Chapter 7 **Single Point Calculations**

Objectives

By this point we have learned a great deal about the thermodynamics of the OLI Software and the internal workings of the simulation engine. We have also learned how to enter data and perform useful calculations.

We now wish to explore some of the other calculations in the OLI Studio. In the process of exploring these calculations, we will introduce some additional features.

In this chapter we will learn about:

1. Isothermal Calculations
    - Using Custom Units
2. Adiabatic Calculation
    - Using the Names Manager
3. Bubble Point Calculations
    - Using new custom units
    - Modifying the report
4. Dew Point Calculations
    - Modifying model options
5. Vapor Amount/Fraction Calculations
    - Using custom report units

Isothermal

In this example we will explore an isothermal calculation. We wish to determine the pH of a 10 weight percent acetic acid solution. The temperature and pressure will be 75 ^{o}C and 1 atmosphere.

We have already entered stream and calculation data in previous examples so we will not dwell on them here. If you have not done so, please start the OLI Studio.

1. Select the **Add Stream** icon.
2. Select the **Description** tab.
3. Replace ***Stream1*** with ***Acetic Acid Solutions.***
4. Select **Definition.** The following grid list should be displayed.

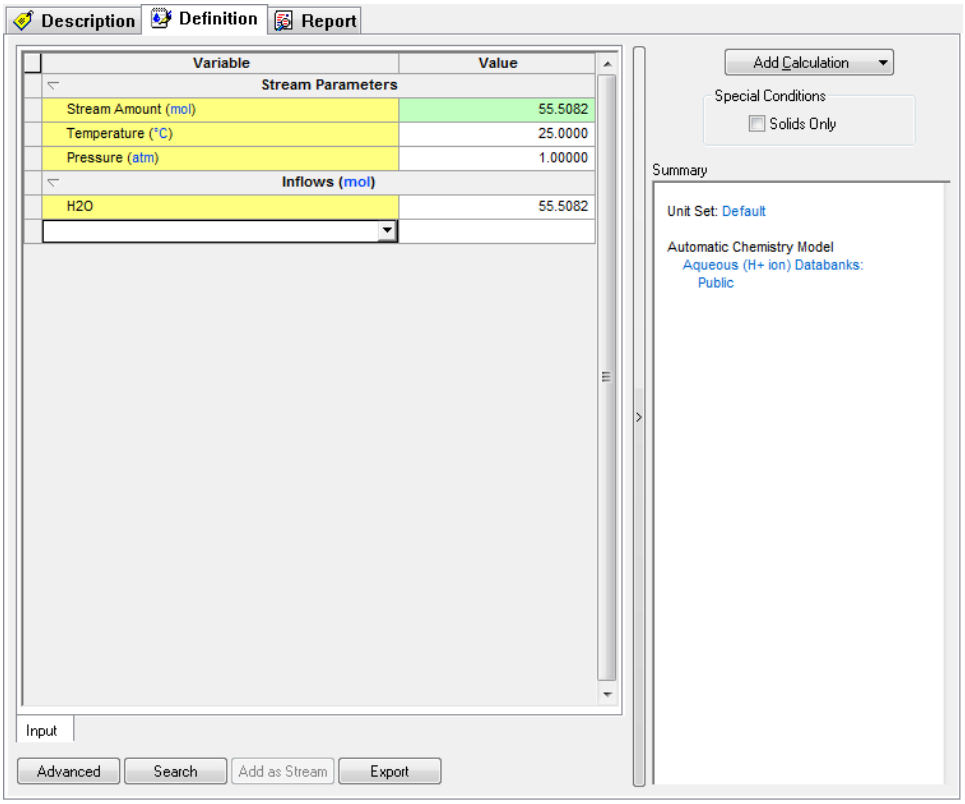


Figure 7-1 Stream Definition Input Grid

Since we wish to determine the pH of a 10 weight percent solution (a fraction type of unit) we should change our input units.

5. From the **Tools** menu item, select **Units Manager.**

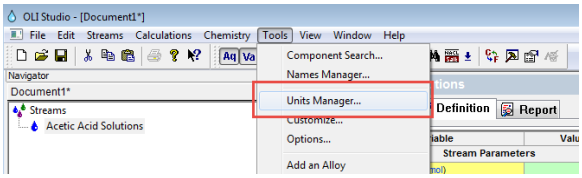


Figure 7-2 Menu Item/Tools/Units Manager

We can now modify the default set of units. The window, displayed in the following figure, shows that the **Standard** set of units are selected. We need to change these units.

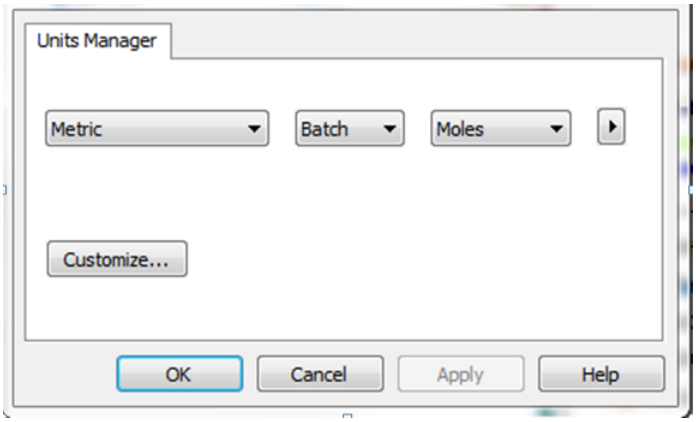
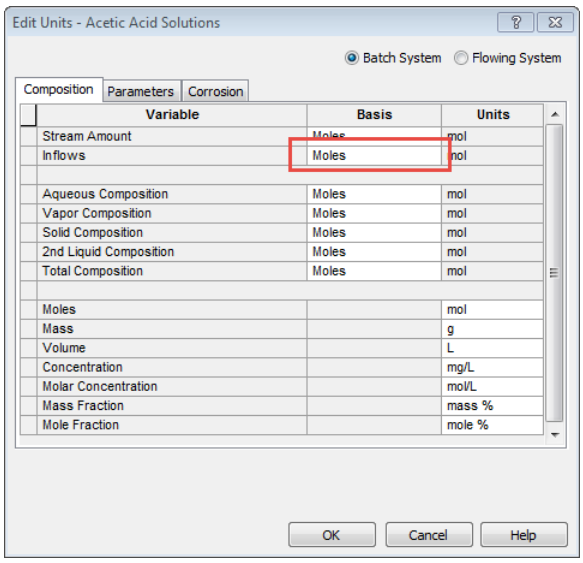


Figure 7-3 Units Manager Dialog

6. ***Click*** on the **Customize** radio button.



