15. Studio ScaleChem Getting Started

Terminology

Before we can discuss how to use Studio ScaleChem we must first discuss some terms. This will help us define some of the concepts in Studio ScaleChem that will be expanded in later sections.

Analysis

There are three analysis types, brines gases, and Oils. Each type must be reconciled.

Brines

Studio ScaleChem refers to all waters and aqueous samples as brines. A brine can be a surface water, an injection water, a formation water, a production water or any other type of aqueous fluid you can create. Brine compositions are entered in terms of ionic concentrations. In addition, the brine pH, density and alkalinity are also specified.

A brine is entered by means of the **Add Water** function, located in the ***Analyses*** menu.

Gases

A gas is any hydrocarbon mixture which may or may not contain water, carbon dioxide or hydrogen sulfide. The default hydrocarbon is methane (CH_4) but the hydrocarbon list may be expanded to include higher carbon numbers.

A gas is entered by means of the **Add Gas** function, located in the ***Analyses*** menu.

Oils

An oil is a non-aqueous phase. The oil sample may consist of pure component hydrocarbons (e.g., alkanes), distillation data, pseudocomponent or all three.

A hydrocarbon is entered by means of the Hydrocarbon function, located in the Analyses menu.

Reconciliation

Corrections must be made for deficiencies in the sample measurements.

Electroneutrality

Due to the nature of experimentation, most, if not all water analyses are incomplete or inaccurate in some manner. Thus, no analysis is electrically neutral. Yet, a real water must be. To solve this problem Studio ScaleChem reconciles each brine analysis for Electroneutrality or charge balance. The reconciliation method will be discussed in a later section.

pH

Many brines have a measured pH. This pH may or may not match the Studio ScaleChem-calculated pH. The cause may be an incomplete and/or inaccurate brine description. Studio ScaleChem reconciles this difference by adding or removing HCl and CO2 to match the measured pH.

Alkalinity

Alkalinity is a brine's capacity to absorb acid to a given pH. In oilfield applications, this pH is 4.5, and the alkalinity is referred to as the Carbonate alkalinity.

The standard alkalinity measurement involves titrating the brine with a known acid to 4.5 pH. Studio ScaleChem performs a mini-titration on the brine to 4.5 (or specified) pH. It then:

1. Calculates the alkalinity for the given water analysis
2. Adjusts HCl and CO2 inflow to match the calculated alkalinity with the reported alkalinity

CO_2 Fraction in Gas

Frequently it is simpler and more stable to measure the gas-phase CO_2 that is separated from the brine at the sampling point. When matched with another measured variable, usually alkalinity, the concentration of the carbonate species and the pH can be calculated. Studio ScaleChem performs a CO2 gas fraction calculation by taking the PCO2 and the calculated alkalinity (based on the water analysis data) to reconcile the system for pH and carbonate properties.

Scaling Tendency

The scaling tendency is defined as the ratio of the activity product to the solubility product for a particular solid. This ratio is related to the saturation index.

When this ratio is greater than 1.0, then there is a thermodynamic tendency for this solid to form. When less than 1.0 then there is no thermodynamic tendency for the solid to form.

The Activity product is the product of all the species on the right hand side of the equation, also known as the Available ions.

The solubility product, usually represented as K_{sp} is the thermodynamic equilibrium constant and is a function of temperature and pressure.

Calculating a Scaling Tendency

The Scaling Tendency is defined as the ratio of the activity product of an equilibrium equation to the solubility product for the same equation. We define the activity product as Q, therefore the Scaling Tendency (ST) = Q/K_{sp}.

As an example, consider the equilibrium for gypsum solubility. The chemical formula for gypsum is $CaSO_4 \bullet 2H_2O$ and the equilibrium expression is:

$CaSO_4 \bullet 2H_2O = Ca^{2+} + SO_4^{2-} + 2H_2O$

The activity product, Q, is defined as:

$Q = a_{ca++}\ a_{so4-2}\ a^2_{H2O}$

Where a_i is the activity of the species.

$$a_i = \gamma_i\ m_i$$

Where γ_i is the activity coefficient for species i. and m_i is the molal concentration.

The solubility product, K_{sp} is a thermodynamic quantity and is a function of temperature and pressure (although in most cases, the pressure functionality for solids can be ignored). Studio ScaleChem has stored the K_{sp} for all of the solids used in the chemistry model.

When the ratio Q/K_{sp} is greater than 1.0, then the solid has tendency to form. When the ratio is less than 1.0, then there is little tendency to form.

For example: consider a 0.01 molal solution of calcium sulfate at 25 C and 1 atmosphere.

The equilibrium concentrations are:

$[Ca^{+2}]$	=	0.008 molal
$[SO_4^{-2}]$	=	0.008 molal
γ_{Ca}	=	0.5
γ_{SO4}	=	0.5
a_{H2O}	=	0.99977
K_{sp}	=	2.68×10^{-5}

The Q value is:

$Q = (0.5)(0.008)(0.5)(0.008)(0.99977)^2$

The Scaling Tendency is Q/Ksp

ST = 0.000016/(2.68E-05) = 0.596

Thus the solution is under-saturated with respect to calcium sulfate.

Why are the concentrations of the ions not exactly equal to 0.01 molal (which is the feed concentration)? The neutral complex $CaSO_4^o$ exists and ties up 0.002 moles of each ion. The ions are not available for precipitation and thus do not appear in the scaling tendency calculation.

Calculating a Scale Index

The scale index is very much related to the Scaling Tendency. The relationship is:

Scale Index (SI) = Log_{10}(ST).

When the SI is less than zero (SI < 0), then the solid is said to be undersaturated. When the SI is greater than zero (SI > 0) then solid is said to be oversaturated.

Putting together a calculation

Now that we have defined some terms we are now ready to begin entering the information required to run a calculation. In this calculation we will be entering the concentrations of a single brine. This sample will be calculated at a range of

temperatures and pressures. The amount of any solids produced will be displayed graphically.

