16. Studio ScaleChem Calculations

Calculations Overview

Studio ScaleChem can be used to calculate scaling at one or more user specified temperatures and pressures. Other calculation options include the ability to mix waters at user specified ratios to find compatible waters, and the ability to saturate a water with respect to one or more solids to simulate reservoir conditions.

We have already entered a scaling calculation in the Studio ScaleChem Tour, you are referred there to review that information

We will need to add some additional brines, gases and oils to continue.

Calculations: Adding a new brine sample

Position the mouse on the Actions Panel and select object name Add brine analysis which looks like a logo above and double click. Rename the brine in Descriptions tab

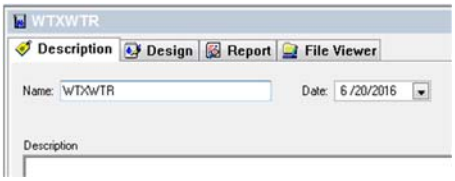


Figure 16-1 The default brine sample description

You must reconcile the sample for both electroneutrality, pH and alkalinity.

Name	WTXWTR	
Type of water	Aquifer Water	
Comment:	West Texas Water Supply	
Species:		
Na^{+}	3074	mg/L
Ca^{+2}	910	mg/L
Mg^{+2}	249	mg/L
Fe^{+2}	0.77	mg/L
Cl^{-1}	4474	mg/L
SO_4^{-2}	2960	mg/L
HS^{-1}	146.2	mg/L
HCO_3^{-}	439	mg/L

Conditions:

pH	7.98
Alkalinity	439 mg/L as HCO_3^-
Titration pH	4.5
Temperature	77 F
Pressure	14.7 PSI
Density 0	(will be estimated)

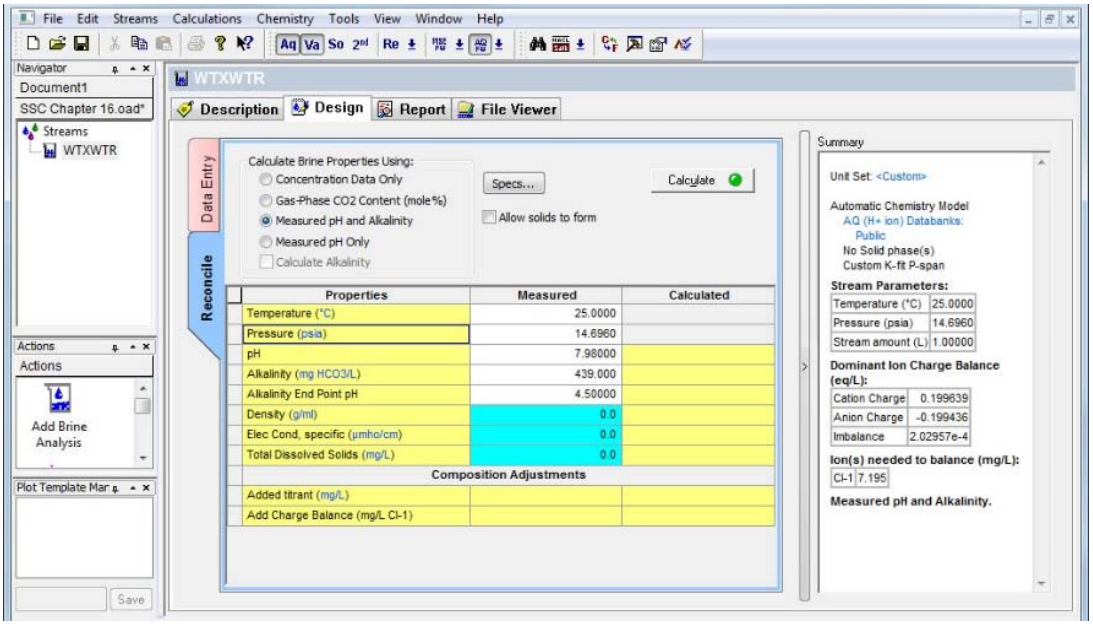


Figure 16-2 The calculated Brine WTXWTR

Calculations: Adding a Gas Sample

From the Actions Panel click on Add Gas Analysis. Input the name in the description tab. We recommend that you use a suitable name

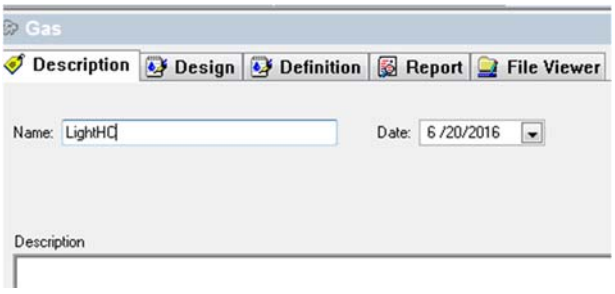


Figure 16-3 Entering a gas sample

To add more descriptive information, click on the Design tab.

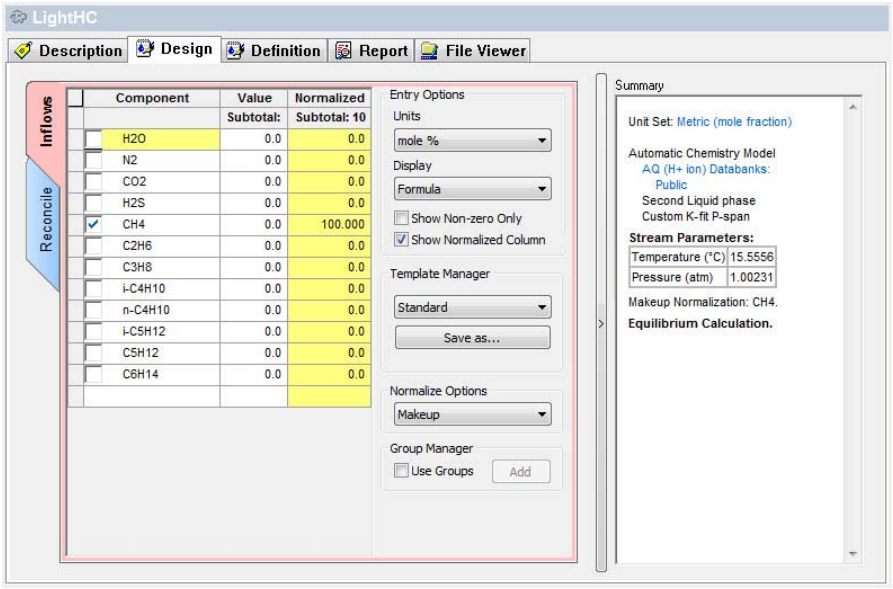


Figure 16-4 The blank gas entry. Initially 100 % methane (CH_4)

Please enter the following composition

Carbon dioxide (CO2)	10	mole %
Water (H2O)	15	mole %

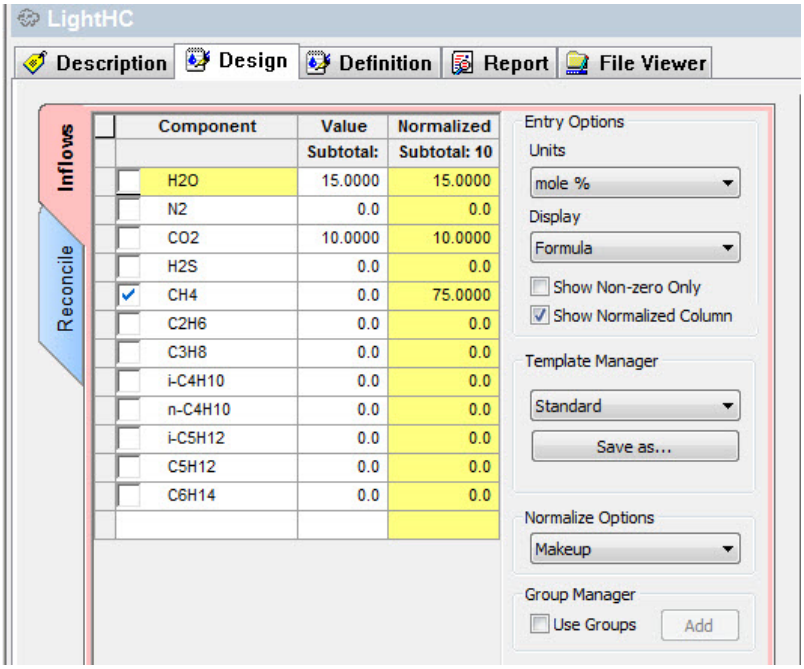


Figure 16-5 Entered gas.

Gas

The gas composition is entered as mole% or volume% (these are equivalent for an ideal gas). The total must be 100% and can be adjusted by normalizing, or by letting the program determine the amount of hydrocarbon gases present. The gases that are displayed here will be either the standard gases or expanded gases . Toggling from the standard to expanded can be achieved by clicking the Gases button.

