23. Modeling the Effects of Complexation on Corrosion

Overview

We continue to review the Corrosion Analyzer and its capabilities in modeling corrosion. In this section we will simulate the reaction of Copper with Ammonia and Gold metal with Cyanide.

This section attempts to answer the question of how strong complexing agents affect the passivation of these metals.

Copper and Ammonia

Create a stream with the following conditions:

Table 23-1 Copper and Ammonia complexing example

Parameter	Value	Comment
Stream Amount (mol)	55.5082	Default value
Temperature (ºC)	25	
Pressure (atm)	1	
H2O (mol)	55.5082	Default Value
Acid Titrant	HCl	No initial value
Base Titrant	NaOH	No Initial Value
NH3	0	No Initial Value used as a complexing agent
Contact Surface	Cu	

As with the other tours, please set the names manger to suit your personal preferences for names display.

Create a stability diagram using the above stream.

Verify that only Copper is the selected redox subsystem using the **Chemistry** menu item and **Model Options**.

The completed grid should look similar to the following figure:

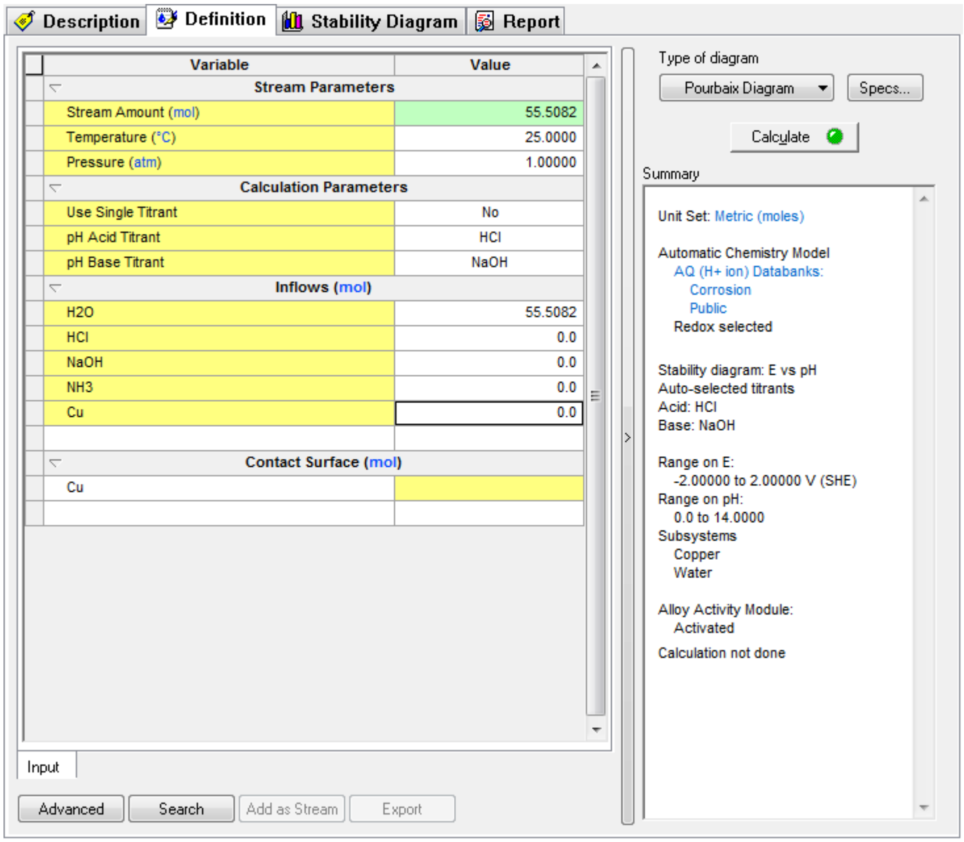

Figure 23-1 The Cu-Ammonia stability diagram definition.

Click on the **Calculate** button when ready.

When the calculation has finished, click on the **Stability Diagram** tab.

The following diagram should be displayed.