7. Locate the **Inflows** line currently displaying ***Moles.*** Click in the cell and change it to **Mass Fraction.**

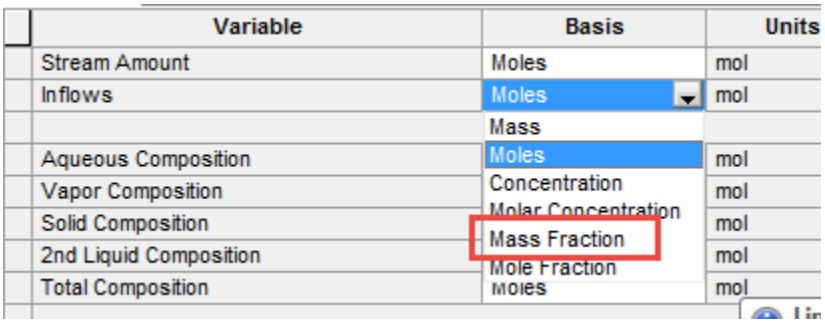
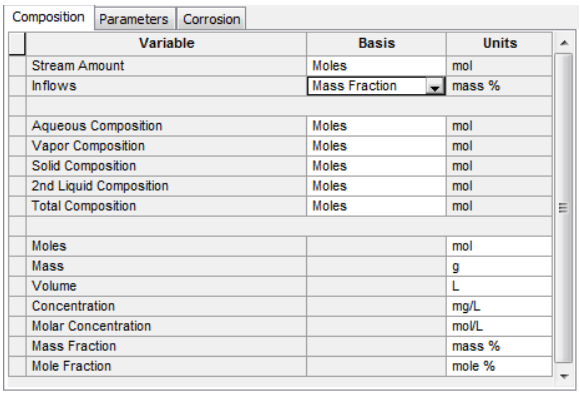


Figure 7-4 Selecting Mass Fraction



8. ***Click* <u>OK</u>** to close the units manager second layer.
9. We are now ready to enter the conditions. When using mass-fraction units, it is assumed that the amount of water will be the difference of the components entered. In this case, the value field is highlighted in yellow to inform you that the value will be determined from the values of the other components.

   Enter a value of 10 % for acetic acid, 75 ^{o}C, 1 atmosphere pressure.

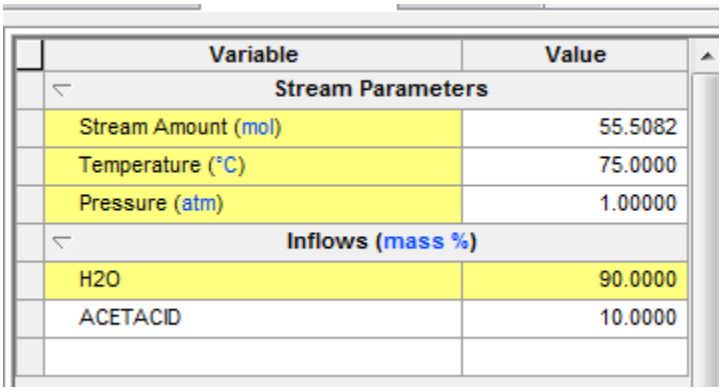


Figure 7-5 the filled out grid for 10 % Acetic Acid

10. ***Click*** on the **<u>Add Calculation</u>** ***button and select*** **<u>Single Point</u>.** Select the default calculation type – **<u>Isothermal</u>.**
11. ***Right-click*** the new object in the tree-view (usually with a name similar to SinglePoint1).

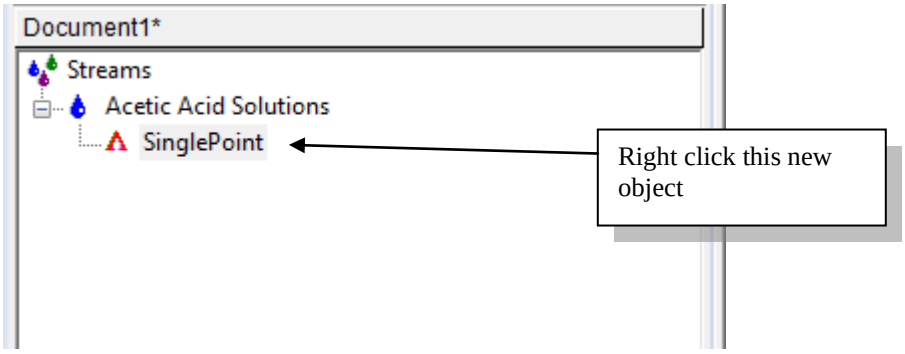


Figure 7-6 Right-click the new object

This will display a menu.

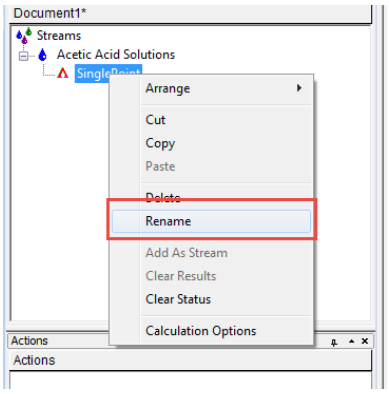


Figure 7-7 Right-click menu choices for the tree-view

Select **Rename** from the list. (Double click on the object name works too)

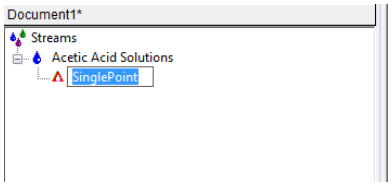


Figure 7-8 Renaming the object

The original text is now high-lighted so you can edit this field. Rename the value to ***pH.***