Normalizing

You can enter just the amounts of carbon dioxide, hydrogen sulfide and water and let the program Calculate Hydrocarbon Percent (default) or enter all values and then normalize to 100%.

Displaying Gases

You can display the name of the gases by Name (the default) or by Formula. Studio ScaleChem will assume that all of the hydrocarbon gas is methane (CH4). If you want to use a more detailed list of hydrocarbon gases, click on Gases to expand the list.

Frequently the data received by the user refers to gas compositions that are reported on a "Dry" Basis. Any water that was present in the actual gas has been removed mathematically and reported as a dry sample.

The dew point corresponds to the temperature or pressure where a gas will begin to condense and form a liquid (aqueous) phase. The Dew Point calculation will allow you to determine the amount of water that could be contained in the gas at the stated temperature, pressure and composition.

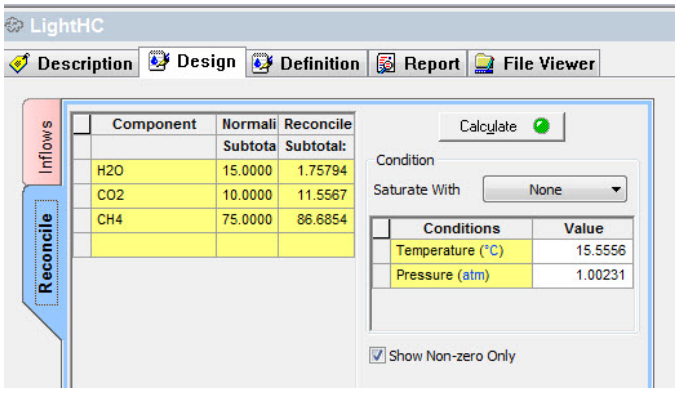


Figure 16-6 Reconcile tab

Type of Calculation

Saturated water Content

At the entered conditions, the amount of water that the gas can contain before an aqueous liquid will form is determined. If the Water Vapor field is entered, then that value is used as an initial guess to the calculation.

The calculated value is NOT updated in the actual gas composition. The user must enter that value manually if desired.

At Conditions

Enter the temperature, pressure and water content of the gas. Click the Calculate button to start the calculation.
You can change the units of the calculation by clicking the Units button. When the calculation is complete, you may view the internal files by clicking the View Files button (currently grayed-out in the above example).

Calculations: Adding an Oil sample

From the Actions Panel click Add Oil Analysis. Enter the name in the Description Tab.

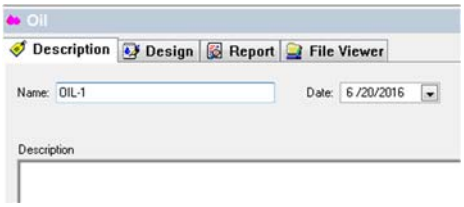


Figure 16-7 Input name for the Oil Analysis

Input the composition information in the design tab.

Calculations: Hydrocarbon - Pseudocomponent approach

There are three entry types. The first is pure components (organic and inorganic), the second is pseudocomponents, and the third is a distillation curve (termed petroleum fraction. Studio ScaleChem groups the pseudocomponent and assays together.

For this example we will enter pure component and pseudocomponent data.

Entering Pseudocomponent data

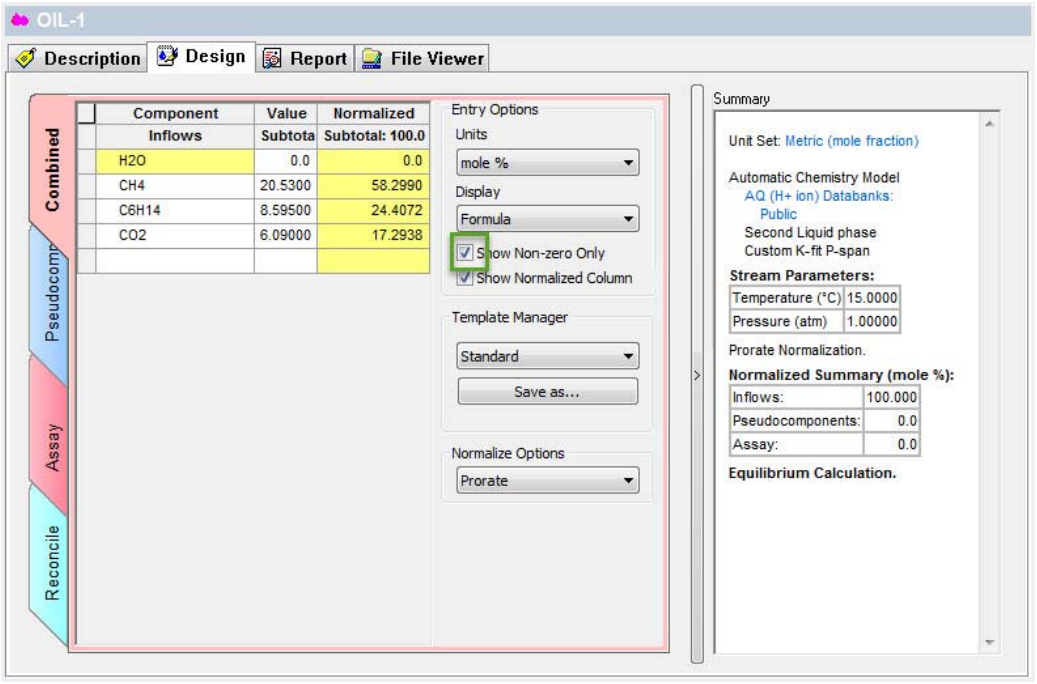
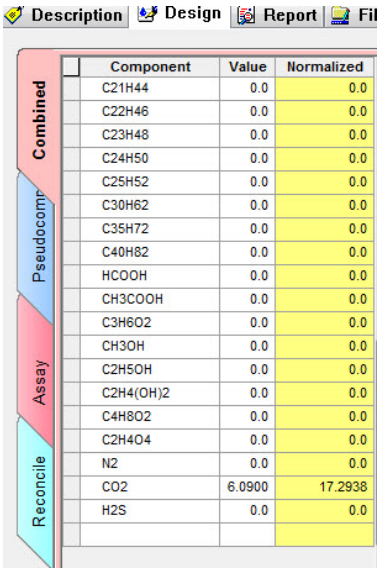


Figure 16-8 Starting to add compositions.

We will start by entering the following composition:

Methane (C1) 20.53mole %
Hexane (C6) 8.595mole %
CO2 6.09mole %

(you will have to scroll down to find the CO2 entry).



Component	Value	Normalized
C21H44	0.0	0.0
C22H46	0.0	0.0
C23H48	0.0	0.0
C24H50	0.0	0.0
C25H52	0.0	0.0
C30H62	0.0	0.0
C35H72	0.0	0.0
C40H82	0.0	0.0
HCOOH	0.0	0.0
CH3COOH	0.0	0.0
C3H6O2	0.0	0.0
CH3OH	0.0	0.0
C2H5OH	0.0	0.0
C2H4(OH)2	0.0	0.0
C4H8O2	0.0	0.0
C2H4O4	0.0	0.0
N2	0.0	0.0
CO2	6.0900	17.2938
H2S	0.0	0.0

Figure 16-9 C1 to C20 entered. Scroll down to find CO2

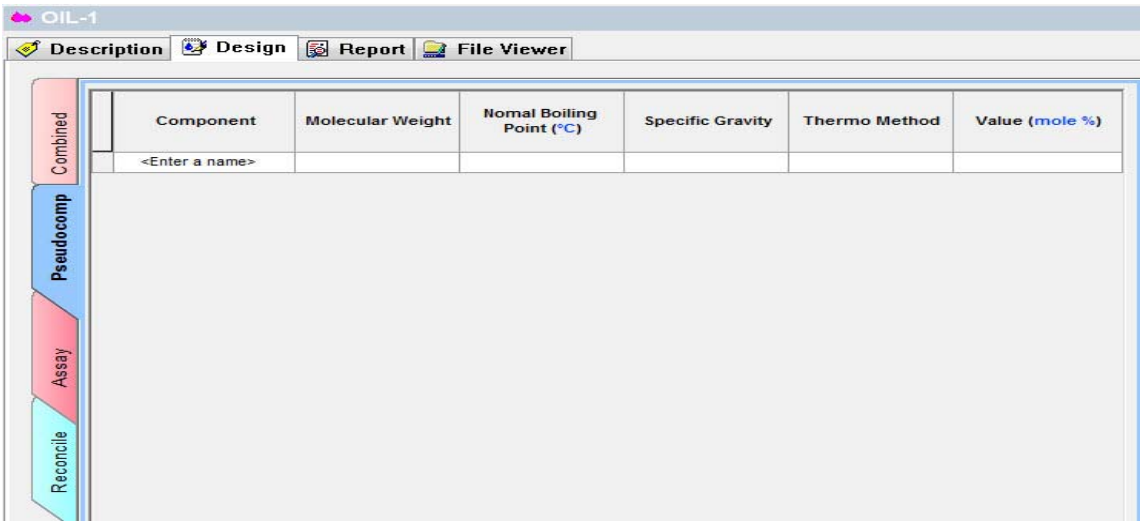


Figure 16-10 Entering pseudocomponents.