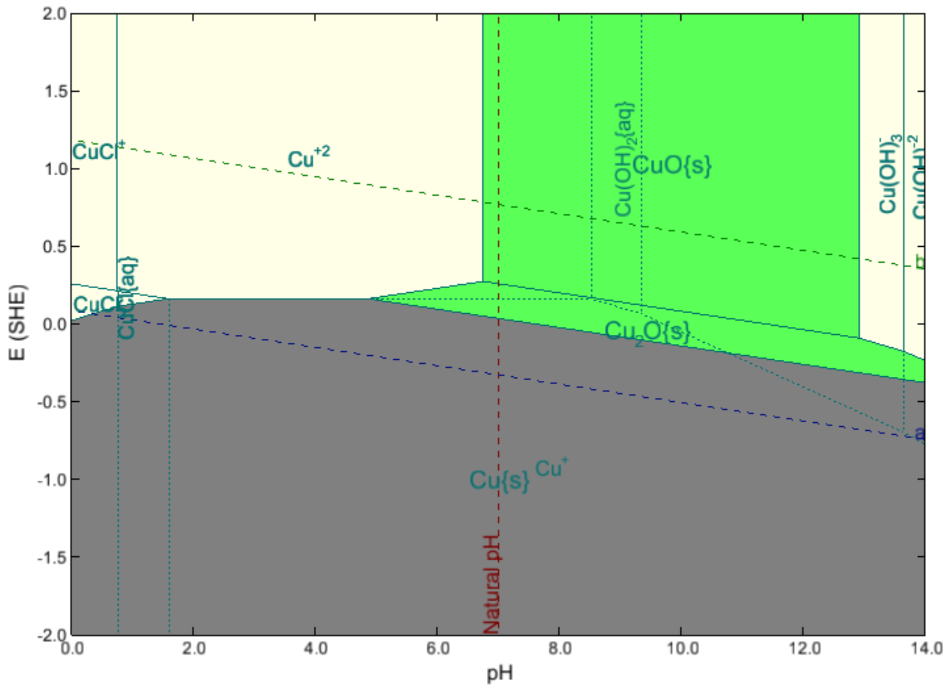

Figure 23-2 The stability diagram of Copper in the presence of Ammonia at 25° C and 1 atm.

In the absence of oxygen (looking at only the ***a*** line). We can see that the copper equilibrium line lays above the hydrogen ***a*** line. This means there is insufficient oxidizing power in the water to corrode copper metal in pure water.

We now wish to see the effects of ammonia on the stability of copper. Click on the **Definition** tab and enter ***0.1 moles of NH3.*** The diagram should still be set up, click on the **Calculate** button to start. When the calculation has finished, click on the **Stability Diagram** tab once again.