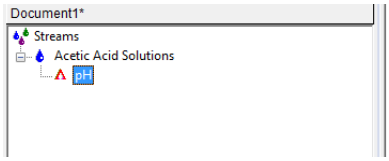


Figure 7-9 The renamed object

12. ***Click*** on the **Calculate** button to start the calculation.
13. After the calculation is complete you may:
    a. ***Click*** on the ***Output*** mini-tab display **Calculated** values.
    b. ***Right-click*** on the grid to display **Additional Stream Parameters**

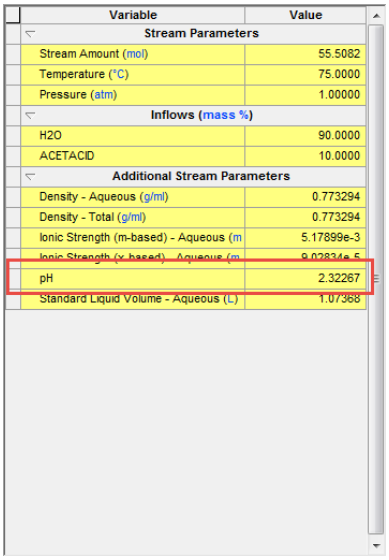


Figure 7-10 Results, the pH is approximately 2.3

The resultant pH is approximately 2.3.

Mix Calculations

In this example we are going to mix two streams of different compositions. In doing so we will determine the temperature rise of a 10 weight percent solution of calcium hydroxide mixed with pure 10 weight percent HCl. To do this, we will need to create both streams separately. Along the way, we will rename a species to a more useful name.

If you have not already done so, please start the OLI Studio. We will be adding a 10 weight-percent calcium hydroxide slurry. By now you should be familiar with adding these components.

1. Create a stream named ***Lime Slurry.***
2. ***Click*** on the **Definition** Tab.

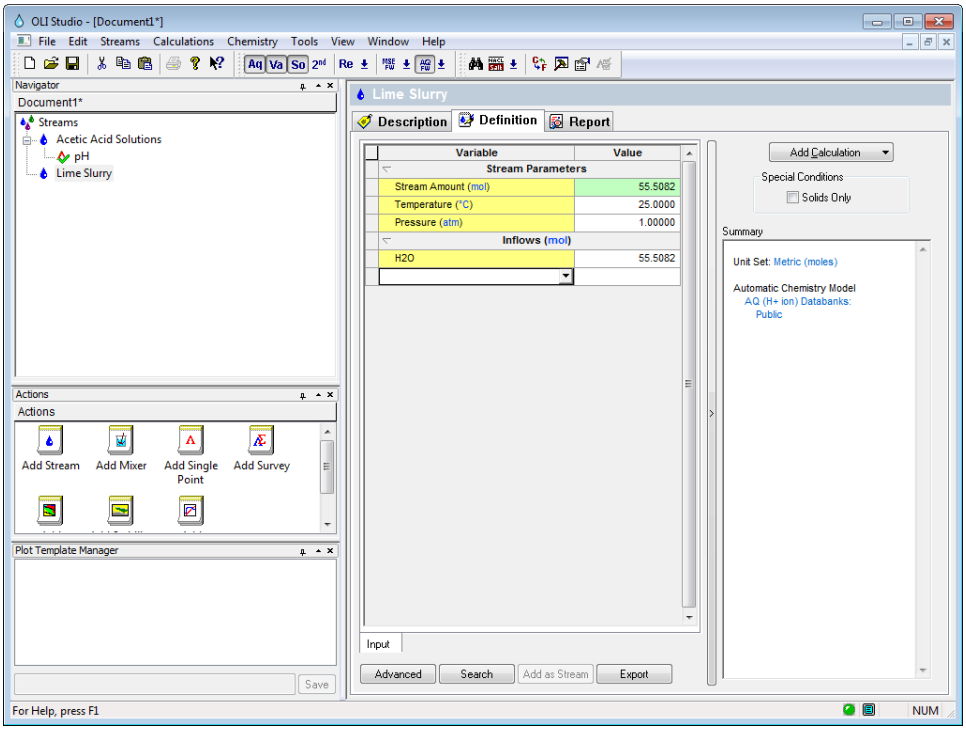


Figure 7-11 Standard Stream Definition

3. ***Click*** on the **Tools/Names Manager** menu item (see next figure).

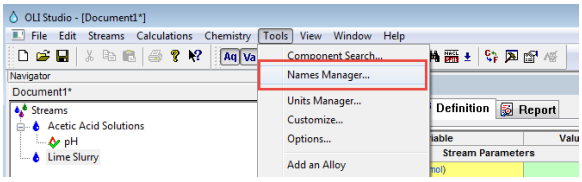


Figure 7-12 Menu Item/Tools/Names Manager

4. ***Click*** on the **Names Dictionary** tab.

We can now enter a name of a species already defined in the software. This will be entered in the **Component** column. We can then rename the species in the **User Name** column.

5. *Scroll down to find an empty cell.*

6. Enter ***$Ca(OH)_2$*** in the **Component** column. ***Left-click*** on the **User Name** column and enter ***LimeSlurry.*** (Note: Do not use spaces or special characters)

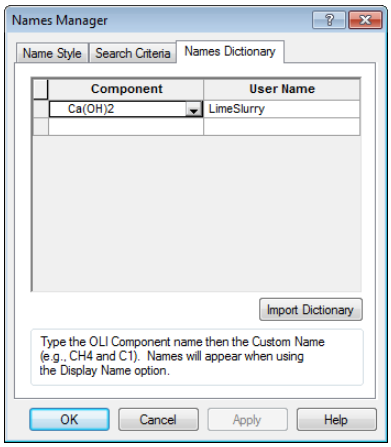


Figure 7-13 Defining Calcium Hydroxide as "Lime Slurry"

7. ***Click*** on **Apply** and then **OK.**
8. As you did in the previous example for the **"**Isothermal**"** calculation. Select **Mass-Fraction** units from the units manager for inflows and mass for stream amount.
9. ***Enter the following conditions***:
   - Temperature = 25 °C
   - Pressure = 1 atmosphere
   - Stream Amount = 1000 g
   - LimeSlurry = 10 mass %

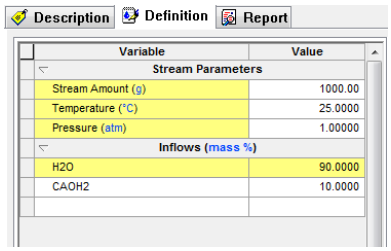


Figure 7-14 Lime Slurry Stream Definition (using display name from Names Manager Tool)

The entered name will revert back to the standard name.