Type the name PC1 in the section <Enter Name> below column heading Component. Please enter the following information. Add a mole percentage of 27.57 %

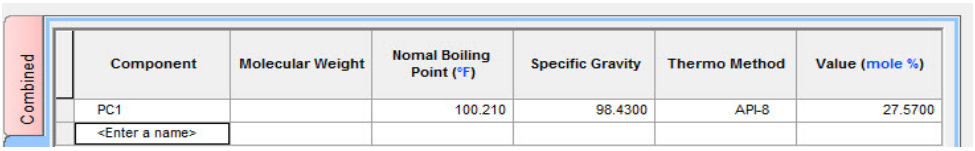


Figure 16-11 Adding the first pseudocomponent.

We have now entered the first pseudocomponent. Keep typing in the Enter Name section to add more pseudocomponents. We have 3 additional entries.

Name	MW (g/mol)	nBP (F)	Method	mole %
PC2	170.34	216.32	API	29.35
PC3	282.55	343.78	API	7.19
PC4	506.0	645.00	API	0.68

The completed input looks like this:

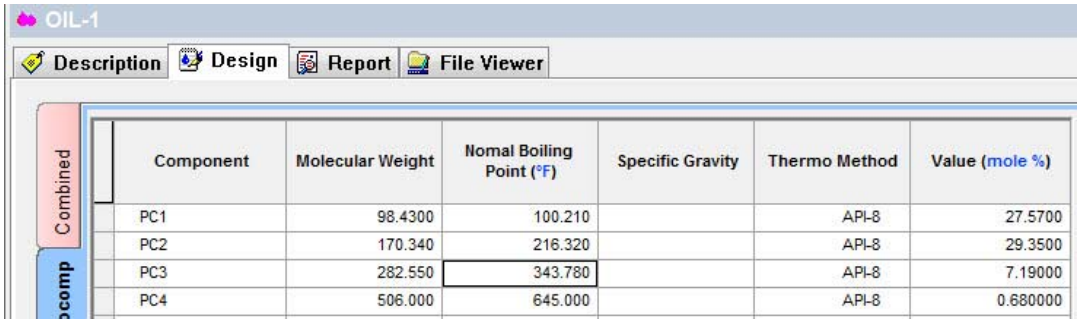


Figure 16-12 Completed input

Reconciling the Pseudocomponent

Click on the ***Reconciliation*** tab to see how well the pseudocomponent will predict the phase behavior of the hydrocarbon sample. You will be presented with the following display:

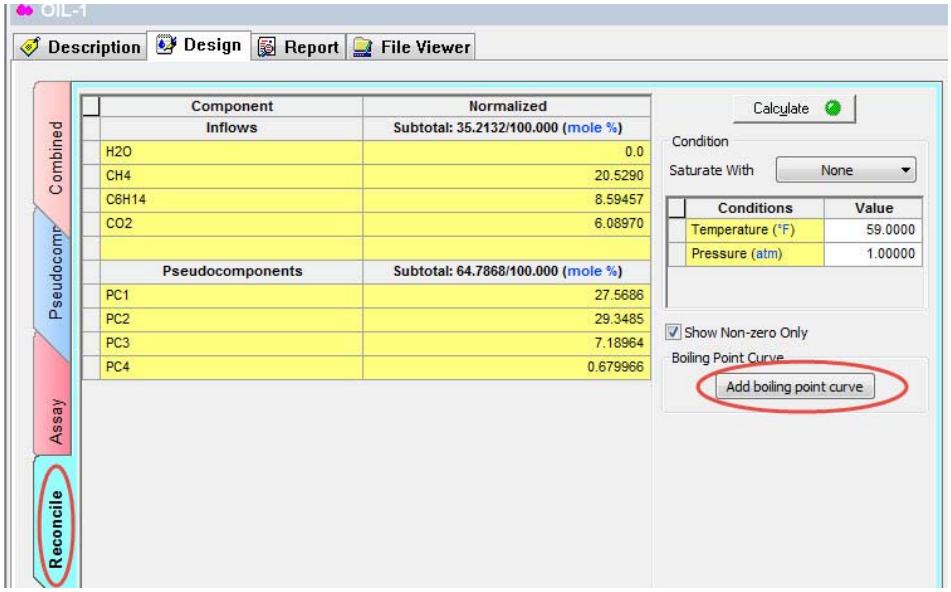


Figure 16-13 Reconciliation Tab

We will hold the temperature constant at 204 F and vary the pressure from 200 to 2000 PSI in 100 PSI increments.

Click the *Boiling point* button. A new calculation appears in the navigation panel below OIL1 Object.

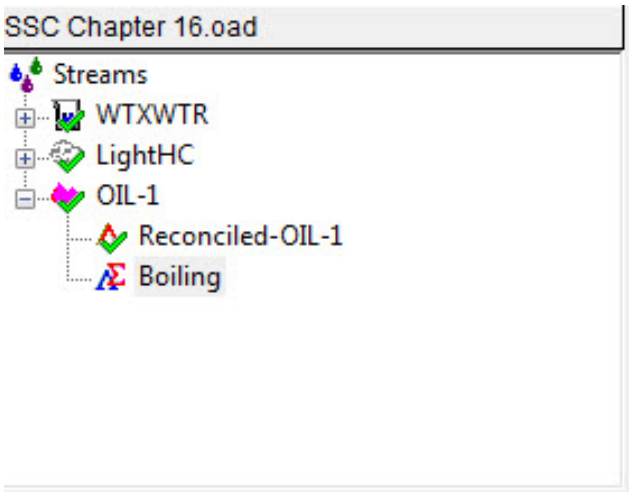


Figure 16-14 Boiling Point calculation

This is a survey by Pressure. Click on the specs button and specify the conditions below.

Enter a fixed value of *204 deg F*

Enter a pressure range:

Start	200 psia
End	2000 psia
Start	100 psia

Click the *Calculate* button.

Click on the plot tab, you will see the following graph: You could adjust the parameters by clicking on curves.

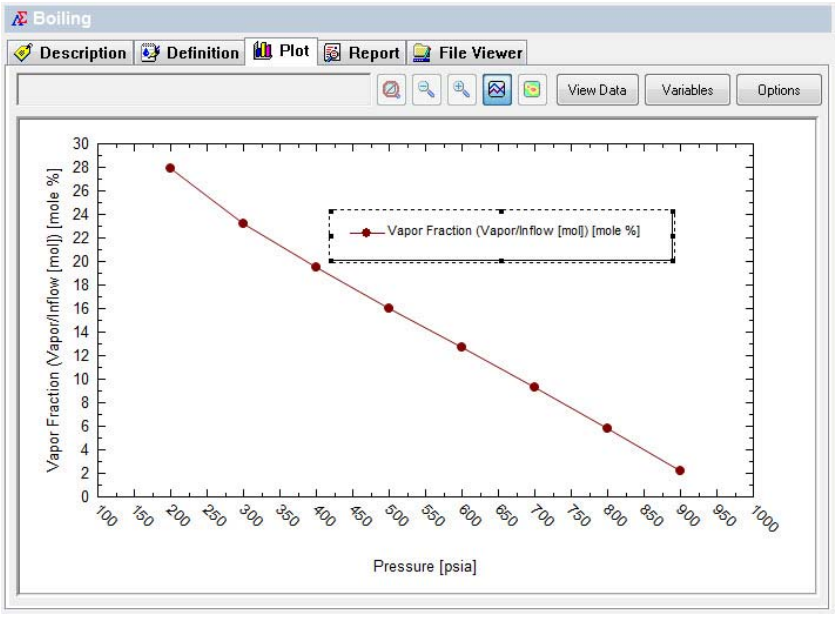


Figure 16-15 Boiling point curve

If the curve does not meet expectations, you will have to adjust the mole percentages or the pseudocomponent properties. This is a manual iterative approach. You can see the actual data by clicking the View data button.

Saturating the hydrocarbon with water

Frequently the hydrocarbon was saturated with water.

