17. Studio ScaleChem Interpreting Results

Overview

Studio ScaleChem reports and displays data in a variety of forms. This information can be confusing to a new user. In this chapter we will examine the various types of output and interpret the meaning of that output.

Some of the data that is reported are reported in summaries and other data are reported in dialog boxes. We will look at several examples of each.

Valid Water Analysis Data

Using valid water (brine) analysis data is the key concept behind using Studio ScaleChem. If the water analysis is not valid then the resulting calculations are not valid.

Assumptions

Reconciliations within the Water Analysis are assumed to be at ambient conditions, 77°F and 14.7 PSIA (25 °C and 1 atmosphere). The default temperature and pressure are set to ambient conditions.

Electroneutrality

Ionic concentrations, even when measured with the best available techniques, tend to have some degree of uncertainty associated with them. These uncertainties will results in an aqueous solution which, when the concentrations are summed together, appears to be not electrically neutral.

In addition to having uncertainties in the measured concentration, some ions may be misreported. For example, the pH of a solution may indicate that the dominant form of carbonate ion in solution should be bicarbonate ion but the reported value is carbonate ion. For the same mass, there is approximately twice as much negative charge in misreporting the carbonate ion.

Correcting for the Electroneutrality of a solution is essential for proper simulations. The following sample is not electrically neutral.

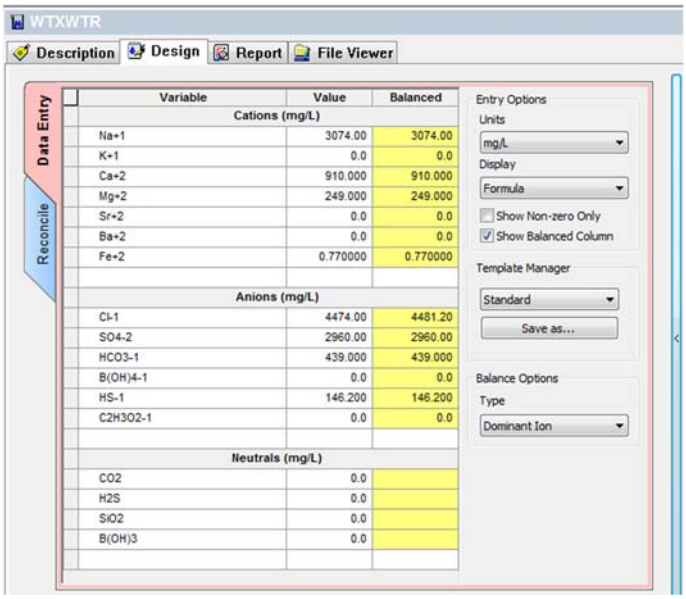


Figure 17-1 A non-electrically neutral sample

In Studio ScaleChem we will receive a report of the required amount of material required to balance the sample in the yellow column headed as Balanced. Stream is balanced as soon as the components are entered.

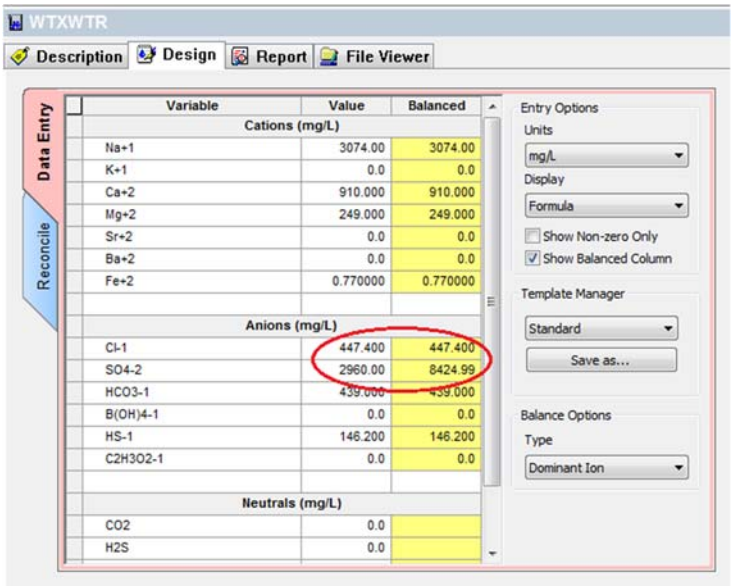


Figure 17-2 Switching of dominant ion

If Cl- quantity is change from 4474 to 447.4 then automatically SO4-2 ion becomes the dominant ion. And its balanced quantity increases by almost 5464

mg/L as opposed to 2960mg/L of SO4-2 ions.

