort sample rows or columns according to any of the analytes on
your Data Sheet, such as Sample ID, the date or time, or by the numerical
value of any of the chemical analytes.

To sort the analytes on your Data Sheet, select **Analytes → Sort**. This
function will arrange the analytes in alphabetical order within the various
categories (Inorganic, Organic, and so on).

"Tip of the Day"

When you start Aq•QA, a dialog box appears with a suggestion on how
to use various features in the program. If you grow tired of seeing this
"tip of the day", uncheck the box labeled **Show Tips at Startup**.

You can resume seeing tips by re-selecting this option on the Preferences
dialog (select **File → Preferences…**).

Appendix: Carbonate Equilibria

About Carbonate Equilibria

This Appendix describes how Aq•QA® accounts for carbonate equilibria when figuring alkalinity, carbonate mineral saturation, CO_2 partial pressure, and so on.

Aq•QA assumes that a water's carbonate concentration [Tot-CO_3] is distributed among the three chemical species CO_2(aq), HCO_3^-, and CO_3^{2-}. In general, [Tot-CO_3] is the sum of the individual species concentrations, or [HCO_3] + [CO_2] + [CO_3]. In this section, the notation [] refers to molal concentration.

Necessary Data

To account for carbonate equilibria, Aq•QA needs to find on the Data Sheet a value for pH as well as a measure of the total carbonate concentration [Tot-CO_3].

Aq•QA takes the value for [Tot-CO_3] from an analysis reported for bicarbonate, carbonate, or carbon dioxide (or the molar sum of these values, if more than one is specified). If none of these analytes is present on the Data Sheet, Aq•QA takes [Tot-CO_3] as the carbon concentration, assuming that most of the carbon in solution is present in oxidized form. Lacking an analysis for carbon, the program figures [Tot-CO_3] from a reported value for alkalinity

Activity Coefficients

Each species in solution has an activity coefficient γ, calculated as follows. The solution's ionic strength is determined in molal units by summing over the charged inorganic analytes, according to

$$I = \frac{1}{2}\sum m_i z_i^2$$

Here, m_i is the species' molal concentration and z_i is its electrical charge (i.e., 2 for Ca^{2+}, –1 for HCO_3^-, etc.). Wherever possible, Aq•QA in calculating ionic strength accounts for the speciation of carbonate to form the species HCO_3^- and CO_3^{2-}. The program also accounts for the contributions of the species H^+ and OH^-, where pH is known.

For each charged species (everything except $CO_2(aq)$), the activity coefficient γ_i is given by the extended Debye-Hückel equation

$$\log \gamma_i = -\frac{A z_i^2 \sqrt{I}}{1 + \mathring{a}_i B \sqrt{I}}$$

where z_i is its electrical charge and $\mathring{a}_i$ is the ion size parameter:

	$\mathring{a}_i$
CO_3^{2-}	4.5
H^+	9
HCO_3^-	4.5
Ca^{2+}	6

The values of A and B vary with temperature (°C) according to

$$A = .4922 + .0003714\,T + 1.083\times10^{-5}\,T^2 - 4.821\times10^{-8}\,T^3$$
$$+ 1.208\times10^{-10}\,T^4$$

and

$$B = .3247 + .0001224\,T + 7.658\times10^{-7}\,T^2 - 2.908\times10^{-9}\,T^3$$
$$+ 5.507\times10^{-12}\,T^4$$

The activity coefficient for the uncharged ion $CO_2(aq)$ is taken as one.

Apparent Equilibrium Constants

The apparent equilibrium constants (K') for the reactions among the three species are calculated from the actual equilibrium constants (K) and the species' activity coefficients, according to

$$CO_2(aq) + H_2O \leftrightarrow H^+ + HCO_3^-$$
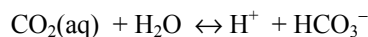
$$\log K_1 = -6.549 + .009002\,T - .0001021\,T^2$$
$$+ 2.762\times10^{-7}\,T^3 - 3.561\times10^{-10}\,T^4$$

$$K_1' = K_1 \cdot \frac{\gamma_{CO2}}{\gamma_{HCO3}} = \frac{[HCO_3^-]\,10^{-pH}}{[CO_2]}$$

and
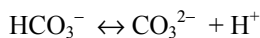
$$HCO_3^- \leftrightarrow CO_3^{2-} + H^+$$

$$\log K_2 = -10.61 + .01277\,T - .0001203\,T^2$$
$$+ 3.017\times10^{-7}\,T^3 - 2.694\times10^{-10}\,T^4$$

$$K_2' = K_2 \cdot \frac{\gamma_{HCO_3^-}}{\gamma_{CO_3^{2-}}} = \frac{[CO_3^{2-}]10^{-pH}}{[HCO_3^-]}$$

Here, T represents temperature in °C.