Click on the *Saturate with* drop down. Select H20

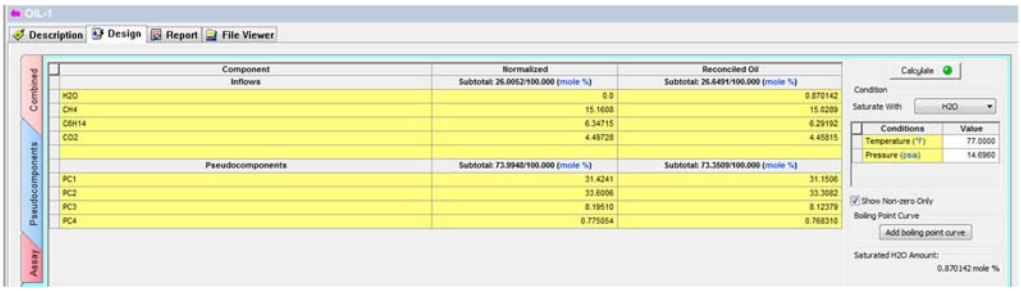


Figure 16-16 Saturate with H2O

In this example we are saturating the hydrocarbon sample at 77 F and 14.7 PSI. The program requires an initial "Guess" for the concentration of the water. When done, we will save the saturated hydrocarbon as the object **SatOIL1**.

Click on the *Calculate* button.

Mix Calculation: Overview

The Mixer calculation determines if two waters (brines) can be mixed. Frequently the mixing of two waters will cause precipitates to form which were not present in original brines. This can lead to the plugging of a formation when an injection water is mixed with the natural fluids in the formation.

Mix Calculation: Set Up

From the Actions Panel, click on the Add Mixing Water logo. After double clicking the logo, you will the object in the Navigation Panel.

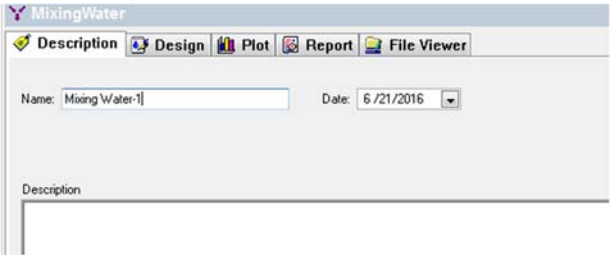


Figure 16-17 Input name for Mixing Water object

Click on the design tab to enter more information.

Selecting objects for the calculation

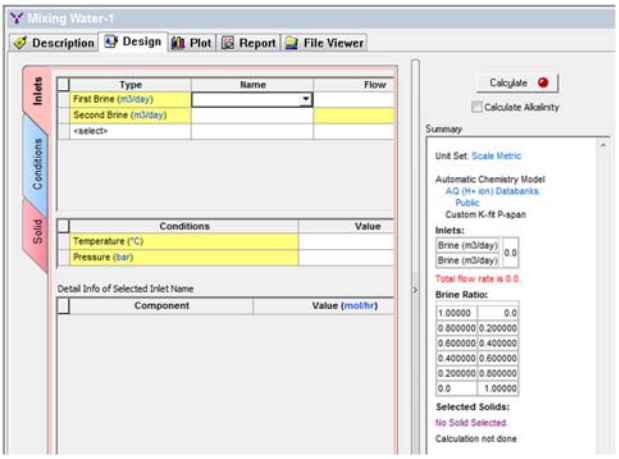


Figure 16-28 Setting up the mix calculation

Select your brines, gases and oils as shown in the next figure. Enter the indicated brine flow rate of 1000 bbl/day, gas flow of 230 stdMft3/day and oil flow of 7 bbl/day.

There are two ways to change the units.

Method 1: To change units on brine, oil and gas, click on the hyperlinked (blue) units inside of the bracket next to Inlets First Brine, Second Brine etc. This is under the column heading Type.

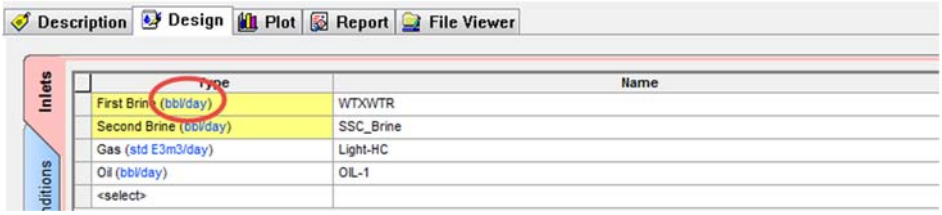


Figure 16-19 Changing units

This should pop the following window up. Click on Inlets tab and change the units.

Inlets tab looks like below. Changing units on Brine:

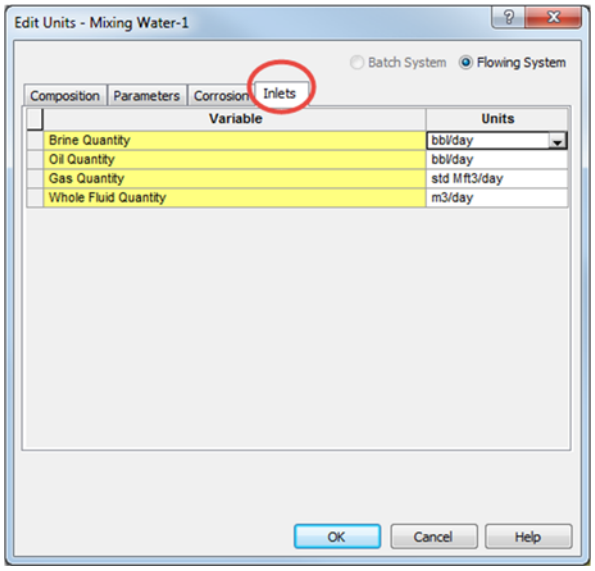


Figure 16-20 Units manager layering

Method 2: This can also be done in one other way, that is through the units manager button on the toolbar. which looks like  .

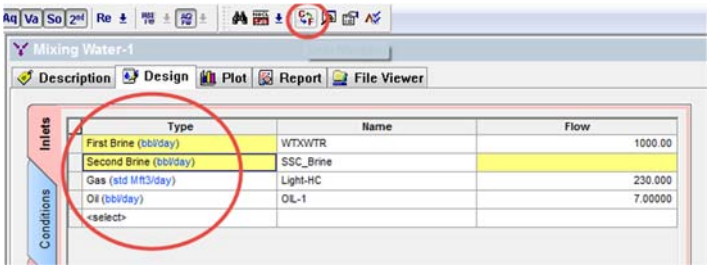


Figure 16-21 Units Manager accessibility

When you click on units manager, following windows pops up.

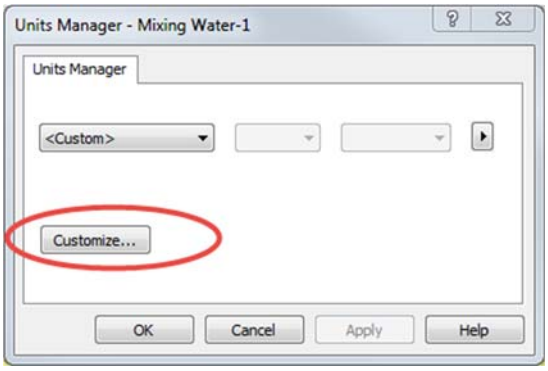


Figure 16-22 Units Manager first layer

Click on Customize. Change the individual parameters as shown below.

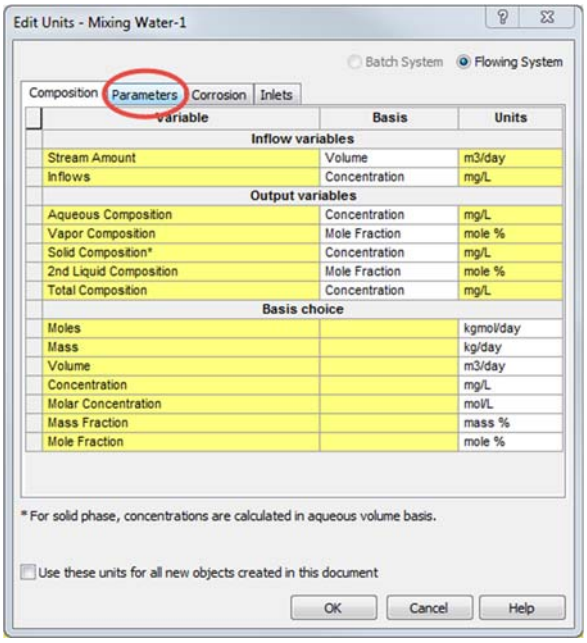


Figure 16-23 Changing units for parameters

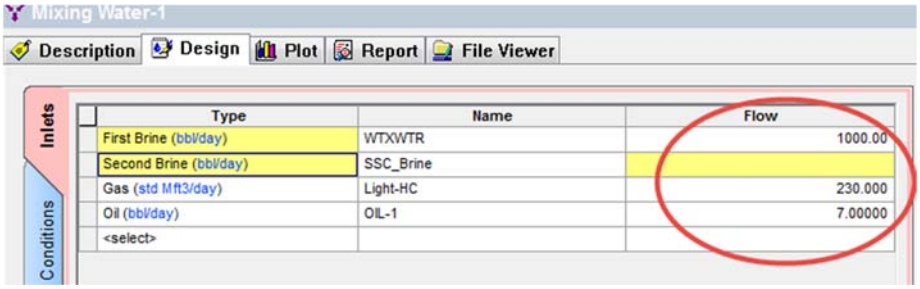


Figure 16-24 Mixer with inflows entered (Inlets Tab)

In this example we will mix two brines, created in other sections at a total brine flow rate of 1000 barrels per day. In addition, we will add a gas and a hydrocarbon to the calculation.