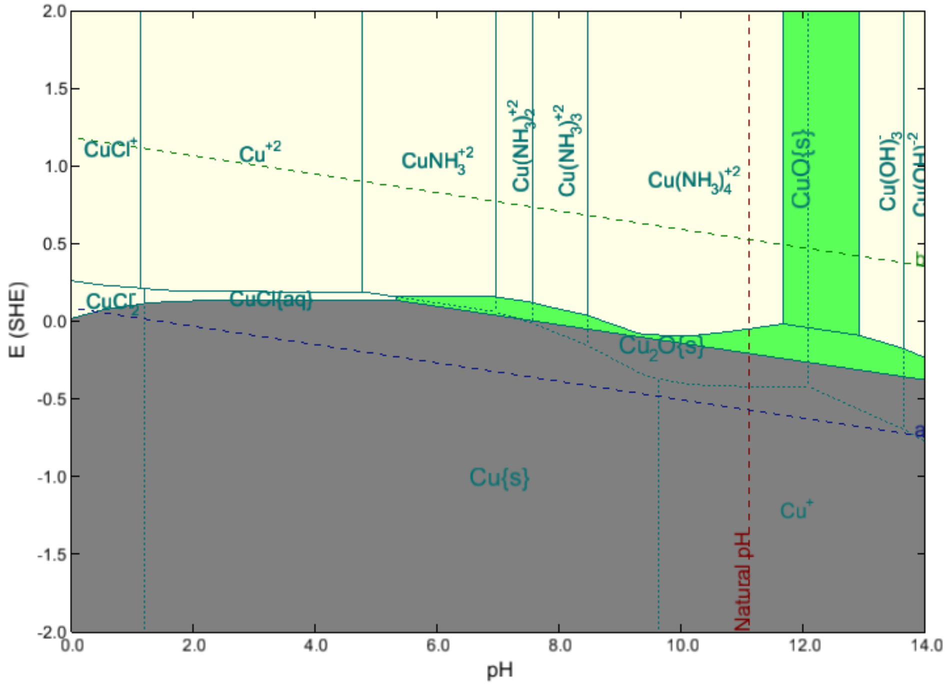

Figure 23-3 The effect of adding 0.1 moles of ammonia on the stability diagram.

A large area of corrosive liquid has appeared in the stability field for the copper oxides. This means that it is thermodynamically possible for the ammonia to break down the passivation layer of copper oxide in the presence of oxygen. Notice that in the absence of oxygen (the ***a*** line only), copper is still stable.

Now repeat the exercise with ***1.5 moles of NH3***.

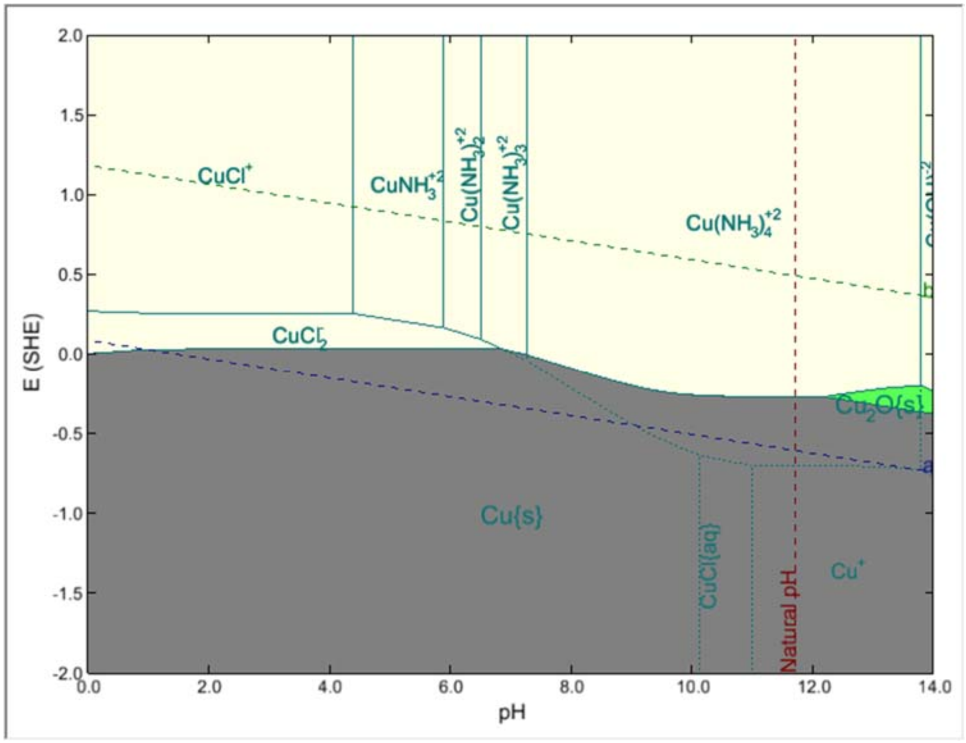

Figure 23-4 The effect of adding 1.5 moles of ammonia on the stability diagram.

At this concentration of ammonia, most, if not all the passivating copper oxide has been reacted away. Only at very high pH values are there any stable oxides.