Starting the Studio ScaleChem Program

Studio ScaleChem can be accessed via the OLI Studio. Objects for Studio ScaleChem are Brine, Gas, Oil, Saturator and Contour plots.

To access these objects click on Streams in the Navigator and you will see these objects amongst others in the Actions Panel.

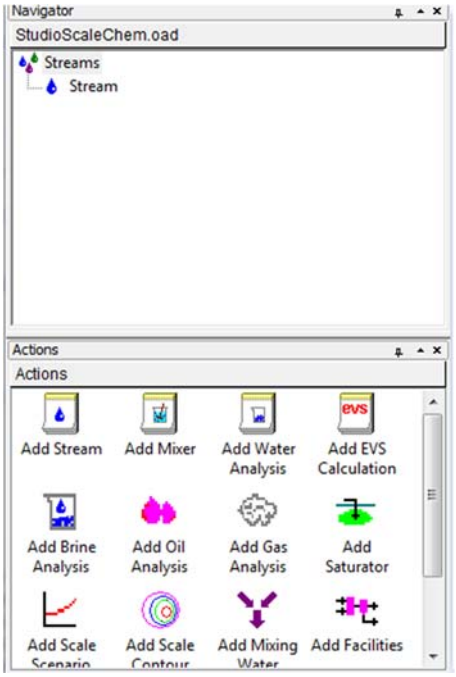


Figure 15-1 Studio ScaleChem objects.

Studio ScaleChem Tour

In this tour we will create a brine (water analysis) and calculate its scale tendency. Let's begin.

Add Brine Analysis from Actions Panel.

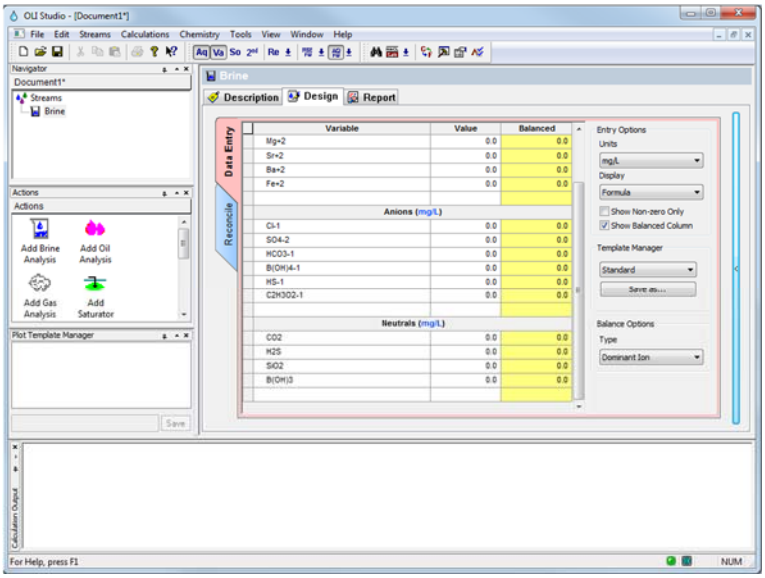


Figure 15-2 Brine Analysis

Brine Analysis Data

The chemistry of the brine needs to be entered. This information includes concentrations, alkalinity, pH and density.

Entering a brine description

Click on the description Tab. If the *Description* tab is not currently displayed, click on the tab.

Figure 15-3 Brine description tab

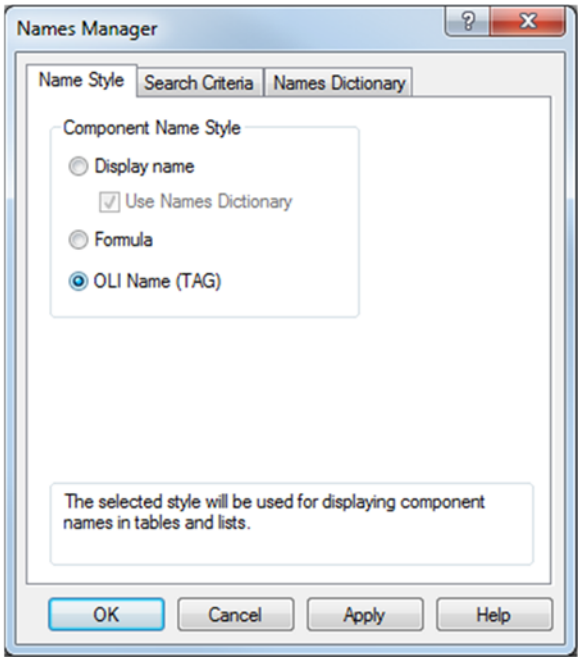
We can fill several items on this screen. All of the items (except the name) are optional.

Well	This name, if entered in a Well View calculation, is the name of the well. It is frequently blank.
Date	The date of the sample. Defaults to the current date.
Comments	Up to 256 characters may be entered as text to describe the well. Brief, direct comments are recommended.

Entering Brine Species

The Design Tab is where you enter the cations, anions and dissolved gases (or neutrals). The species formulas (default) or species names may be displayed. This display By Formula or By Name can be changed by clicking the names manager logo on the toolbar which looks like this:

A window will pop up where you can choose to select what display method you prefer. The pop up window will look like below:



Data entry tab under Design tab is designed to provide means to input cation/anion and neutrals composition.