Entering Conditions

In this example, we are mixing the brines at 100 F and 200 PSIA. The first brine specified (brine1 in the example) is the one we compare to when evaluating the ratios. In this case we start out with all brine1 and none of the brine WTXWTR and end up with none of brine1 and all of WTXWTR.

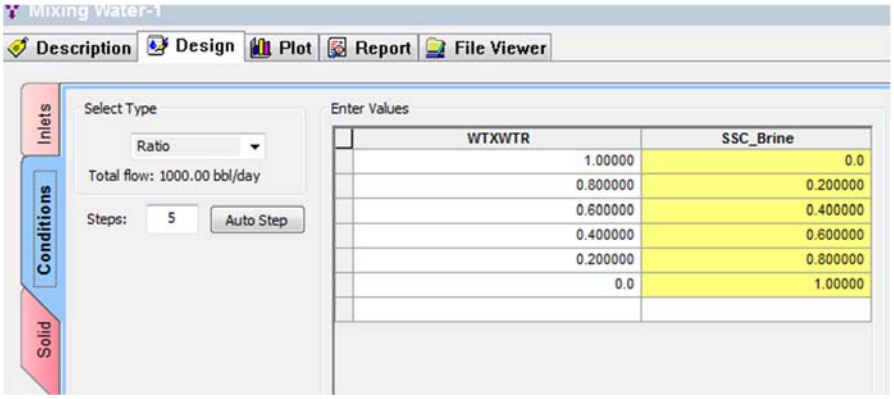


Figure 16-25 the mixing conditions (Conditions tab)

Selecting Precipitates

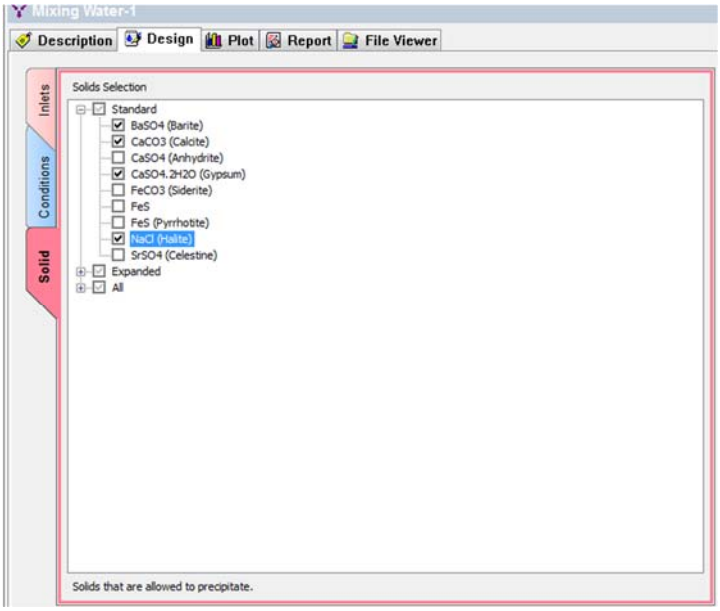


Figure 16-27 Selecting a few solids. (Solids tab)

For this calculation we are only selecting a few of the possible solids. Mark a check box next to desired solids (BaSO4, CaCO3, CaSO4.2H2O, NaCl).

Click on the Calculate button.

View the report. Click on the Plot tab and view Plot

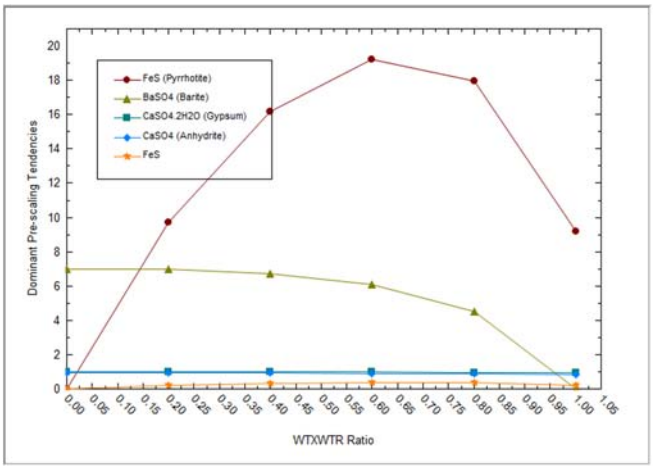


Figure 16-28 Default plot

To study the effects better go to the variables button and eliminate other solids precipitated by the << arrow. Keep only one solid (in this case BaSO4). The ratio is relative to the first brine specified. This means at a ratio of 0.0 (all the first brine and none of the second) we have no BaSO4 scaling. As we add the second brine, the amount of BaSO4 increases. These waters are perhaps incompatible.

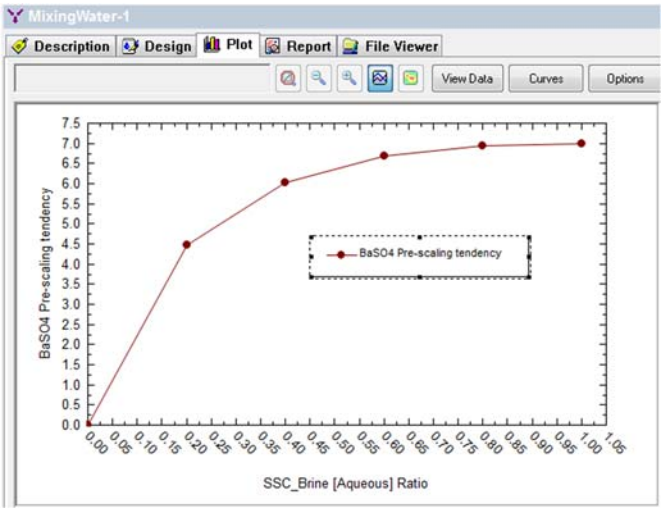


Figure 16-29 Mixing results

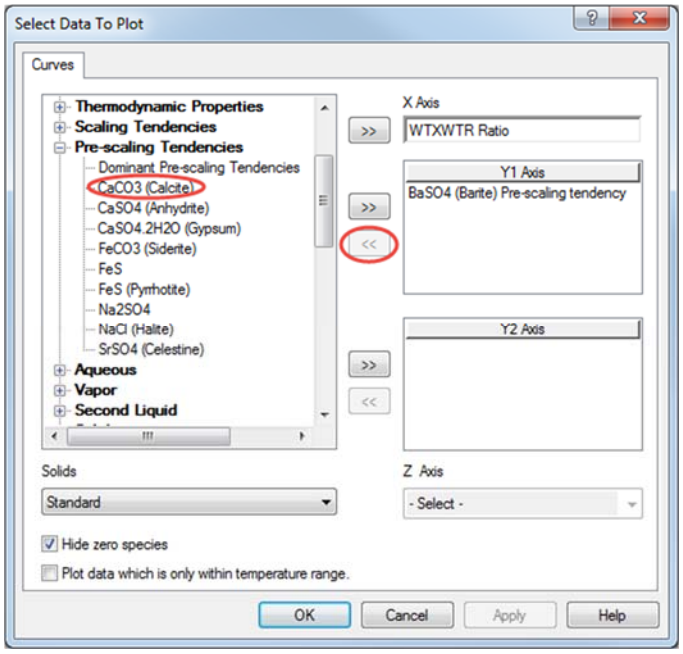


Figure 16-30 Editing the plot via variables button

You could choose to select any of the other solids that could be precipitated from the above pre-scaling tendencies. The red marked << arrow removes the existing component from Y1-axis and >> arrow adds components to axis. Simply double clicking the component/parameter name under axis works for removing it from the list to display on plot too.

Saturate Calculations: Overview

Water and gas samples at the surface are not necessarily representative of conditions in the reservoir. The processing of the samples may involve significant changes in the chemistry.