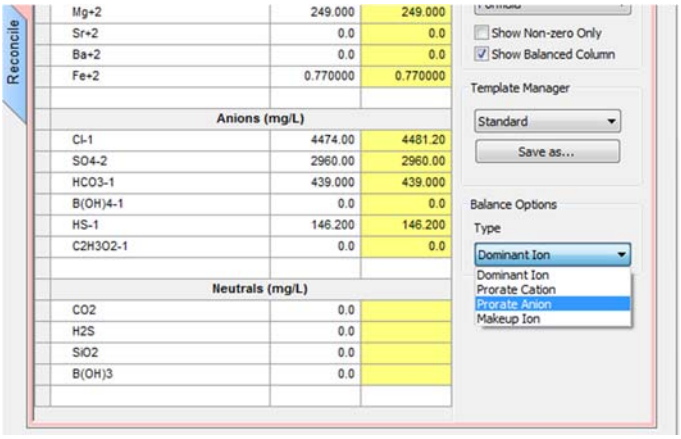


Figure 17-2a Balance options

This report shows us that 5464mg/l of SO4-2 ions must be added. Since the original sample only had 2960 mg/l of SO4-2 ion (see Figure 17-12a) there is probably an error.

In general, an added value of less than 10% of an ion concentration is acceptable. In this case we would have expected a value of less than 45 mg/l and that of chloride ion rather than Sulfate ion.

Another consideration is the type water that this analysis represents. This water is an aquifer water. The concentration of the sodium and chloride ions, on a mole basis, tends to be roughly equal. If we have 3074 mg/l of sodium (see Figure 17-1) or 134 mmoles (1000 mmoles =1 mole), then we would expect 4481 mg/l of chloride.

Therefore the concentration of the chloride seems to be in error. Perhaps a typographical error occurred either in the analysis or in the input. Change the value of the chloride concentration by increasing the number one order of magnitude from 447.4 mg/l chloride ion to 4474 mg/l chloride ion.

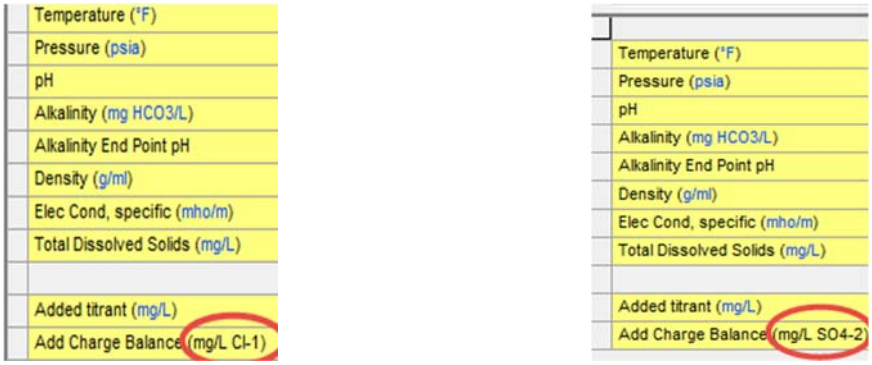


Figure 17-3 Reconcile tab when Chloride ion quantity is 4474 mg/L and Chloride ion is 447.4 mg/L(SO4-2 becomes adjustment parameter in the second image on the right).

Each species concentration has been altered.