Gold in the presence of Cyanides

Create a new stream with the following composition:

Table 23-2 Gold in the presence of cyanide

Parameter	Value	Comment
Stream Amount (mol)	55.5082	Default value
Temperature (ºC)	25	
Pressure (atm)	1	
H2O (mol)	55.5082	Default Value
Acid Titrant	HCl	No initial value
Base Titrant	NaOH	No Initial Value
NaCN	0	No Initial Value used as a complexing agent
Contact Surface	Au	

The input grid should be similar to this:

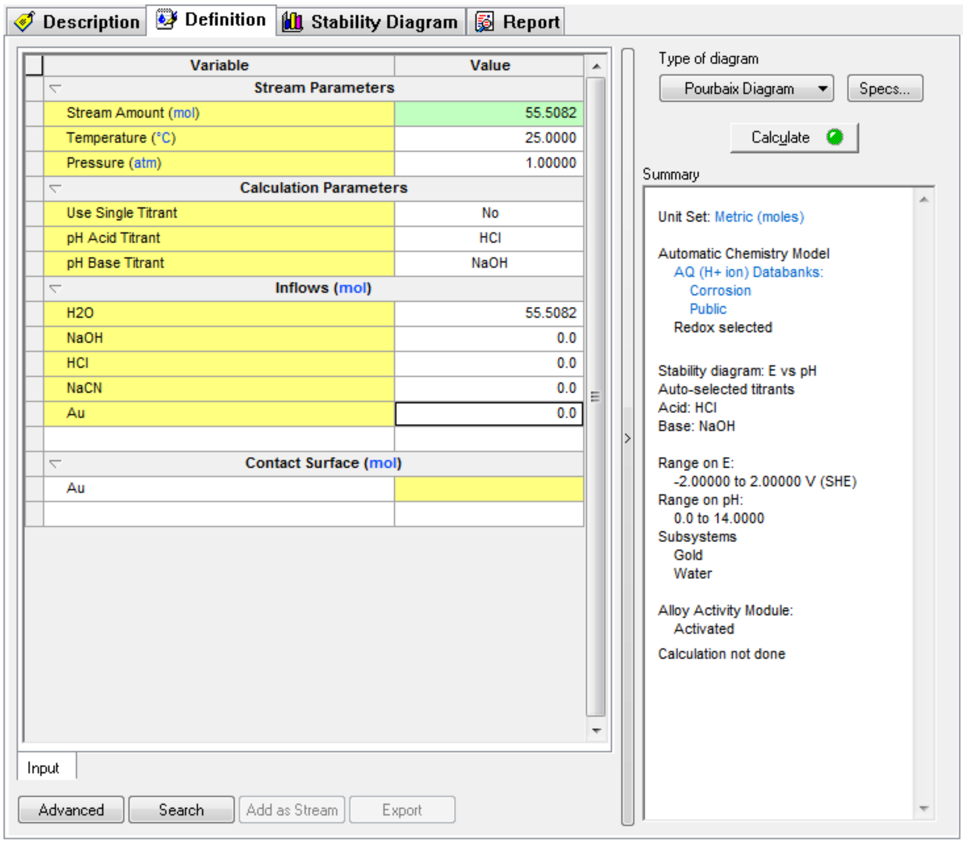

Figure 23-5 The Gold-Cyanide stability diagram definition.

Click on the **Calculate** button when you are ready. When the calculation has finished, click on the **Diagram** tab.