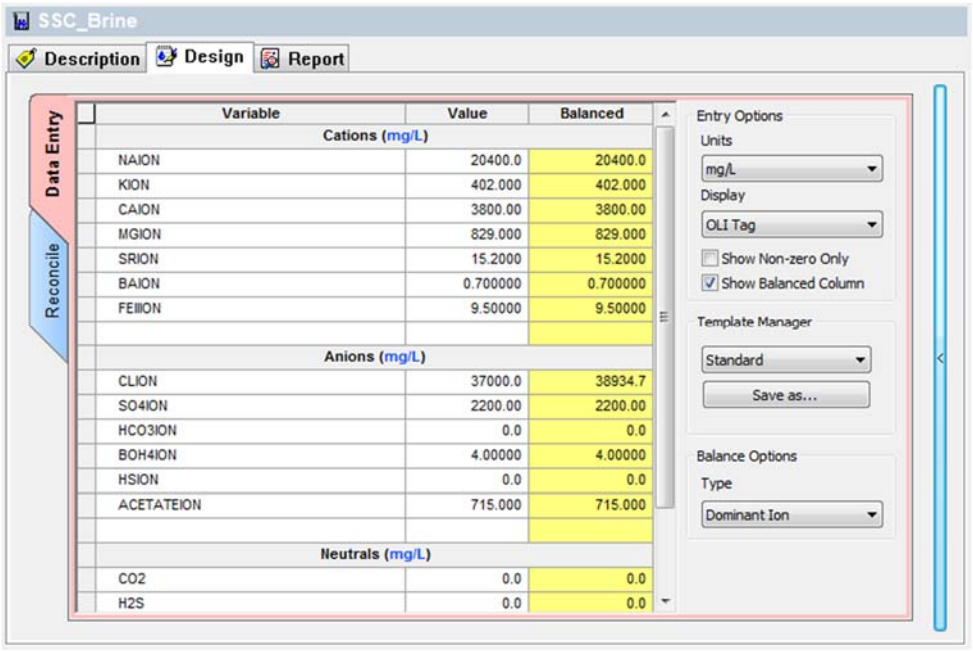


Figure 15-4 Brine data entry

Fields

Cations: The positive ions are entered in grid. The units may be changed by clicking on the Units button under entry options. The default units are mg/l (milligrams per liter).

Anions: This field is similar to the Cations field except that negative ions are added.

Neutrals: Neutral gases such as dissolved CO_2, H_2S and methane (CH4) are added. These dissolved gases do not affect the Electroneutrality of the sample but can have an overall affect on pH and alkalinity.

Reconcile tab: This tab gives options from three calculation types:-
Equilibrium calculation
CO2 Fraction in Gas
pH Alkalinity Reconcile

Entering Brine Species - Balance Button

It is highly unusual for the data to be electrically neutral. Therefore. samples are reconciled for Electroneutrality. After entering each species concentrations, you will notice that Balanced values show up in the column next to values. The Column header says Balanced.

Ionic samples measured experimentally are almost always not electrically neutral. Before we can proceed we must reconcile this sample for Electroneutrality.

Data Entry
Reconcile

Variable	Value	Balanced
Cations (mg/L)		
Na+1	20400.0	20400.0
K+1	402.000	402.000
Ca+2	3800.00	3800.00
Mg+2	829.000	829.000
Sr+2	15.2000	15.2000
Ba+2	0.700000	0.700000
Fe+2	9.50000	9.50000

Figure 15-5 Electroneutrality balance column

When adding or removing ions to balance charge, the solute mass is altered. We must make a decision as to whether we keep the mass of the solution constant (thereby adjusting the amount of water) or keeping the amount of water constant and adjusting the solution mass.

The user can select from a variety of balancing methods

Dominant Ions The deficient charged species with the largest concentration is added.

Proration Equal ratios of the deficient charge is added.

Make Up Ion The selected ion is either added or removed to balance the solution.

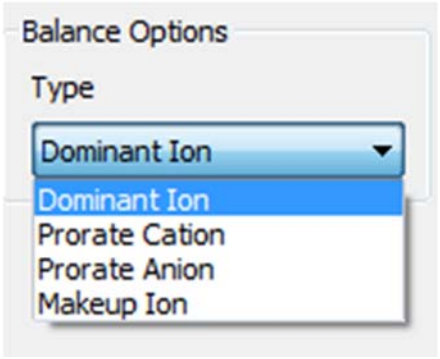


Figure 15-6 Balance Options

Reconciling a brine

We are now ready to reconcile the sample for pH and alkalinity.

Click the ***Reconciliations*** tab. Make sure if you are choosing the pH and Alkalinity type of calculation, you need to specify the HCO3 concentration in the grid under reconciliation tab.

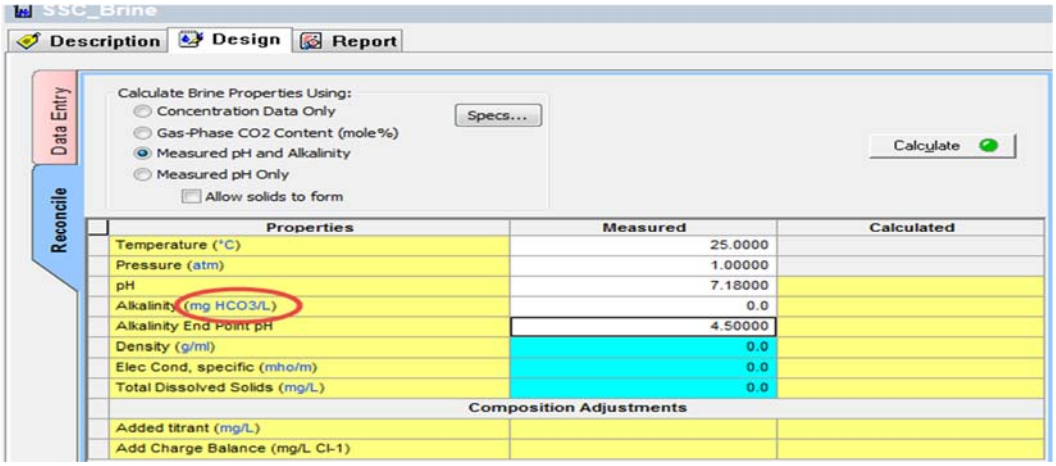


Figure 15-7 The reconciliations tab

Reconciliations (Select one).

Due to experimental uncertainty and error, the measured values for a water sample may not match the calculated values. Therefore, we need to reconcile the calculated values. There are four reconciliation types.