Only the chloride concentration value changed

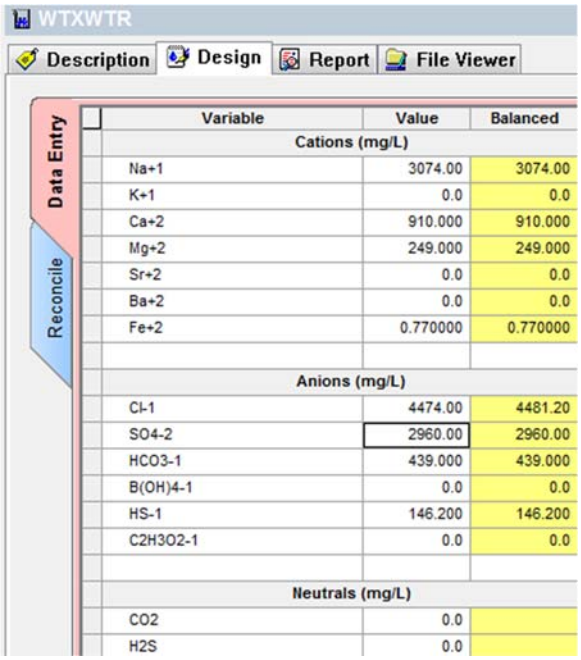


Figure 17-4 The chloride ion has been increased to 4474 mg/l

pH/Alkalinity

The pH of a solution is related to the alkalinity of the solution. In the simplest terms, the alkalinity is the acid neutralizing capacity of the solution. In practice we often refer to the alkalinity as the concentration of carbonate species in the sample.

The actual alkalinity experiment involves the titration of a known acid concentration against the sample. A predetermined Titration End Point (usually a pH of 4.5) is the end of the experiment. The Titration End Point is set sufficiently low to ensure that all of the neutralizing species in solution have been neutralized.

The pH/Alkalinity reconciliations have many options.

Reconciling pH/Alkalinity

The measured pH and alkalinity can be reconciled The user enters a measured pH and an alkalinity.

Alkalinity

The alkalinity can be entered as:
meq/l
mg/l as HCO3
mg/l as CaCO3

The units meq/l is the actual base capacity of the solution regardless of speciation. The units mg/l as HCO3 are the most common unit in the industry. It is important to note however, that the sample does not have to contain carbonates to have the alkalinity reported as HCO_3^-. The last unit, mg/l as CaCO3 is also used frequently.

Titration pH

The titration pH is the end point of the actual alkalinity experiment. Normally this value is a pH of 4.5. The only requirement here is that the alkalinity pH must be less than the measured pH. An error will occur if this is not true.

Clicking on ***Calculate*** will execute the procedure.

When the calculation is complete, Studio ScaleChem will report the values required to reconcile the sample.

The calculated pH is somewhat higher than the measured pH. HCl will have to be added to adjust the pH.

The calculated alkalinity is approximately 700 mg/l as HCO_3^-

The reconciled values are approximately 159 mg/l HCl added and 183 mg/l of CO_2 removed

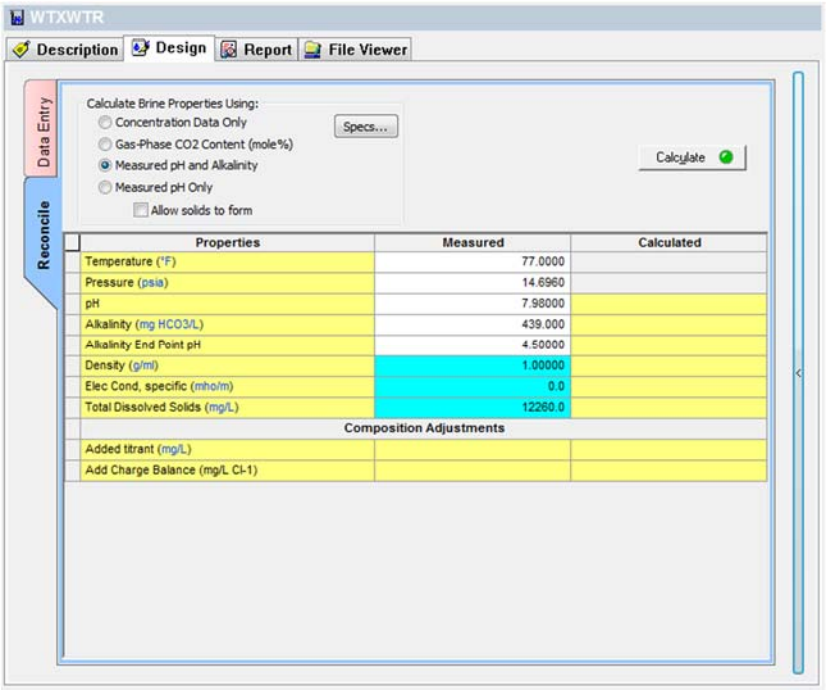


Figure 17-5 Reconciled pH and alkalinity

Calculating pH and Alkalinity

Sometimes it is desirable to determine the pH and alkalinity of the solution prior to reconciling.