Speciation

Aq•QA calculates the distribution of carbonate among the species by rewriting the mass action equations above as follows:

$$[CO_2] = \frac{[HCO_3^-]10^{-pH}}{K_1'}$$

and

$$[CO_3^{2-}] = \frac{K_2'[HCO_3^-]}{10^{-pH}}$$

Then, the mass balance equation

$$[Tot\text{-}CO_3] = [CO_2] + [HCO_3^-] + [CO_3^{2-}]$$

can be expressed

$$[Tot\text{-}CO_3] = \frac{[HCO_3^-]10^{-pH}}{K_1'} + [HCO_3^-] + \frac{K_2'[HCO_3^-]}{10^{-pH}}$$

Knowing the pH and the free concentration of the HCO_3^- species, then, Aq•QA uses this equation to calculate the total carbonate concentration directly. Likewise, knowing pH and [Tot-CO_3], it calculates the HCO_3^- concentration

$$[HCO_3^-] = [Tot\text{-}CO_3] \bigg/ \left(\frac{10^{-pH}}{K_1'} + 1 + \frac{K_2'}{10^{-pH}} \right)$$

and from it the concentrations of $CO_2(aq)$ and CO_3^{2-}.

Titration Alkalinity

Titration alkalinity is a measure of the ability of a water to resist acidification as strong acid is added. The two species HCO_3^- and CO_3^{2-} are taken to provide alkalinity. Each mole of HCO_3^- can neutralize one equivalent of acid by reacting to form $CO_2(aq)$, and each mole of CO_3^{2-} can likewise neutralize two equivalents of acid.

Titration alkalinity is generally reported as an equivalent mass of $CaCO_3$ per kg solution, even though $CaCO_3$ isn't involved in an alkalinity titration. Each mole of $CaCO_3$ can neutralize two equivalents of acid, and the mole weight of calcium carbonate is 100.09 g/mol. Hence, the alkalinity in units of mg $CaCO_3$/kg solution is related to the molal concentrations of the two species by

$$\text{Alk} = 1000 \times \frac{50.05}{(1-10^{-6} \times \text{TDS})} \times \left([\text{HCO}_3^-] + 2\,[\text{CO}_3^{2-}] \right)$$

Or, substituting,

$$\text{Alk} = 1000 \times \frac{50.05}{(1-10^{-6} \times \text{TDS})} \times \left([\text{HCO}_3^-] + 2\,\frac{K_2'\,[\text{HCO}_3^-]}{10^{-p\text{H}}} \right)$$

The free HCO_3^- concentration, then, can be calculated from the alkalinity according to

$$[\text{HCO}_3^-] = \text{Alk} \left/ \left[1000 \times \frac{50.05}{(1-10^{-6} \times \text{TDS})} \times \left(1 + \frac{2\,K_2'}{10^{-p\text{H}}} \right) \right] \right.$$

From this value, the free concentrations of CO_3^{2-} and $\text{CO}_2(\text{aq})$ can be determined immediately.

Mineral Saturation

The minerals calcite and aragonite have the same chemical composition (CaCO_3), but different chemical structures. The saturation indices of these minerals

$$SI = \log Q/K = \log Q - \log K$$

tells whether they are supersaturated ($SI > 0$), saturated ($SI = 0$), or undersaturated ($SI < 0$). Here, Q is the ion activity product, and K the equilibrium constant.

For calcite, the reaction

$$\text{Calcite} \leftrightarrow \text{Ca}^{2+} + \text{CO}_3^{2-}$$
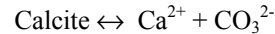
has an equilibrium constant vs. T (°C) given by

$$\log K = -8.539 - .001499\,T - .0001263\,T^2$$
$$+ 4.477 \times 10^{-7}\,T^3 - 6.883 \times 10^{-10}\,T^4$$

For aragonite, the reaction and equilibrium constant are

$$\text{Aragonite} \leftrightarrow \text{Ca}^{2+} + \text{CO}_3^{2-}$$
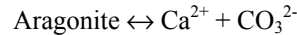
$$\log K = -8.371 - .001671\,T - .0001253\,T^2$$
$$+ 4.466 \times 10^{-7}\,T^3 - 6.884 \times 10^{-10}\,T^4$$

In each case, the ion activity product is determined by the activity coefficients and molal concentrations of the CO_3^{2-} and Ca^{2+} species:

$$Q = \gamma_{\text{CO3}}\,[\text{CO}_3^{2-}] \times \gamma_{\text{Ca}}\,[\text{Ca}^{2+}]$$

and the saturation index follows from the definition above.

CO₂ Partial Pressure

Knowing the free concentration of $CO_2(aq)$, the partial pressure of carbon dioxide can be calculated immediately from the reaction

$$CO_2(g) \leftrightarrow CO_2(aq)$$
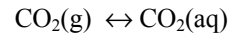
The log equilibrium constant for this reaction is given as a function of T (°C) as

$$\log K = -1.134 - .01363\, T + 6.614 \times 10^{-5}\, T^2$$
$$- 1.286 \times 10^{-7}\, T^3 + 7.348 \times 10^{-11}\, T^4$$

Since the activity coefficient for CO_2 is unity,

$$K = \frac{[CO_2]}{P_{CO2}}$$

the CO_2 partial pressure (in atm units) is

$$P_{CO2} = \frac{[CO_2]}{K}$$

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