We will now repeat these steps but using a 10 weight percent Hydrochloric acid solution. The input for this step is shown in the following figure.

10. Create a new Stream named ***Acid.***

11. Enter the following conditions:
    - Temperature = 25 °C
    - Pressure = 1 atmosphere
    - Stream Amount = 1000 g
    - HCl = 10 mass %

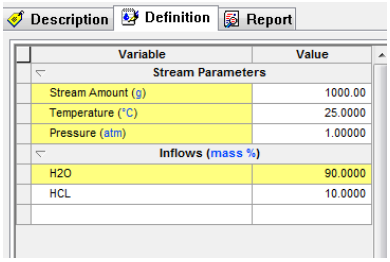


Figure 7-15 Standard stream definition for 10 wt % HCl

We will now have to add a mix calculation to determine the temperature raise.

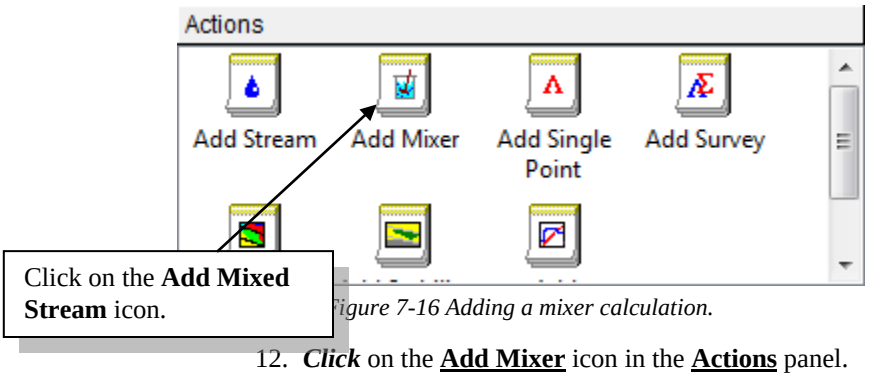


Figure 7-16 Adding a mixer calculation.

12. ***Click*** on the **Add Mixer** icon in the **Actions** panel.

This will display all possible streams for the mix calculation. There is no limit to the number of streams to be mixed. We will only select two streams.

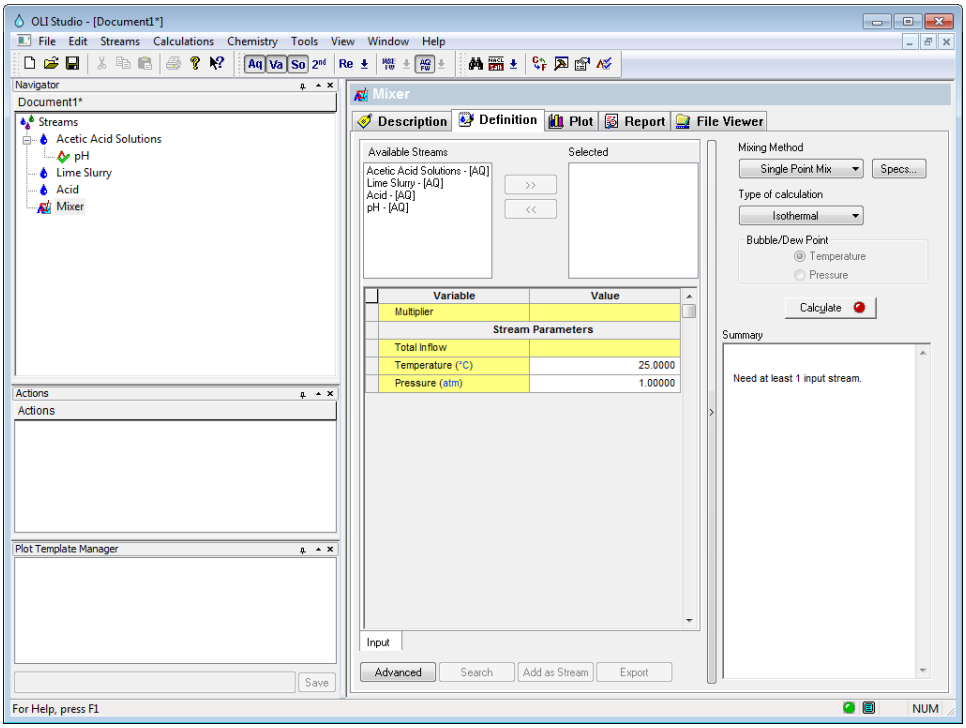


Figure 7-17 The input for the mix calculations.

13. Select the **Limeslurry** stream from the available list and ***click*** on the >> button.
14. Select the **Acid** ***stream*** and ***click*** on the >> button. The display should look like this:

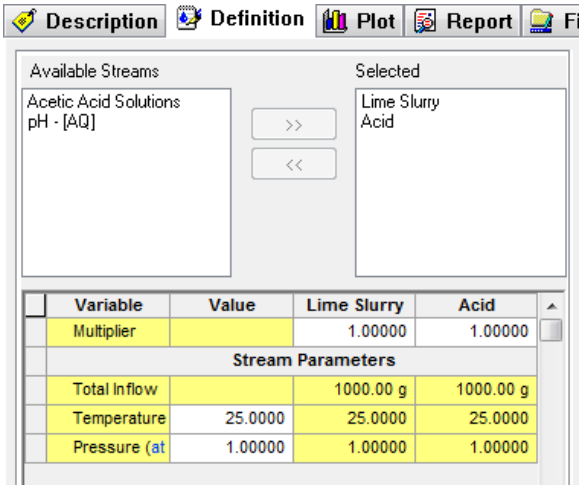


Figure 7-18 Selecting streams. You may have a different list.

The default calculation is to hold a single point calculation at isothermal conditions.

15. ***Click*** on the second **Type of Calculation** button.