Select the Equilibrium option

Click on ***Calculate*** to begin.

Studio ScaleChem will then return the calculated pH and alkalinity.

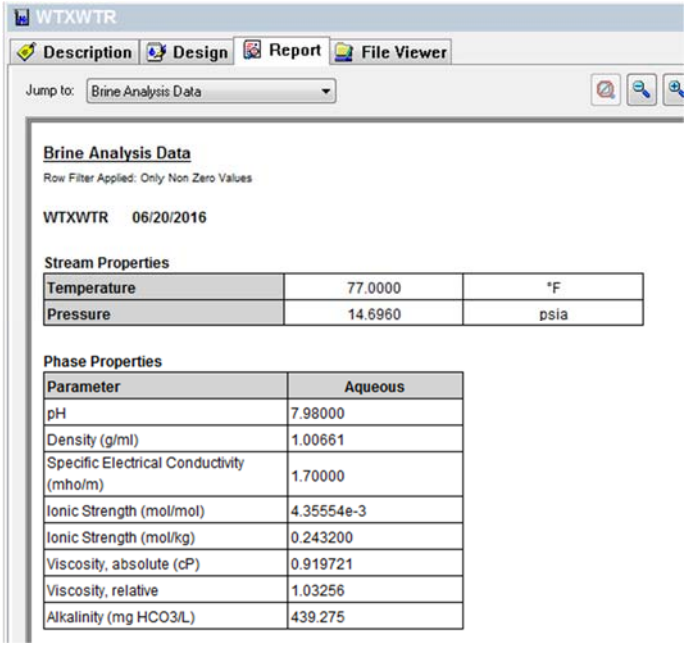


Figure 17-6 Calculated pH and alkalinity.

Speciation

The display of the ionic species can be altered to meet user requirements. By default the display of the ionic species are the standard list and the reconciled values.

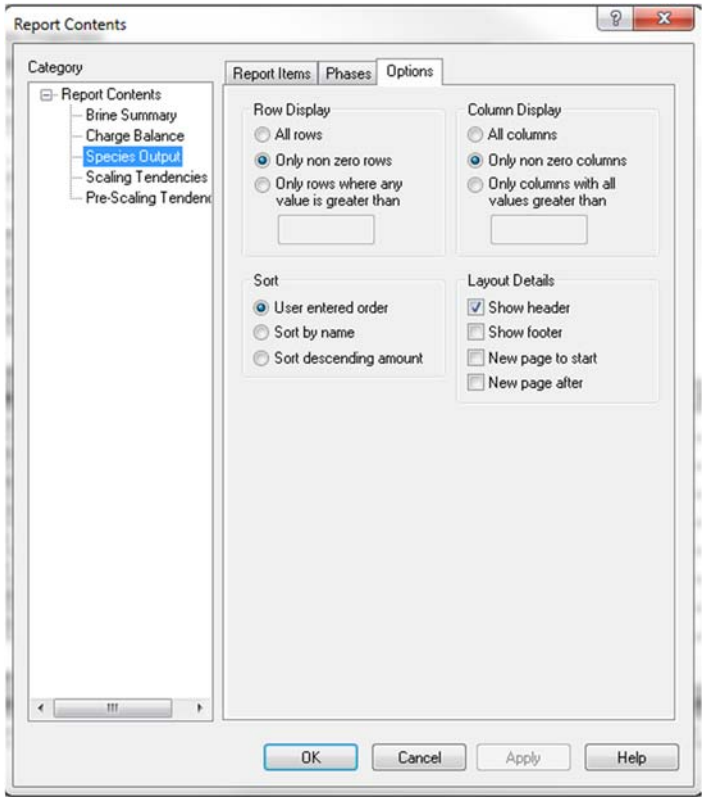
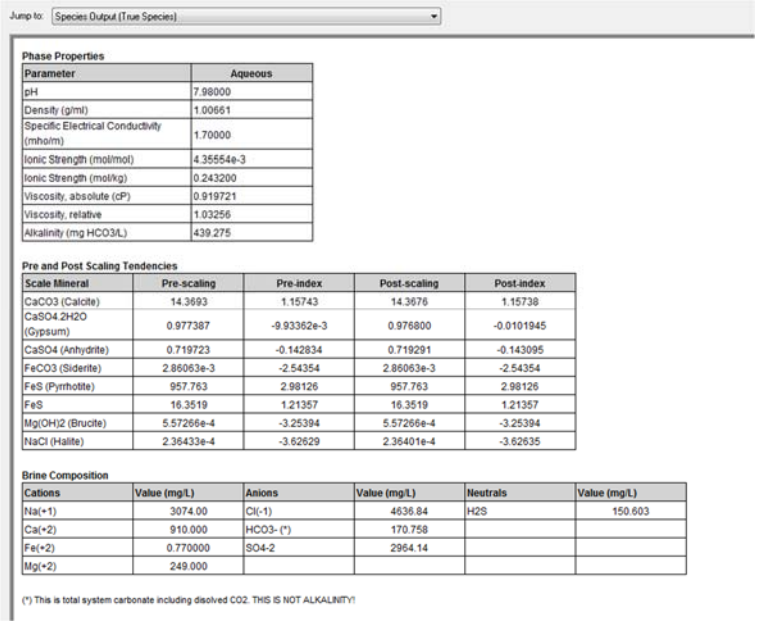