Concentration Data Only	Using the entered ionic and neutral compositions, the pH, density and alkalinity are calculated for this sample.
Gas-Phase CO2 Content	The CO2 is adjusted to match a saturated gas composition
Measured pH and Alkalinity	This adds or removes Hydrochloric Acid (HCl) to match the specified pH and alkalinity. This is default calculation.
Measured pH Only	The pH of the solution can be specified by adjusting the titrant/s.

Radio buttons for the above types can be found under reconciliation options

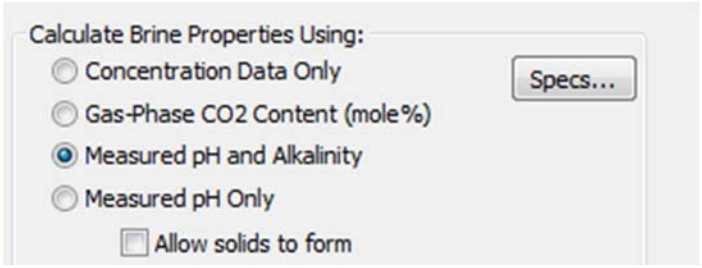


Figure 15-8 Radio buttons

Variables

	The following variables are part of the Reconciliation step. Several variables are user-entered and other are calculated.
Temperature	The default temperature is at ambient conditions. The user may change these values as required.
Pressure	The default pressure is at ambient conditions. The user may change these values as required.
pH	A measured pH is considered to be an unreliable value.. Therefore, users enter the measured pH and compares it to the calculated pH. A user can also force Studio ScaleChem to adjust the concentrations so that the calculated pH matches the measured pH.
Density	The water density is a very reliable number. The program can adjust the total volume or amount of water to match this value. If no density information has been entered, then a calculated density will be used.
Alkalinity	This is generally a reliable value, unless solids have precipitated in the sample. Alkalinity is often but not always the same value as the bicarbonate ion ($HCO3^-$). Studio ScaleChem can reconcile on a measured alkalinity by adjusting the solution composition.
Titration pH	This is the end point for the experiment used by the lab to determine the Alkalinity. The default value is 4.5.
CO2 Fraction in Gas	This is the gas phase, partial pressure of CO2 on a mole-fraction basis. Studio ScaleChem adjusts the dissolved CO2 concentration to match this measured CO2 mole fraction. The CO2 value is assumed to be on a dry basis (no water) and that the complimentary gas is methane (CH4).
HCl Added	This is the amount of HCl either added or removed to match the measured pH and Alkalinity. This value is calculated by Studio ScaleChem.
CO2 Added	This is the amount of carbon dioxide either added or removed to match the measured pH and alkalinity. This value is calculated by Studio ScaleChem.
Total Dissolved Solids	This is the calculated TDS as reported by Studio ScaleChem. It is used as a check to see if all the solutes were properly accounted for in the analysis. This value is calculated by Studio ScaleChem.
Electrical Conductivity	This is the solution electrical conductivity. This value is calculated by Studio ScaleChem.

.

Once the reconciliation options have been selected, the Calculate button is clicked.

Buttons	Calculate Button This button begins the reconciliation calculation.
Allow Solids to form	This check box allows solids to form
	Enter a value of pH = 7.1 and alkalinity = 715 as HCO3-, mg/L

Figure 15-9 Entering pH and alkalinity

Click the *Calculate* button.

The OLI calculation orbit will now display.

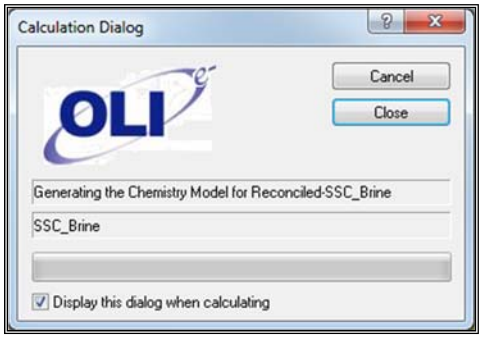


Figure 15-20 the revolving electron

This dialog will close automatically.

Super saturation Warning

Experimental inaccuracies in sample measurement may, on occasion, result in a calculation that indicates that solid is supersaturated. This can normally be ignored providing that the super saturation is not excessive.

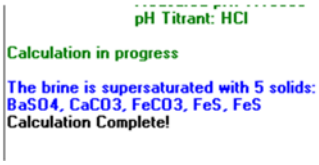


Figure 15-31 Super saturation warning.

Phase Properties

Parameter	Aqueous
pH	7.10000
Density (g/ml)	1.04481
Specific Electrical Conductivity (mho/m)	9.13274
Ionic Strength (mol/mol)	0.0225482
Ionic Strength (mol/kg)	1.30103
Viscosity, absolute (cP)	1.02323
Viscosity, relative	1.14877
Alkalinity (mg HCO3/L)	715.032

Pre and Post Scaling Tendencies

Scale Mineral	Pre-scaling	Pre-index	Post-scaling	Post-index
BaSO4 (Barite)	9.38663	0.972510	9.38334	0.972357
CaCO3 (Calcite)	11.3078	1.05338	11.3072	1.05335
CaSO4.2H2O (Gypsum)	0.929837	-0.0315932	0.929426	-0.0317851
CaSO4 (Anhydrite)	0.732900	-0.134956	0.732577	-0.135147
FeCO3 (Siderite)	1.26295	0.101386	1.26292	0.101376
Fe(OH)2 (Amakinite)	2.52726e-4	-3.59735	2.52710e-4	-3.59738
KCl (Sylvite)	6.70525e-4	-3.17359	6.70426e-4	-3.17365
NaCl (Halite)	0.0121056	-1.91701	0.0121042	-1.91706
SrSO4 (Celestine)	0.203533	-0.691365	0.203444	-0.691554

Brine Composition

Cations	Value (mg/L)	Anions	Value (mg/L)	Neutrals	Value (mg/L)
K(+1)	402.000	Cl(-1)	38665.4	B(OH)3	3.13840
Na(+1)	20400.0	HCO3- (*)	472.817		

Figure 15-4 Reconciled Brine report

The results show that the pH has been reconciled to 7.18 and the alkalinity to 715 mg HCO3-/L. To do this approximately 20 mg/L of HCl was removed (i.e., H+ and Cl-) and approximately 24.66mg/L CO2 was added.