The Saturate option (often referred to as "Saturate at reservoir conditions") allows the user to "Back" calculate the conditions down hole.

Saturate Calculations: Set Up

Select Add Saturator from the Actions Panel. Rename the object in the descriptions tab.

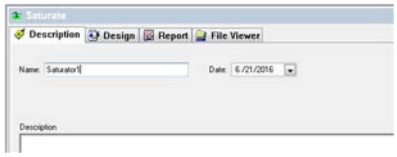


Figure 16-31 Description tab

The default location will be the ***Component*** tab.

We will select objects that we have already defined.

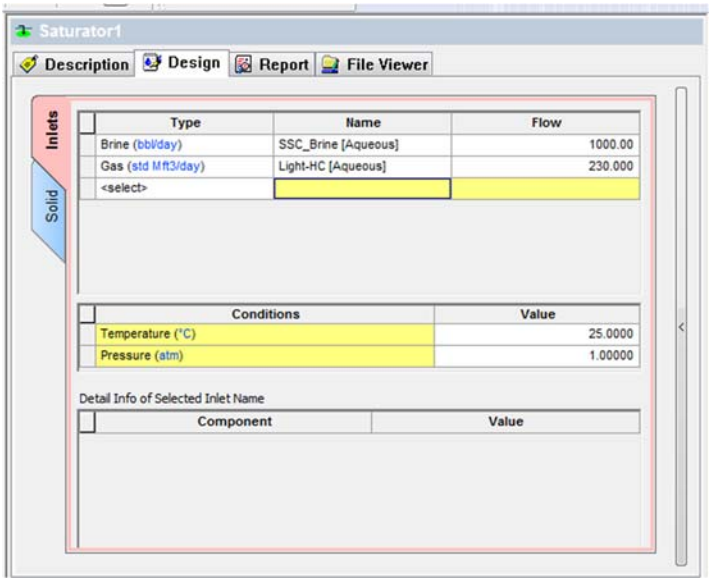


Figure 16-32 Selecting saturating components

For the Gas and Brine flow and Conditions units for temperature and pressure, we have to make sure to have bbl/day, Mft3/day and F, PSIA respectively. Set these units as custom units for all new objects in Units manager.

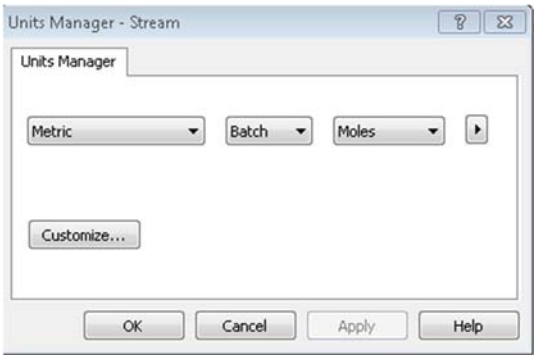


Figure 16-33 Customize the unit sets

We have to select solids inflow to vary for Saturator1. Under the solids tab select the solids allowed to be formed. Under the table select inflows to vary, choose the solid to vary from the dropdown list.

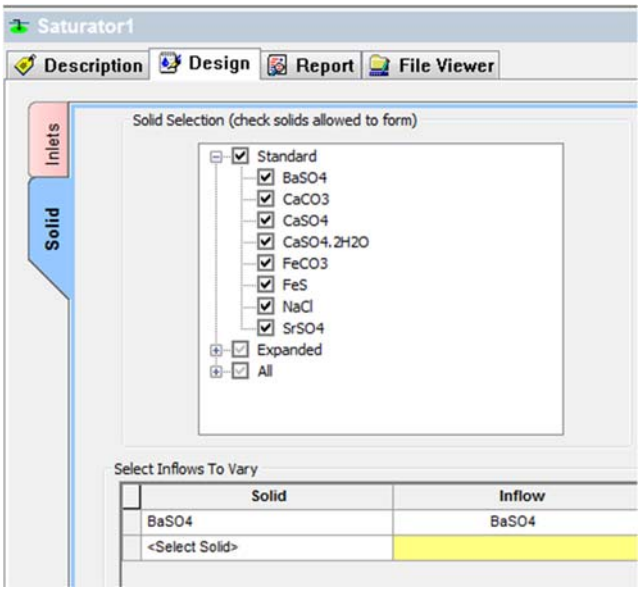


Figure 16-34 Selecting solids to vary

To study the saturator brine at various locations we need to add a Scaling Scenario from the saturator.

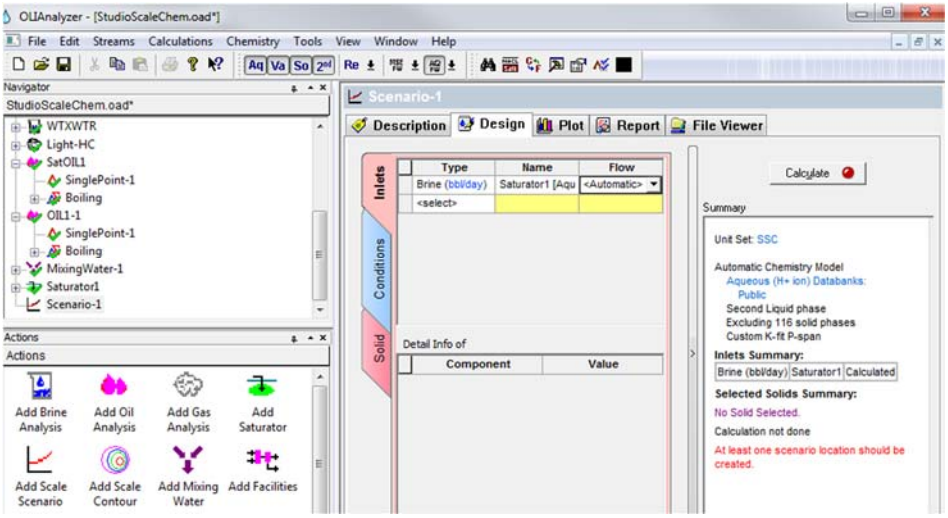


Figure 16-35 Adding a scaling Scenario

We have to make sure when we add brine under the inlets tab, under Type column, that we are selecting brine from Saturator1 and not SSC brine or WTXWTR brine. Flow will be automatically controlled. Locations can be input under the conditions tab.

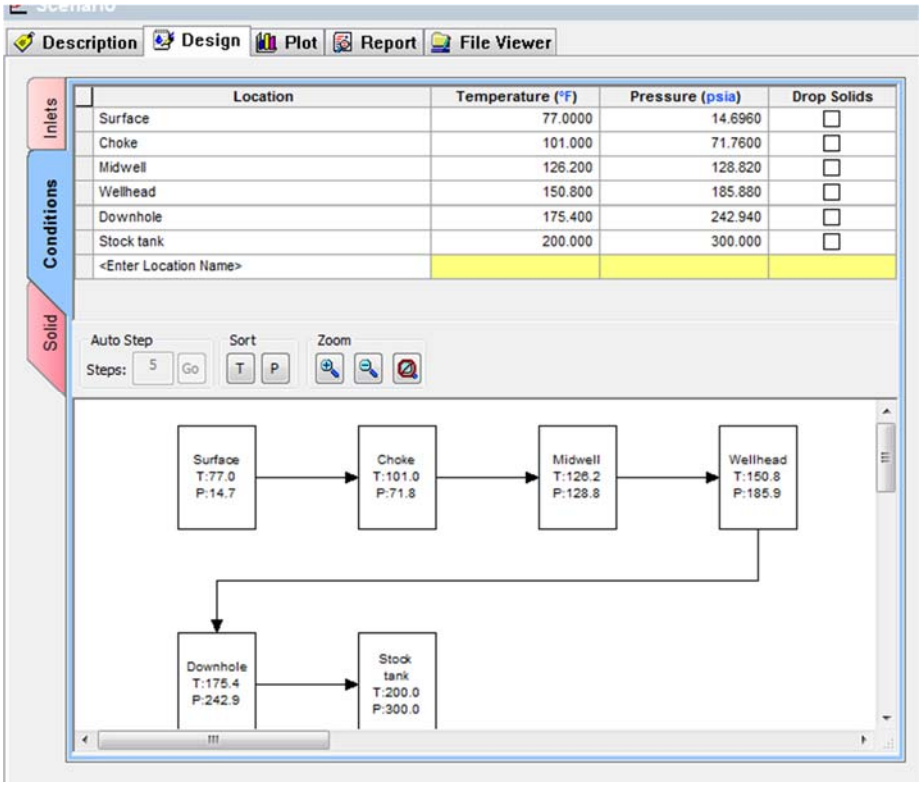


Figure 16-36 Conditions set up

We will start at 77 °F and 14.696 PSIA and end at 200 °F and 300 PSIA. We will use 5 steps.