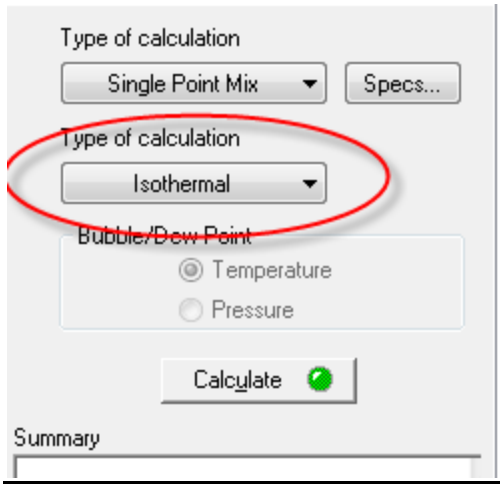


Figure 7-19 Changing the type of calculation

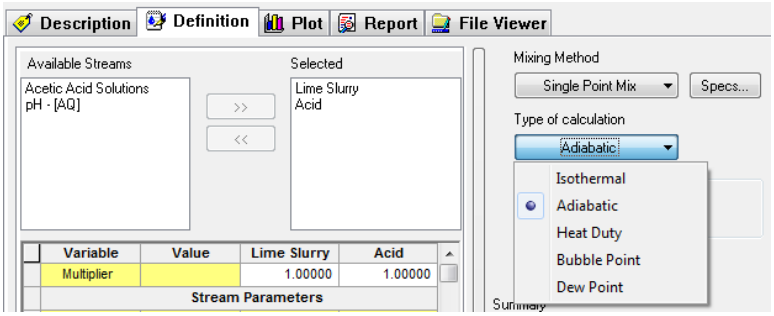


Figure 7-20 Selecting the mix calculation type.

***Select* <u>Adiabatic</u>.**

16. Click on the **<u>Calculate</u>** button.

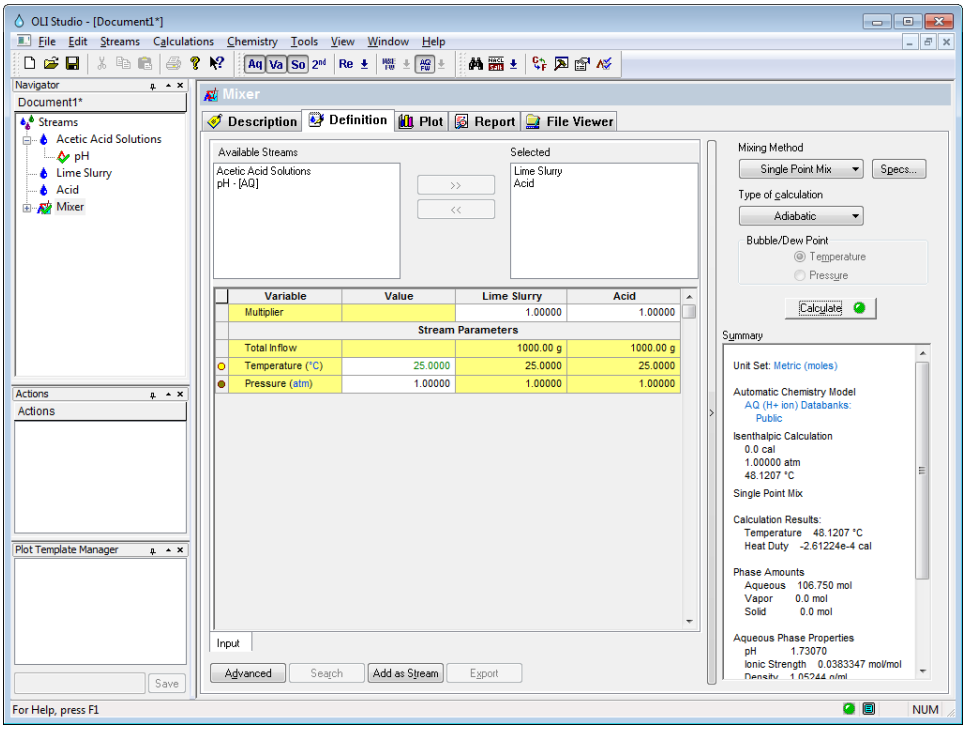


Figure 7-21 The results of the mix.

The **<u>Summary Box</u>** shows the results of the calculation. You can see that the temperature increased from 25 degrees centigrade to approximately 48.1 degrees centigrade. There was a considerable heat of reaction.

Bubble Point

Bubble points calculations are a calculation where the temperature or pressure of the system is adjusted such that a very small amount of vapor will form. This is another way of saying that the bubble point calculation is a determination of the boiling point.

Normally we determine the temperature at which a solution will boil. If the pressure is set to 1 atmosphere, then we are calculating the **Normal Boiling Point**. If we hold the temperature constant then we can determine the bubble point pressure.

Bubble point calculations are useful for determining the saturation pressure or temperature of a system. Many systems will have a vapor phase when we least expect it. Calculating the saturation pressure or temperature will allow us to set our conditions appropriately.

In this example we are using a 1 molar Acetone solution in water. Remember the molal concentration scale has moles of solute per kilogram of water. So we have 1.0 moles of Acetone and 1 liter of solution.

We are going to let you set up this calculation primarily on your own. The following is a set of steps to help you along.

1. Define a new stream and call it ***Bubble.***

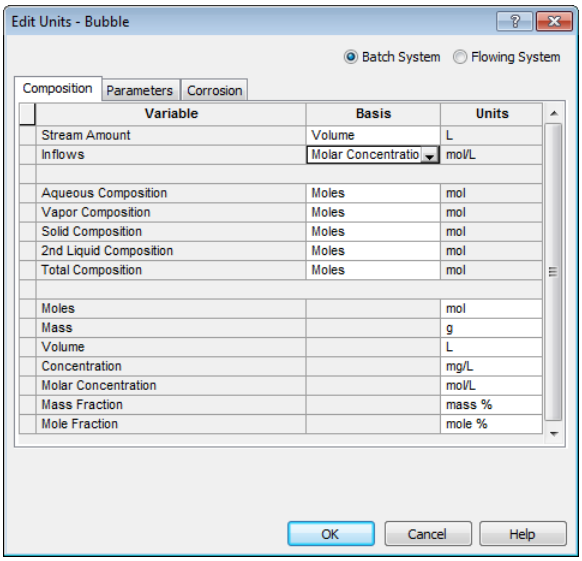
2. ***Click*** on the **Definition** tab.