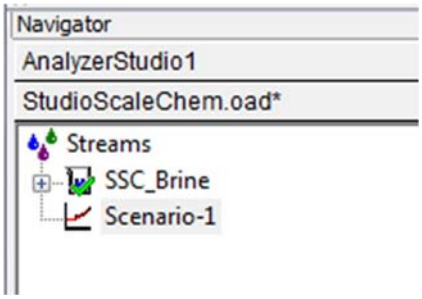
Report is one of the peculiar features of Studio ScaleChem. Navigation and customization of the output data has been made much easier in this format.

Now that we have specified the flow rate of the brine, we need to specify the temperatures and pressures that we wish to simulate as shown in the following example.

Scaling Scenario

Once the Brine Analysis data is entered and the sample reconciled, we can begin the scaling calculation. We now begin to describe the conditions of the calculation.

Select Add Scale Scenario from Actions panel.



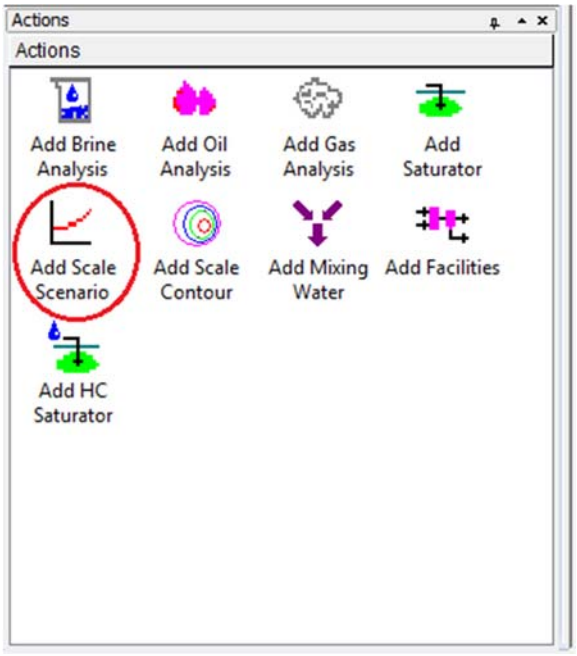


Figure 15-53 Scaling Scenario object

Click on the description tab and rename the Scale Scenario as " SSC-Brine Scale Scenario".

Your screen should now look like image 3-14

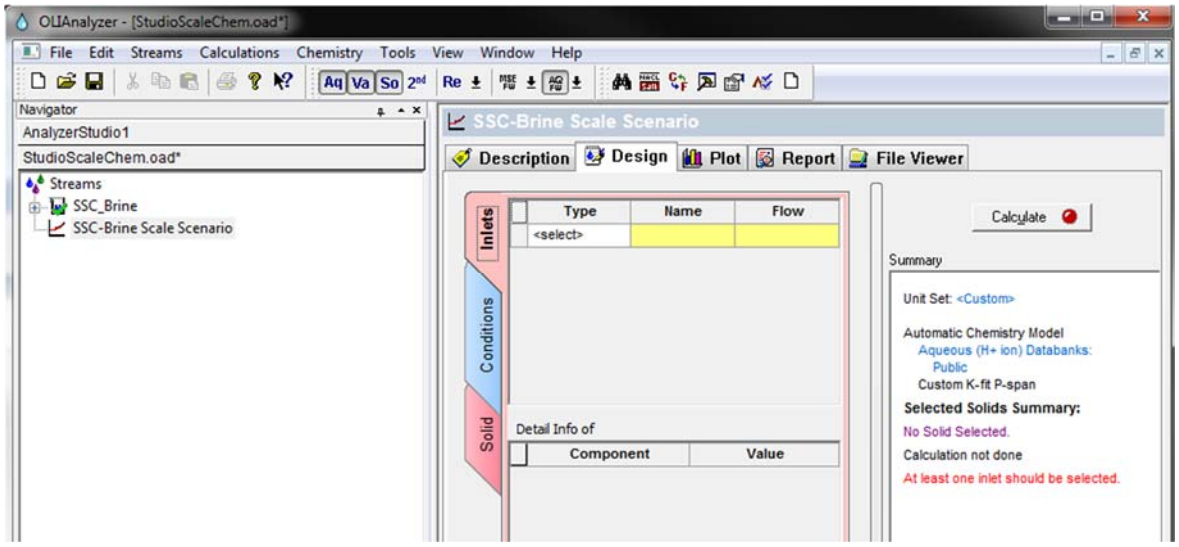


Figure 15-14 Scaling Scenario Design tab

Brine and Gases

The brines and gases that are to be considered for this calculation must now be selected.

Click the *Drop-Down* arrow in the box next to the word *"Select"* under the *"Type"* heading.

This will display all the available brines in this document.

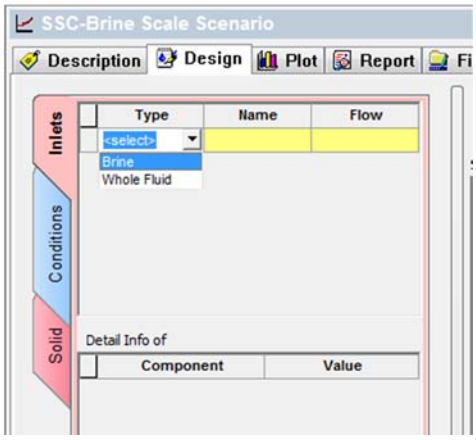


Figure 15-15 Selecting a brine

In this example we are going to use only a single Brine SSC- Brine at 1000L/hr.