Figure 17-7 The default species display

Default Speciation Display

See **Chapter 2: Thermodynamics** for a more complete description of the standard chemistry.



Jump to: Species Output (True Species)

Phase Properties

Parameter	Aqueous
pH	7.98000
Density (g/ml)	1.00661
Specific Electrical Conductivity (mho/m)	1.70000
Ionic Strength (mol/mol)	4.35554e-3
Ionic Strength (mol/kg)	0.243200
Viscosity, absolute (cP)	0.919721
Viscosity, relative	1.03256
Alkalinity (mg HCO3/L)	439.275

Pre and Post Scaling Tendencies

Scale Mineral	Pre-scaling	Pre-index	Post-scaling	Post-index
CaCO3 (Calcite)	14.3693	1.15743	14.3676	1.15738
CaSO4.2H2O (Gypsum)	0.977387	-9.93362e-3	0.976800	-0.0101945
CaSO4 (Anhydrite)	0.719723	-0.142834	0.719291	-0.143095
FeCO3 (Siderite)	2.86063e-3	-2.54354	2.86063e-3	-2.54354
FeS (Pyrrhotite)	957.763	2.98126	957.763	2.98126
FeS	16.3519	1.21357	16.3519	1.21357
Mg(OH)2 (Brucite)	5.57266e-4	-3.25394	5.57266e-4	-3.25394
NaCl (Halite)	2.36433e-4	-3.62629	2.36401e-4	-3.62635

Brine Composition

Cations	Value (mg/L)	Anions	Value (mg/L)	Neutrals	Value (mg/L)
Na(+1)	3074.00	Cl(-1)	4636.84	H2S	150.603
Ca(+2)	910.000	HCO3- (*)	170.758		
Fe(+2)	0.770000	SO4-2	2964.14		
Mg(+2)	249.000				

(*) This is total system carbonate including disolved CO2. THIS IS NOT ALKALINITY!

Figure 17-8 The standard display

Expanded Species Display

Click on Customize under the report tab. Click on ***Species output*** and then by checking boxes before the species name will display ***Species List***. Click on ***OK*** to redisplay the **Report** tab.