This case differs from the other calculations in that we will force a scale to appear just at its solubility limit. The scaling tendency is forced to be equal to 1.0 exactly. See report tab on the Saturator 1where Pre and Post Scaling Tendency table shows more details.

Pre and Post Scaling Tendencies

Scale Mineral	Max Scale (lbmol/day)	Pre-scaling	Pre-index	Post-scaling	Post-index
Na[C2H3O2].3H2O	0.0	8.13548e-4	-3.08962	8.11722e-4	-3.09059
MgCO3.3H2O (Nesquehonite)	0.0	2.87353e-4	-3.54158	2.07936e-4	-3.68207
CaSO4.2H2O (Gypsum)	0.0	0.930189	-0.0314286	0.926655	-0.0330819
CaCO3 (Aragonite)	0.0	0.586274	-0.231900	0.419877	-0.376878
FeCO3 (Siderite)	0.0	0.159419	-0.797461	0.114829	-0.939950
NaHCO3 (Nahcolite)	0.0	5.00092e-3	-2.30095	4.27561e-3	-2.36900
SrSO4 (Celestine)	0.0	0.203427	-0.691592	0.203606	-0.691209
BaSO4 (Barite)	5.29109e-8	1.00000	3.50074e-11	1.00000	0.0
Na2SO4.10H2O (Mirabilite)	0.0	7.19368e-3	-2.14305	7.20588e-3	-2.14231
MgSO4.7H2O (Epsomite)	0.0	8.47496e-4	-3.07186	8.53133e-4	-3.06898
CaSO4 (Anhydrite)	0.0	0.733302	-0.134717	0.730447	-0.136411
CaCO3 (Calcite)	1.28496	1.39630	0.144977	1.00000	0.0
Na2SO4 (Thenardite)	0.0	1.12143e-3	-2.95023	1.12280e-3	-2.94970
MgCO3 (Magnesite)	0.0	3.03330e-4	-3.51809	2.19466e-4	-3.65863
NaCl (Halite)	0.0	0.0121050	-1.91704	0.0121087	-1.91690
KCl (Sylvite)	0.0	6.70480e-4	-3.17361	6.70604e-4	-3.17353

Figure 16-37 Pre and post Scaling tendencies at location one-surface

We want to force the BaSO4 (barite) solid to appear. It is generally a good idea to select a maximum of one or two solids. As we can see above, BaSO4 has a scaling tendency of exactly one.

After the calculation is complete, the plot for scale scenario shows that other solids are appearing. In this case both Anhydrite and calcite and disordered dolomite are appearing.

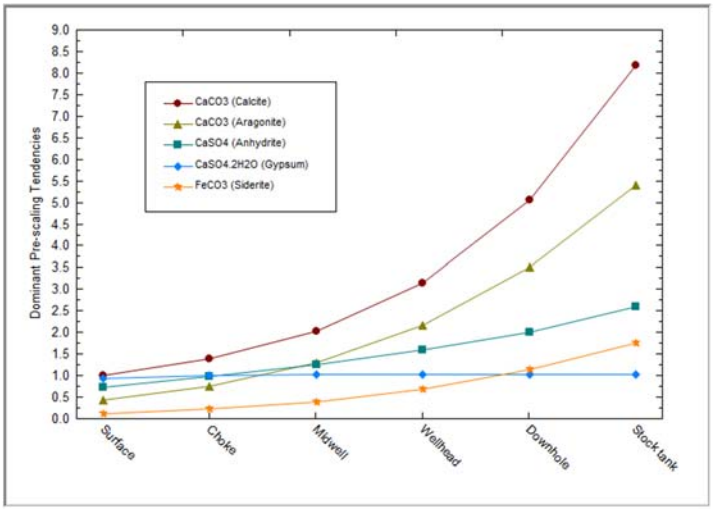
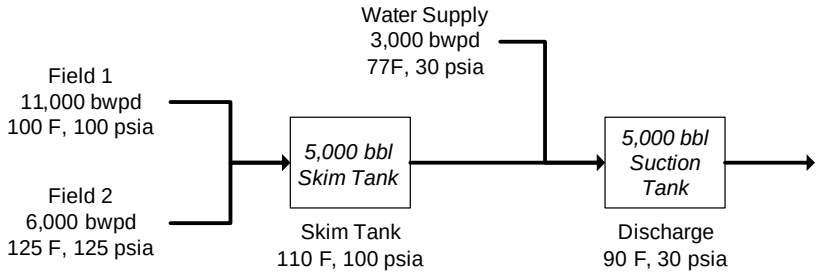


Figure 16-38 The plotted results

At this point it may be beneficial to saturate with other solids. We will leave that as an exercise for the user.

Facility Calculation: Overview

Studio ScaleChem has the ability to link together several individual calculations to create a flow sheet facility. An example of a facility calculation is shown in the figure below.



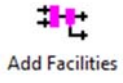
It is a simple process in which two field brines mix in a skim tank. The discharge from this tank then mixes with a water supply in a discharge tank. Below are the compositions and conditions of the inlet fluids

Name	Field1	.	Field2	.	Water Supply
Na+	38209		27078		3074
Ca+2	6600		4480		910
Mg+2	1531		1191		249
Fe+2	120		6.6		0.77
Cl-1	73150		51134		4474
SO4-2	2453		1840		2960
HS-1	244		146.2		0
HCO3-	421		677		439
Conditions					
Temperature	100F		125 F		77 F
Pressure	100 PSI		125 PSI		30 PSI
Alkalinity (As HCO3 mg/L)	421		677		439
Titration pH	4.5		4.5		4.5
Sample pH	6.97		7.53		7.98

Create the above brines

You start this example by first creating the above three brines:. Use the Add Brine Analysis object as you have done before to create them. *Reconcile these three brines for **measured pH and alkalinity***. Make sure that the *Allow solids to form* box is uncheck at the bottom of the reconciliation options for all the brines.

Facility Calculation: Set Up



The facilities calculation is based upon transferring information between calculations through nodes. These nodes can be thought of as pseudo brines and gases.. These pseudo brines are not stored as individual brine rather they are used internally in the calculation. The concentration and flow rates for these nodes can be viewed in the output.

Select ***Add Facilities*** from the Action Panel.

Figure 16-39 The Description tab for the Facilities

Under design tab, within Inflow Specs, we can add Nodes via Node input options. There will be one default node added. Click on the node name and type "Skim Tank" That populates the name field below Node Input section.

At the start the panel contains Node #1. It has default conditions and no inlet streams. This node will be the Skim Tank.

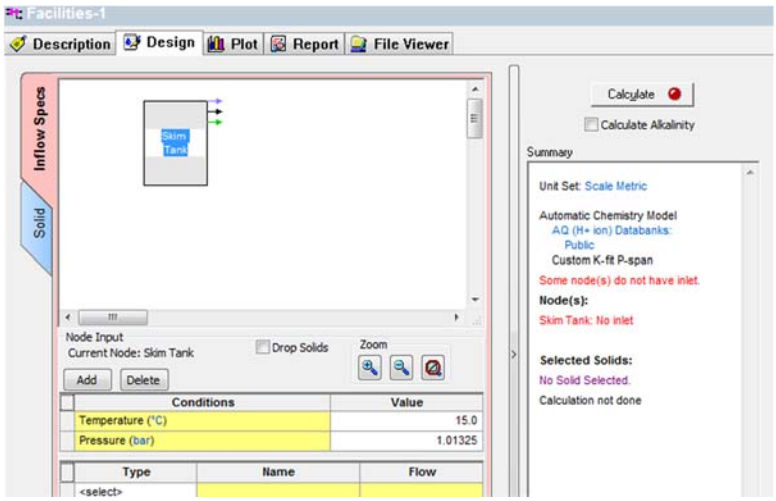


Figure 16-40 Node input Screen

Enter the name, description, conditions, and streams for the Skim Tank shown above. When complete, your screen should look like this.

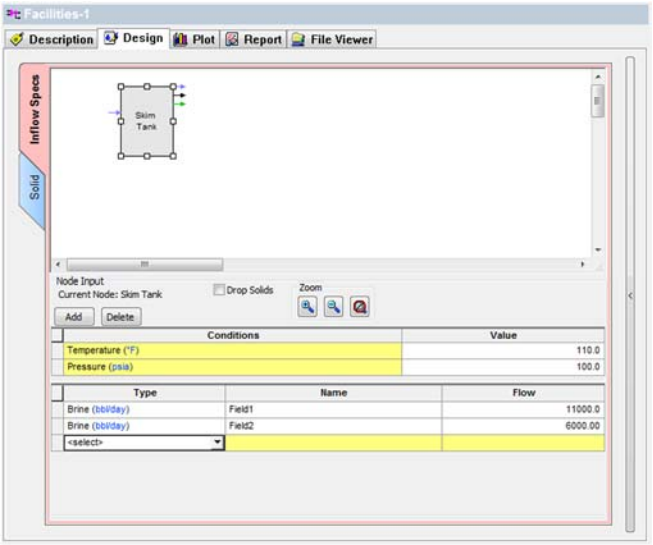


Figure 16-41 Node 1 is complete

The temperature and pressure of the calculation is 110 F and 100 PSI. A default node name is supplied and it is sufficient for our use. The output of this calculation will go to the next node. Make sure to select drop solids checkbox at the Skim Tank node.