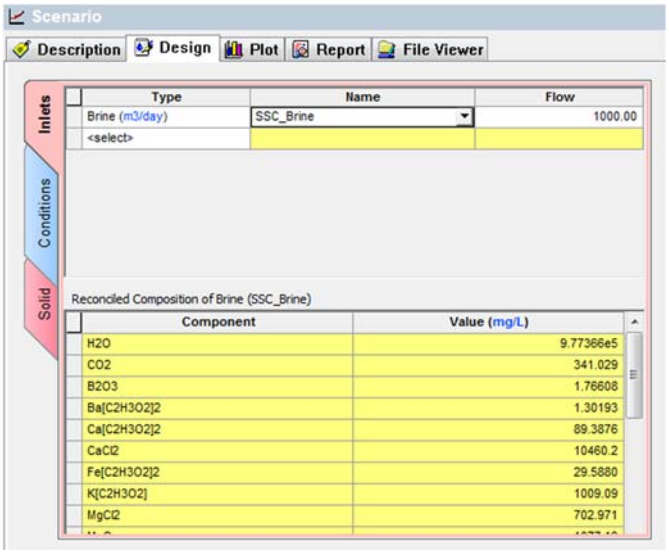


Figure 15-16 The completed case

Input Box

Type You can select the brine, gas or hydrocarbon of interest

Name Click in the Name field. As you position the cursor in the field, a Down Arrow will appear. You can then select from a list of brines, gases or oils already entered into this Studio ScaleChem document.

Flow Enter the flow rate for the gas, hydrocarbon or brine.

Conditions

Now that we have specified the flow rate of the brine, we need to specify the temperatures and pressures that we wish to simulate as shown in the following example.

Click on the *Conditions* tab.

For our example we are going to perform a temperature survey at constant pressure.

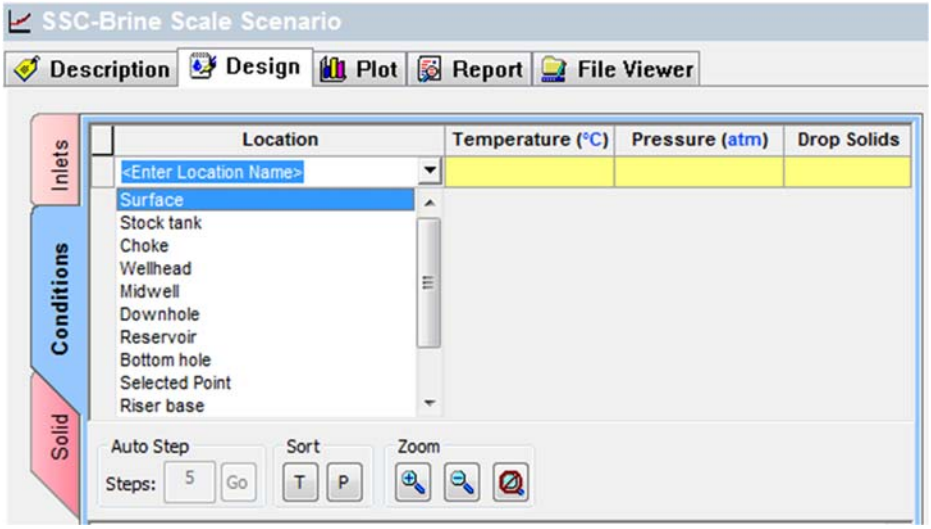


Figure 15-67 The empty conditions tab.

Click on surface and move on to the temperature tab. Change the units by clicking the hyperlinked (^{0}C) and (atm) via units manager second layer. Input the temperature as 77 ^{0}F. Change the Pressure field to 250 psia. Add second point at a temperature of 300 F.

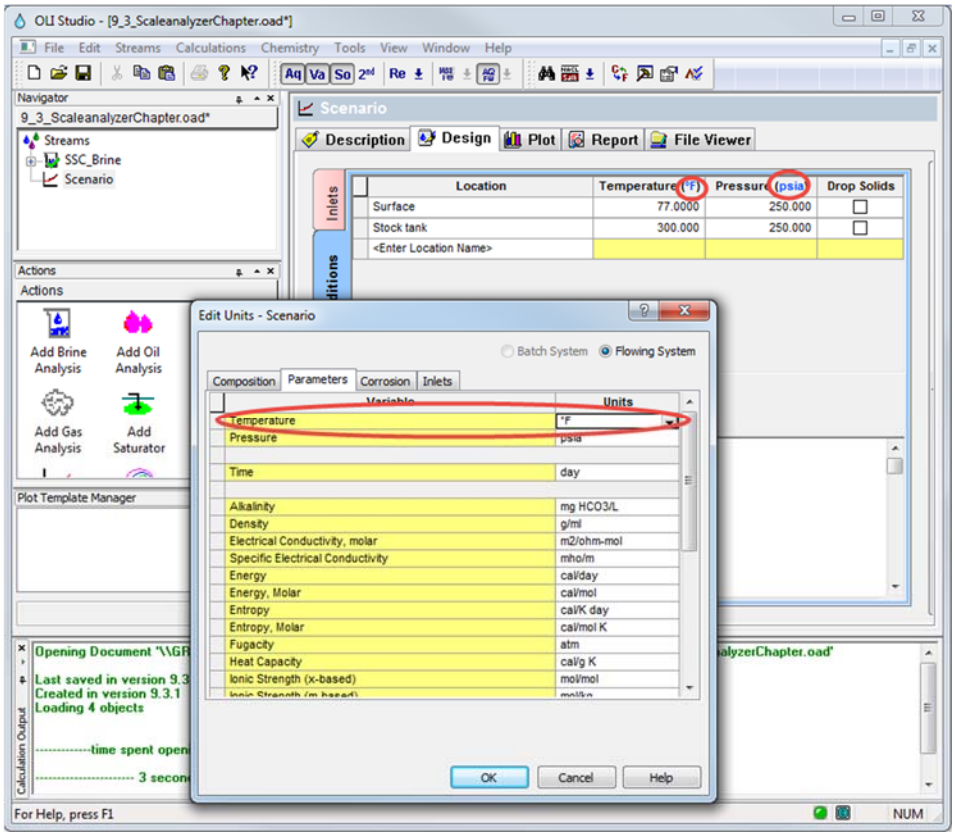


Figure 15-18 The first and second point added.