The expanded species lists are scrollable

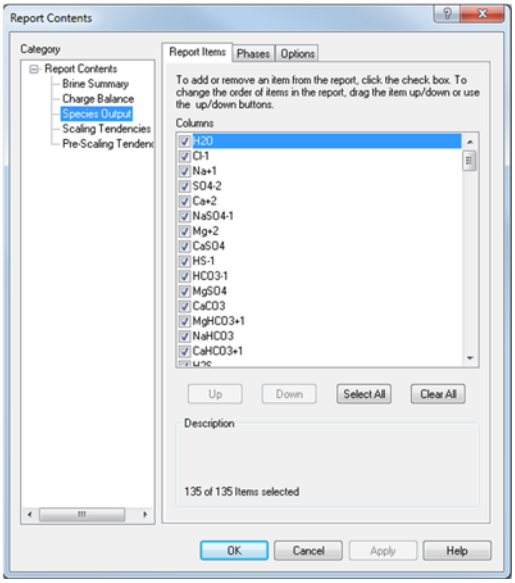


Figure 17-9 Displaying the Expanded Species lists

The complete list of the expanded ions can be found in **Chapter 2: Thermodynamics.**

The Non-Zero species Display

Sometimes viewing species with zero concentrations can be difficult to read. The Species Display dialog allows the user to mask zero valued species. Customize report-> Species Output->Options leads to display options where we can select to

view species only greater than value 0. Column and rows are adjustable according to the user's preference.

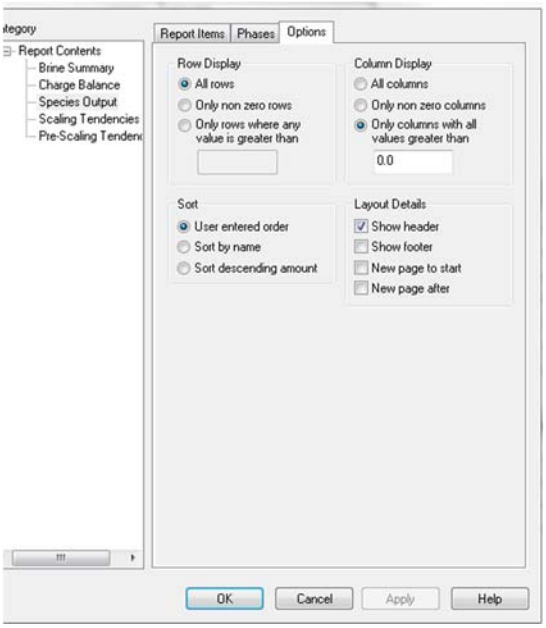


Figure 17-10 Water Analysis with zero values masked

Supersaturation of Solids

Frequently a measurement of a water sample (brine) may have a small uncertainty associated with the measurement. This uncertainty, especially when the sample was in contact with solid minerals, may lead to Studio ScaleChem reporting that the sample is supersaturated.

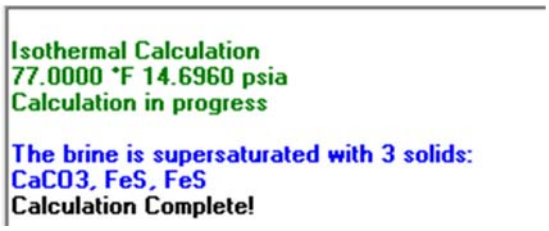


Figure 17-11 A warning that the sample is supersaturated.

Summary Content

Reconciliation summary

Water Analysis

The results of a reconciliation for pH, alkalinity and neutrality are reported for each sample.

This field has been "Scrolled Down" to display the dew point temperature

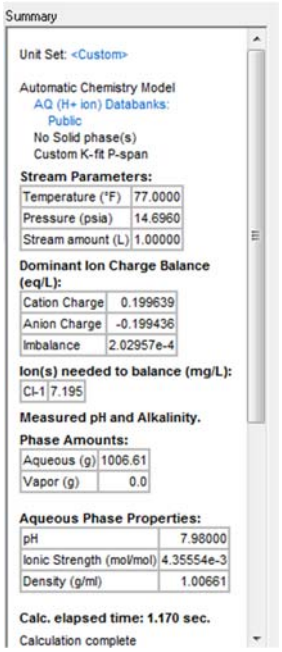


Figure 17-12 The summary for a water analysis

Gas Analysis

The information that can be displayed for a gas analysis is rather limited. Unless a **Dew Point** calculation had been performed, the output is an echo of the input.