3. Create a new set of units (see the Isothermal example for more details).

4. Select **Tools/Units Manager** from the **Tools** menu item.

5. Select the **Customize** button.

6. Set the **Inflows** to *Molar Concentration*



7. ***Click*** on **Apply, OK** or **Close** as appropriate.

8. Enter the following conditions:

- Stream Amount = 1 L
- Temperature = 25 C
- Pressure = 1 Atmosphere
- Water = (adjusted)
- Acetone = 1.0 molarity

9. Add a **Single Point** calculation.

10. From the **Type of Calculation** button, select **Bubble Point.**

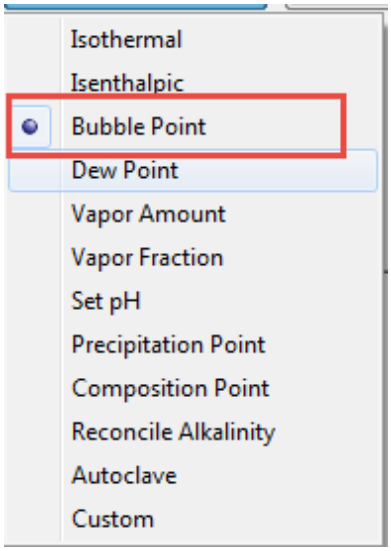


Figure 7-22 Selecting Bubble point calculations

11. Previously grayed out radio buttons are now active. Make sure that the **Temperature** radio button is selected.

Notice the presence of a "Free Dot" next to **Temperature** to indicate that value will be adjusted.

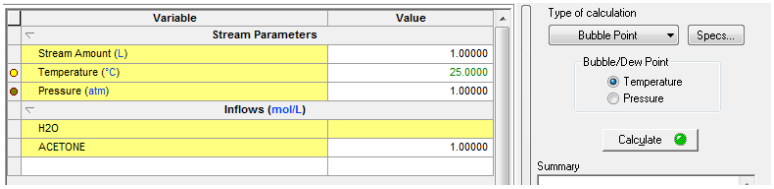
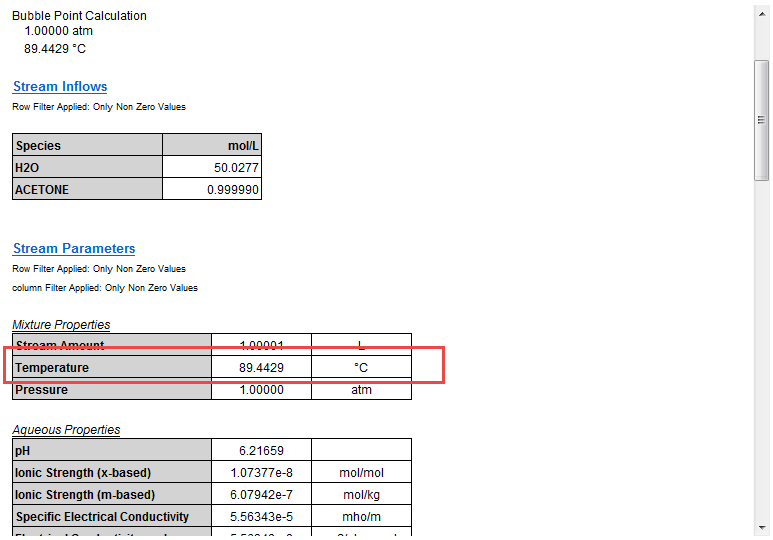


Figure 7-23 Bubble point temperatures are selected

12. ***Click*** on the **Calculate** button.
13. ***Click*** on the **Report** tab to see the results. The temperature is 89.4 C.
14. Scroll down to see more information.



Bubble Point Calculation
1.00000 atm
89.4429 °C

Stream Inflows

Row Filter Applied: Only Non Zero Values

Species	mol/L
H2O	50.0277
ACETONE	0.999990

Stream Parameters

Row Filter Applied: Only Non Zero Values

column Filter Applied: Only Non Zero Values

Mixture Properties

Stream Amount	1.00001	L
Temperature	89.4429	°C
Pressure	1.00000	atm

Aqueous Properties

pH	6.21659	
Ionic Strength (x-based)	1.07377e-8	mol/mol
Ionic Strength (m-based)	6.07942e-7	mol/kg
Specific Electrical Conductivity	5.56343e-5	mho/m

Figure 7-24 The bubble point is 89.4 C

There is a lot of information that is displayed just for this relatively simple case. The user does have the option to limit the display of data. Remember that the data is not lost, merely not displayed.

15. ***Click*** on the **Customize** button.

16. By default, all the options are selected. Clear all the **Check Boxes** leaving only **Calculation Summary**, **Stream Inflows** and **Stream Parameters** selected.

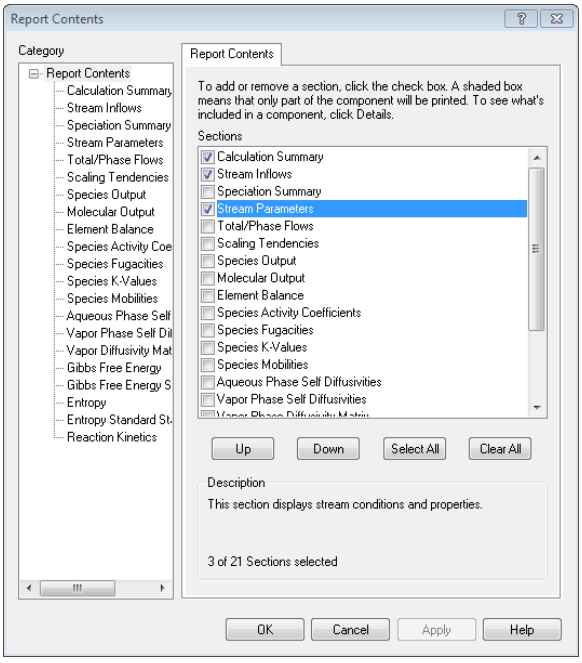


Figure 7-25 Customizing information displayed in a Report

17. ***Click*** the **OK** ***button.*** Scroll down to see that some of the information has been suppressed.