We now want to add additional points between the two we've just entered.

Click the *Auto Step* button.

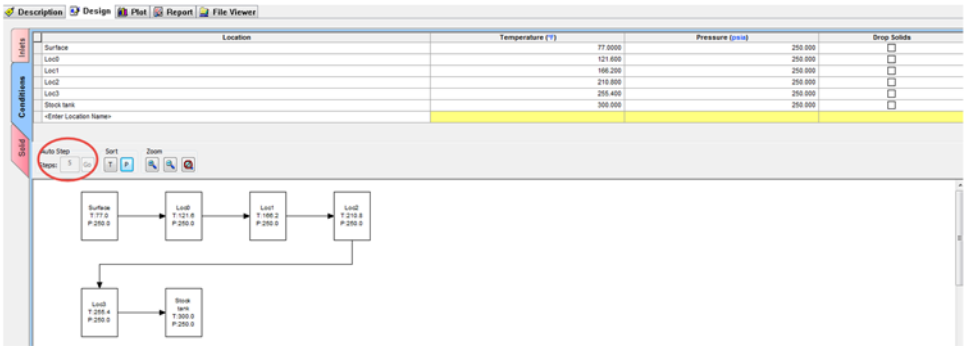


Figure 15-19 The completed conditions tab.

Sort options

Temperature/Pressure Sort the list according to the temperature or pressure fields.

The graphical view clearly shows the five locations and their Temperature and pressure conditions. The Drop Solids checkbox column at the very end of the grid is designed to help the users decide if they want to carry forward solids from certain locations or not.

Precipitates

Studio ScaleChem allows for many solid phases to be considered in the actual calculation. For this example we want to consider all the available solids

In Studio ScaleChem, you have to manually turn the solids on at the top of the toolbar in order to enable the solids tab.

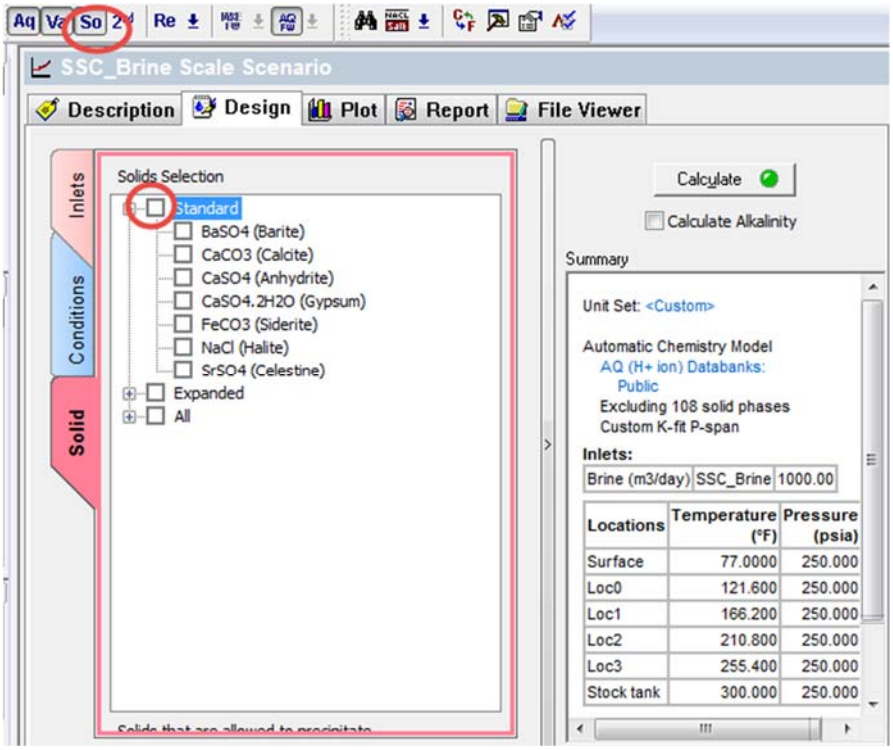


Figure 15-20 possible precipitates

All the possible precipitates could be seen if + sign before all is clicked.

Figure 15-71 All solids selected.

Calculate

We are now ready to calculate

Click on the *Calculate* tab.

Results

After Studio ScaleChem has finished calculating, there will be information of the type shown below available for review. Click on any report tab to display more information.

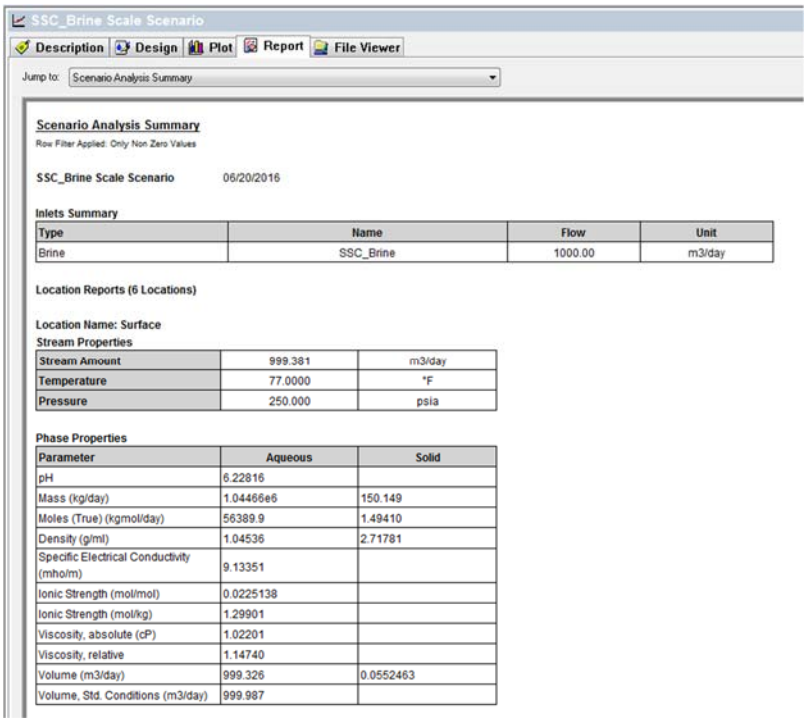


Figure 15-82 The report tab.