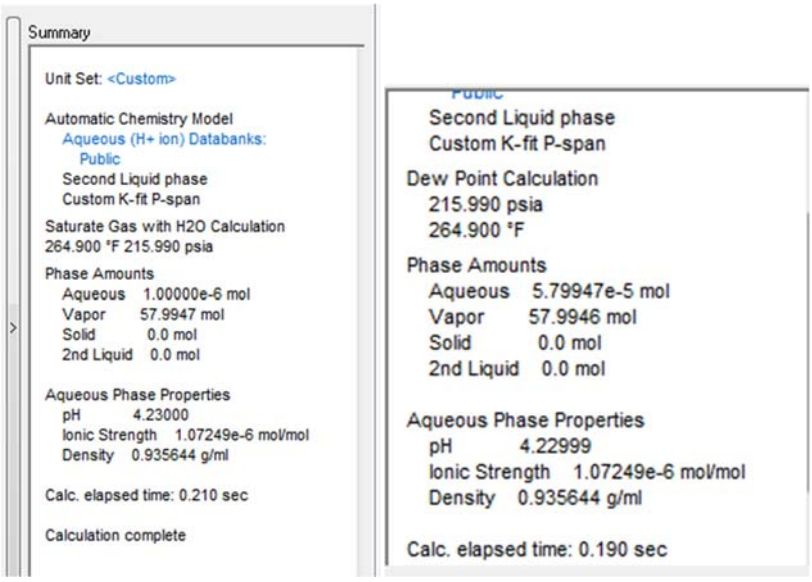


Figure 17-13 Gas Analysis Summary and the Dew Point summary

Node Summary

The brines and/or gases collected at the node are displayed along with the flow rate of each item. The temperature and pressure of the node is also displayed.

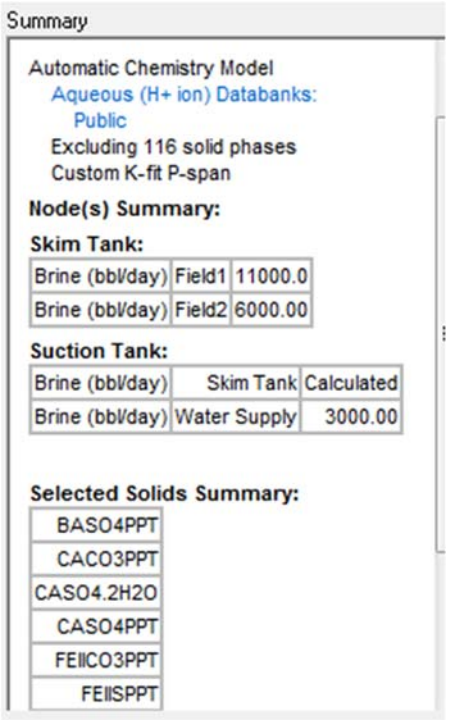


Figure 17-14 Node Summary Report

Overview of Studio ScaleChem Output

There are three types of output which a user can request after a Studio ScaleChem calculation: Plot, Reports, or File Viewer.

Summaries

Summaries is the default Studio ScaleChem output. It is located on the right most corner of the software window under the calculate button.

After a successful calculation, internal files produced by the OLI Solver are scanned for available sections of data which can be viewed. A list of the available sections is displayed when customize section is clicked open under the reports tab. This includes check boxes which can include, or eliminate a section in the report.

Report Section Selection

Clicking on the individual check boxes toggles between including and eliminating that section from the report.

Facilities Summary

Report for each node and dropped phases are shown.

Pre-Scaling tendencies

Solids to be displayed can be chosen from an extensive list of possible precipitants.

Scaling Tendencies

Sorting options are more to choose from. TRANGES can be displayed. The solids analysis gives a report of the solids which precipitated (Scaled out), and of the pre-precipitation and post-precipitation scaling tendency.

If the solid was not selected as a possible precipitate, but if the scaling tendency is greater than 1.0E-04, the solid is included in the analysis list. The amount of solid precipitated is left as 0.0, and the scaling tendency is reported.

Survey Parameters

Stream Amount, Temperature, pressure etc is reported.

OLI Speciation Report

When this report is available, the full speciation which the OLI Solver uses to perform an equilibrium calculation is given. This report is activated by requesting detailed output, using the Tools… Options menu choice.