Dew Point

It is frequently useful to determine the temperature or pressure at which a gas will condense. In this example we have a simple hydrocarbon laden gas. We wish to determine the condensation temperature otherwise known as the dew point temperature.

In this example we have the following conditions:

Initial Temperature	=	25	°C	(This is an initial guess)
Pressure	=	1	atmosphere	
H_2O	=	1	mole	
CO_2	=	1	mole	
CH_4	=	95	moles	
H_2S	=	3	moles	

In previous examples you have entered data for the stream. We will not repeat them here. The following figure is the set up for the Dew Point calculation. Please enter the data.

Click on the <u>Calculate</u> button when ready.

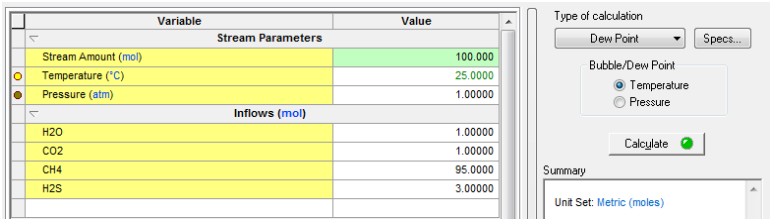


Figure 7-26 Bubble Point Temperature Stream Definition

After the calculation is complete, the resultant temperature is approximately 7.01483 C.

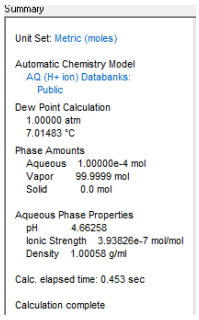


Figure 7-27 Results with standard model options

The mathematical model that the OLI Studio uses is the Helgeson equation of state (see Chapter 6). To evaluate this equation of state, the OLI software has "pre-generated" a set of values for each equilibrium constant as a function of temperature.

Occasionally, the operating temperature may be outside the default temperature and pressure ranges. These default ranges are: **25 – 225 °C** and **1 – 200 Atmospheres.** In this example, the new temperature is lower than the defaults. This may have caused some offset in our answer.

To check to see if our answer changes we need to modify the model options.

1. ***Click*** on the **Menu Item: Chemistry**
2. ***Click*** on **Model Options**

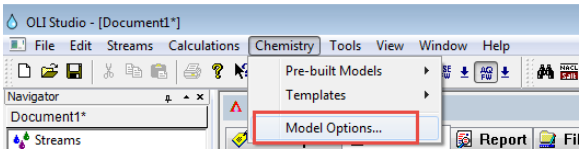


Figure 7-28 Menu Item: Chemistry

Below is the default **Model Options** screen.

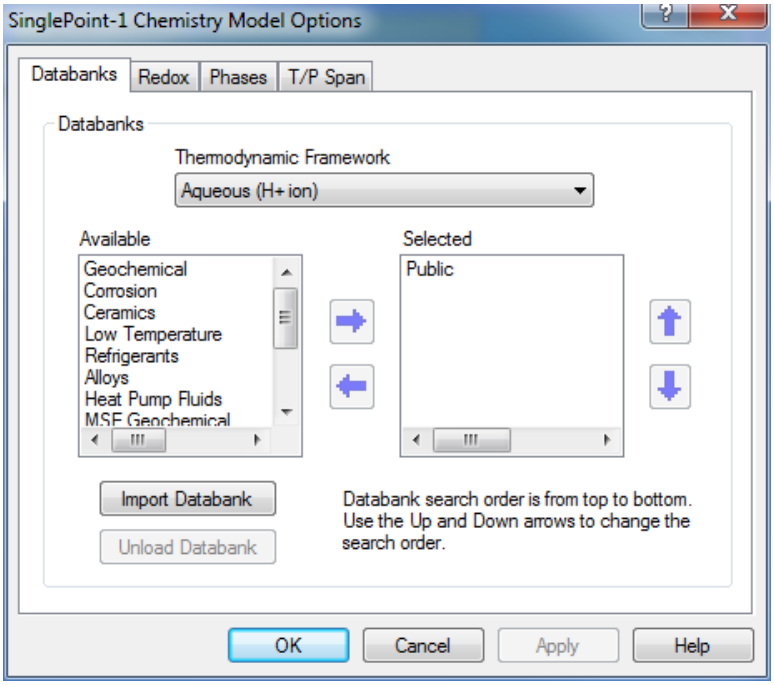


Figure 7-29 The Model Options screen.

3. ***Click*** on the **T/P Span** tab.

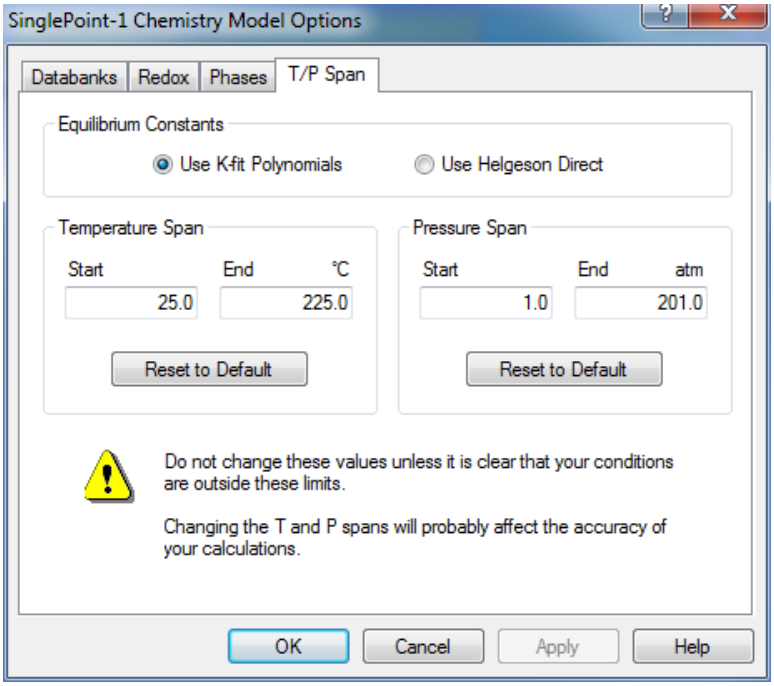


Figure 7-30 The Temperature and pressure span model options

4. Change the lower temperature from ***25*** to ***0*** and then ***click* <u>OK</u>.**

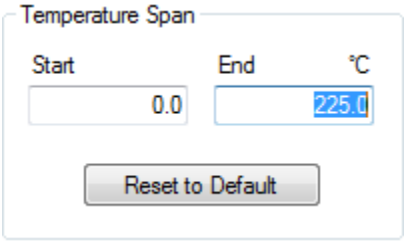
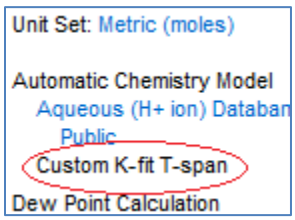