Next, enter the information for the second node, Suction Tank. We will select the output brine of the Skim tank, which is a ***brine from node*** The temperature and pressure as well as the flow of the brine are calculated.

When a brine is calculated in a facilities calculation, we have the option of allowing any produced solids to be considered (that is they traveled along with the brine) or to ***eliminate*** them as they precipitate out. We will eliminate the solids in this case. The orange downward arrow from Skim Tank indicate dropped solids.

We are also adding the **Water Supply** to this tank.

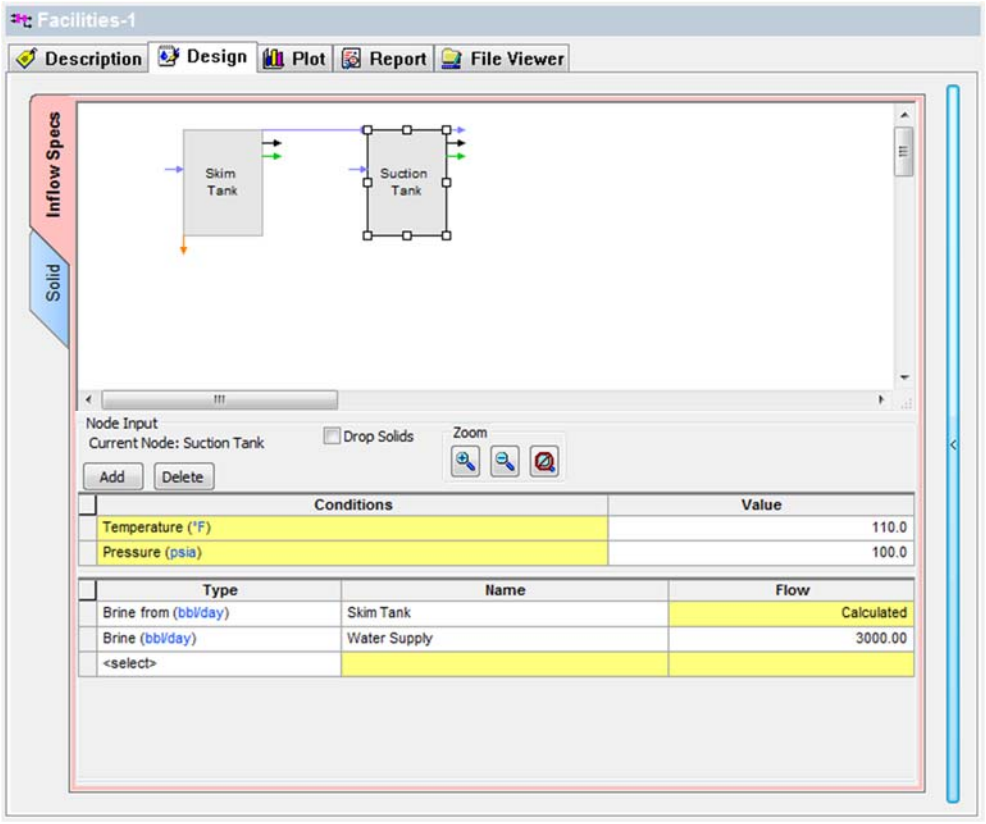


Figure 16-42 Node 2 is entered

The program assigns a default node name of **Node2** which is sufficient for our use. We have added the description **"Suction Tank"**.

Click on the Calculate button. Or press Ctrl+F9.

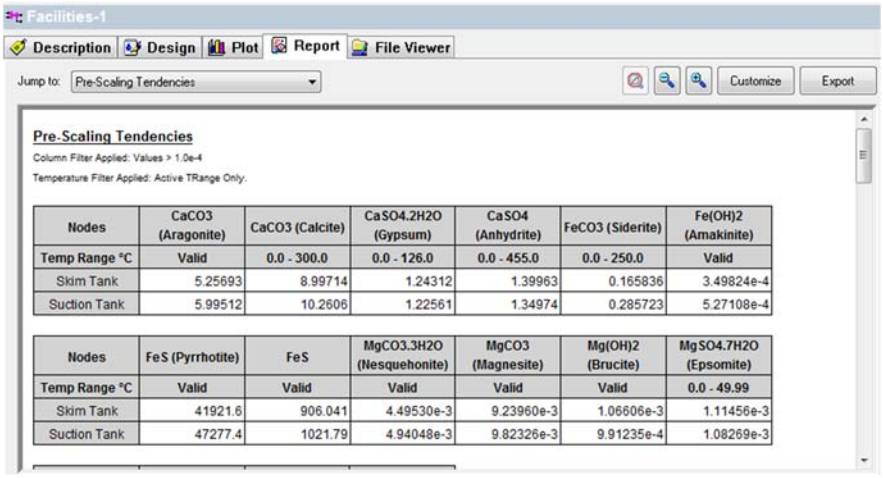


Figure 16-43 the reports tab

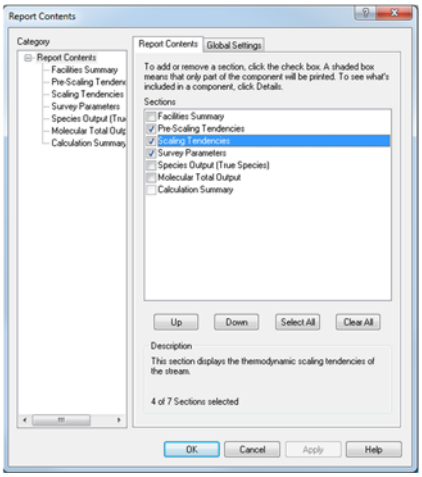
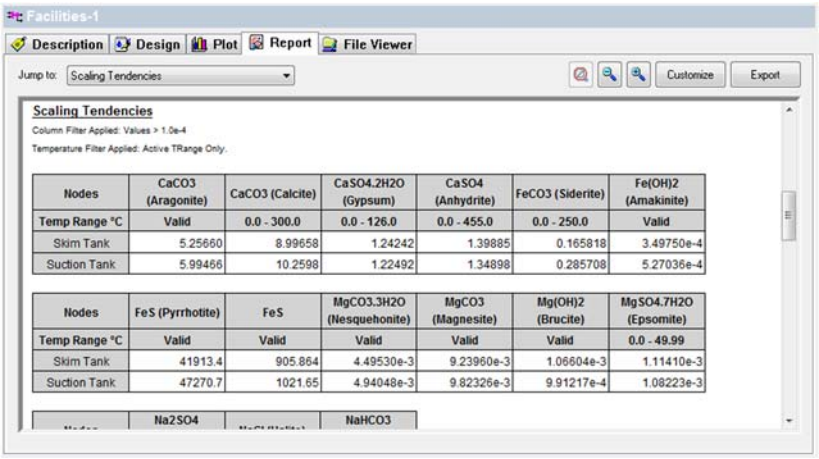


Figure 16-4 Results for nodes



Nodes	CaCO3 (Aragonite)	CaCO3 (Calcite)	CaSO4.2H2O (Gypsum)	CaSO4 (Anhydrite)	FeCO3 (Siderite)	Fe(OH)2 (Amakinite)
Temp Range °C	Valid	0.0 - 300.0	0.0 - 126.0	0.0 - 455.0	0.0 - 250.0	Valid
Skim Tank	5.25660	8.99658	1.24242	1.39885	0.165818	3.49750e-4
Suction Tank	5.99466	10.2598	1.22492	1.34898	0.285708	5.27036e-4

Nodes	FeS (Pyrrhotite)	FeS	MgCO3.3H2O (Nesquehonite)	MgCO3 (Magnesite)	Mg(OH)2 (Brucite)	MgSO4.7H2O (Epsomite)
Temp Range °C	Valid	Valid	Valid	Valid	Valid	0.0 - 49.99
Skim Tank	41913.4	905.864	4.49530e-3	9.23960e-3	1.06604e-3	1.11410e-3
Suction Tank	47270.7	1021.65	4.94048e-3	9.82326e-3	9.91217e-4	1.08223e-3

	Na2SO4		NaHCO3

Figure 16-45 Scaling tendencies