Convergence Pattern

When this report is available, the mathematical convergence pattern which was used in performing the equilibrium calculation is given. This report is not normally requested. It is included as a debugging aid when trying to identify convergence problems. This report is activated by requesting detailed output, using the Tools.. Option menu choice.

Plot

To view Studio ScaleChem Plot Options click on Plot tab. This is located next to the design tab. This will show a default plot.

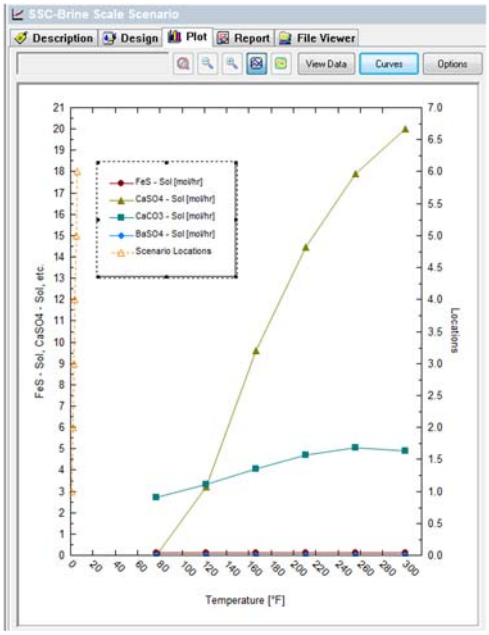


Figure 17-15 Displaying the Default plot

Determining the Default Plot

After returning from the OLI Solver, Studio ScaleChem analyzes the output file to determine an acceptable default plot. The precedence followed is this:

X axis Variable	Y axis variable
If the temperature varying, use Temperature else if Pressure varying, use Pressure else use Case number or Mix Ratio	If any precipitates, use the solids else user any pre-scaling indices > 0 to a maximum of 8 variables

Viewing Data

The data which is used to create the plot can be viewed by using the View Data button. In general, the View Data button shows the report which has been created. Use the View Plot button to return to the plot.

Selecting Data

To add to the variables displayed or to change the variables which are displayed, use the Select Data button, which is to the right of the Plot. Right click on the X or Y axis will pop up a format plot window. It has options like Format X-axis, Adjust Scale, Label Axes etc. Curves Button will prompt a Select data window.

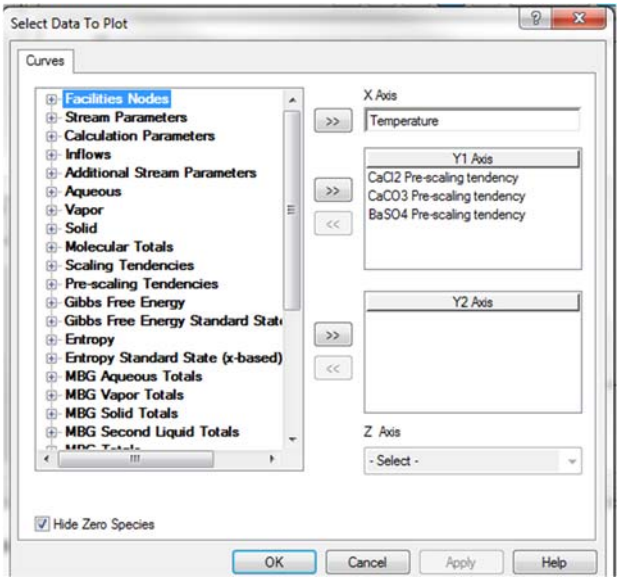


Figure 17-16 Selecting Data

Data Available

The list of variables which can be displayed are shown as Data Available. Stream parameters include Temperature and Pressure etc. Additional Stream parameters contain density, viscosity etc.

Selecting Data

To select different X and Y axis variables, highlight the variable in the Data Available box, and then click on >> button either before X or Y Axis. Of course,

variables can also be removed from the axis variables by highlighting the selected variable, and clicking the << button.

Minimum Data Required

A minimum of one X variable and one Y variable must be selected from the Select Data facility, in order to leave Select Data. Of course, you always have the option of canceling, and returning to the original plot.