Figure 7-31 Modified temperature model options

5. From the **<u>Definition</u>** screen, re-calculate the problem.

The new temperature is 7.03 ^{o}C. This is only slightly different from our original value of 7.016 ^{o}C.

Please note that once you change the Temperature or Pressure span, you are going to see a message in the summary section



This just means that you have changed the default setting. All ScaleChem objects have this because the pressure range has been changed up to a 1500 atm internally.

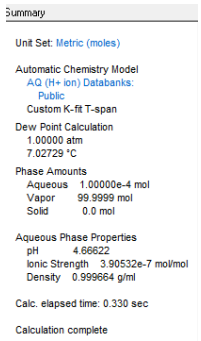


Figure 7-32 Results with modified model options

Vapor Amounts/Fractions

In this example we have a brine in which we want to evaporate to concentrate the brine. To do this we will adjust the temperature (or pressure) to create a specified amount of vapor (or vapor fraction).

In this case we want to adjust the temperature such that our system is 95 percent vapor (on a mole basis). Please enter the following conditions into a stream definition:

Temperature	=	25	^{o}C
Pressure	=	1	Atmosphere
NaCl	=	9.0	mass %
$CaSO_4$	=	1.0	mass %
Vapor Fraction	=	0.95	mole/mole

The component compositions are grams of species per 100 grams of solution (a weight fraction). The vapor fraction is in moles of vapor per mole of solution and is a mole fraction.

You must change the units for this example. You already have done this previously.

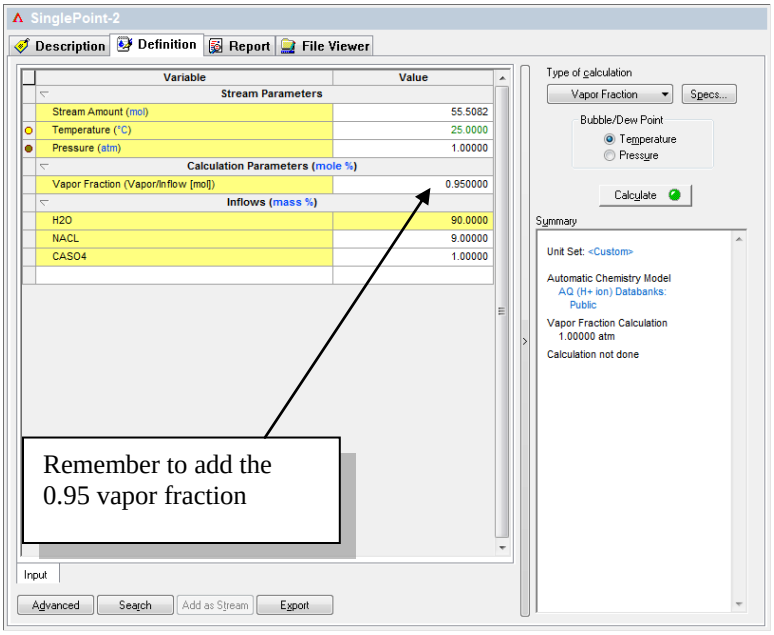


Figure 7-33 Vapor Fraction Stream Definition

Click on **<u>Calculate</u>** to start.

After the program finishes the calculation, the temperature is approximately 101 ^{o}C. At this temperature, 95 percent of the system will be vapor.

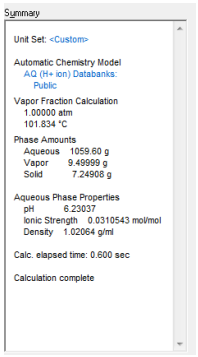


Figure 7-34 Summary of Vapor Fraction

Desalinating brines often create solids known as scales. These scales are often detrimental to the operation of the desalination unit. We should review the reports to see how much solid has been produced.

Click on the **<u>Report</u>** tab.

The following figure shows that both solid sodium chloride (halite) and calcium sulfate (anhydrite) have scaled out. The operator may wish to divide the desalination unit into smaller units to prevent scaling.

Species Output (True Species)

Row Filter Applied: Only Non Zero Values

column Filter Applied: Only Non Zero Values

	Total	Aqueous	Vapor	Solid
	mol	mol	mol	mol
H2O	53.7716	53.2443	0.527328	0.0
HION	6.95925e-7	6.95925e-7	0.0	0.0
OHION	1.57322e-6	1.57322e-6	0.0	0.0
CLION	1.65748	1.65748	0.0	0.0
HCL	1.46697e-10	1.69224e-11	1.29774e-10	0.0
NAION	1.65754	1.65754	0.0	0.0
CACL2	2.13394e-12	2.13394e-12	0.0	0.0
CACLION	5.61472e-5	5.61472e-5	0.0	0.0
CAION	0.0250859	0.0250859	0.0	0.0
CAOHION	4.50552e-7	4.50552e-7	0.0	0.0
CASO4	0.0539185	6.71912e-4	0.0	0.0532466
H2SO4	1.07728e-23	1.07623e-23	7.05533e-26	0.0
HSO4ION	1.33671e-6	1.33671e-6	0.0	0.0
NASO4ION	1.8635e-8	1.8635e-8	0.0	0.0
SO3	7.10783e-27	7.10766e-27	1.6772e-31	0.0
SO4ION	0.0251412	0.0251412	0.0	0.0
Total (by phase)	57.1909	56.6103	0.527328	0.0532466

Figure 7-35 Vapor Fraction results