Information in reports

Reprint of individual brines Each brine as it was entered and reconciled will appear in the report. All known information about the brine will be displayed. Input gases will also be displayed.

Input brine mixture Prior to each calculation, brines may be mixed with other brines and gases. The sum of these mixtures is displayed in the report.

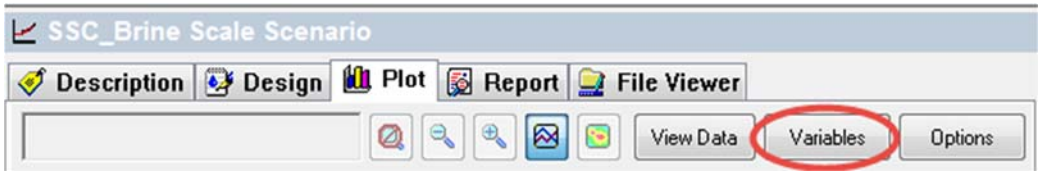
Output brine and gas mixture After each calculation, the resultant brine and gas compositions are displayed.

Pre and Post Scaling tendencies and solids The resultant formation of solids and their tendency to form is displayed.

Location reports Parameters like Temperature, pressure, viscosity etc will be calculated for both aqueous and solid phase existing at each individual location is calculated and reported.

Plot This tab when selected, will display a plot of scaling scenario.

Go to plot and click on Variables.



A window will pop up named Select Data to plot. Get rid of the pre-scaling tendencies and plot Solids against Temperature on X-axis.

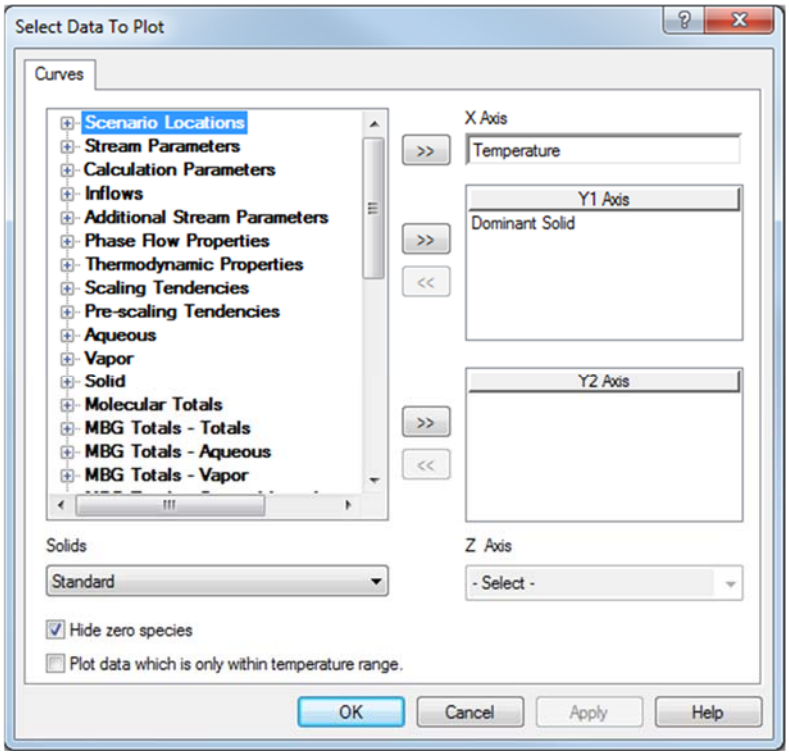


Figure 15-93 Editing the plot.

Plot looks as below:

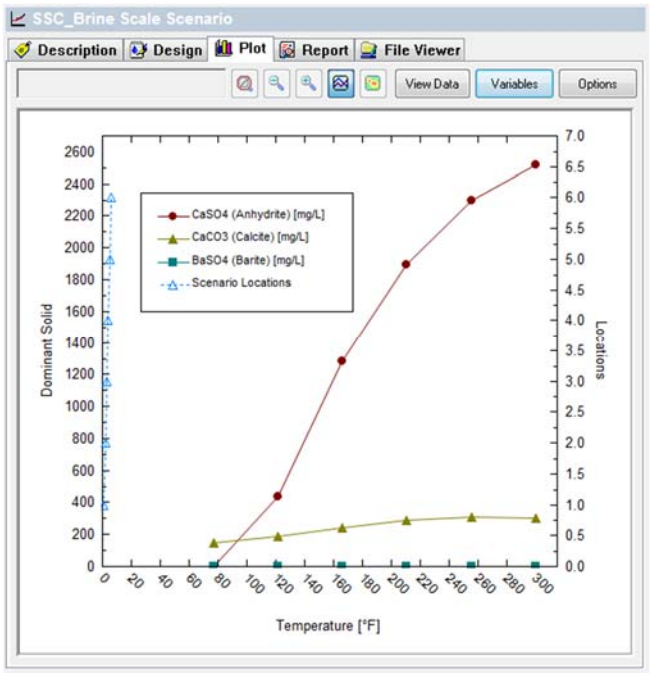


Figure 15-104 The resultant plot.

Most importantly name your file SSC_tutorial and save!save!save!