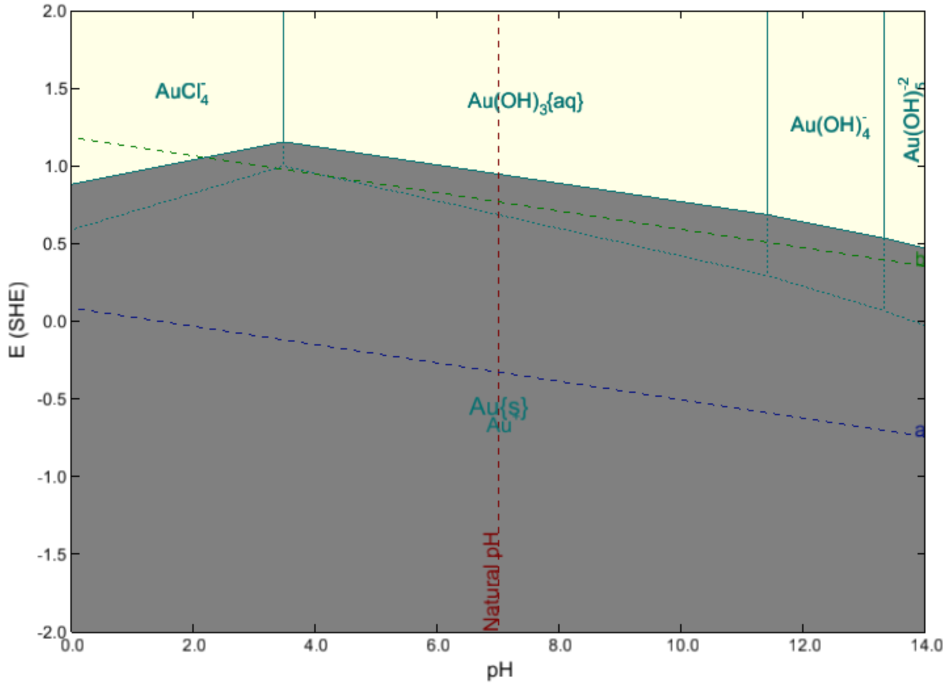

Figure 23-6 The stability diagram of Gold in the presence of Cyanide at 25° C and 1 atm.

You can see that without oxygen, gold metal is immune to corrosion. The hydrogen line ***a*** is below the gold equilibrium line. In the presence of oxygen, gold is still immune to corrosion except at very low pH.

Now repeat the exercise with ***1.0E-04 moles of NaCN.***

The figure should look like this:

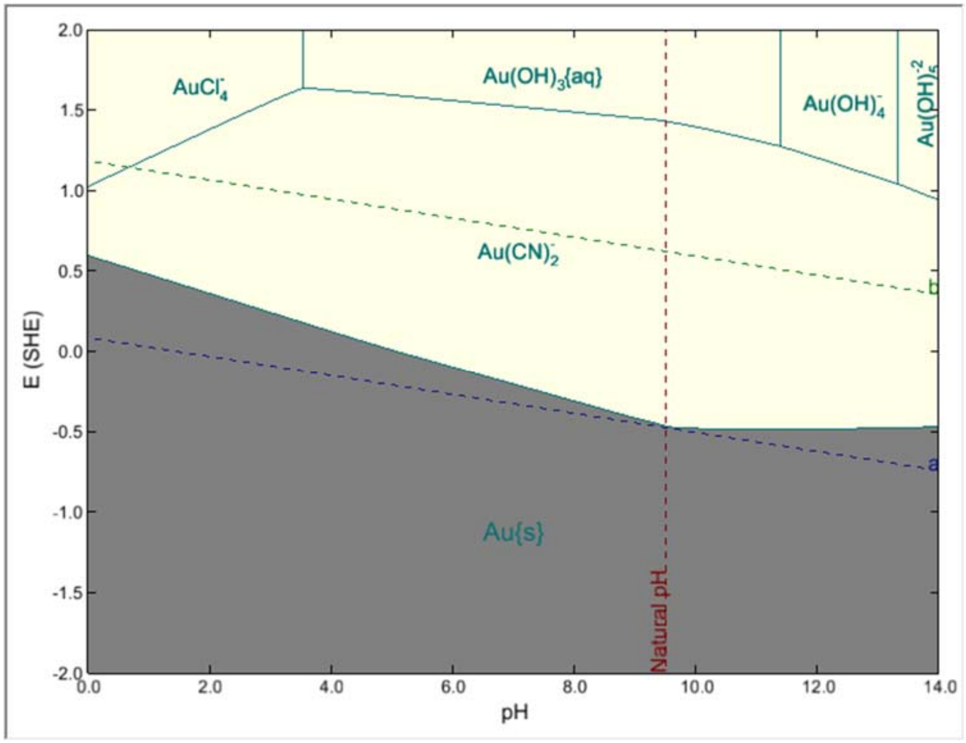

Figure 23-7 The effect of adding 1.0E-04 moles of NaCN on the stability diagram.

In the presence of oxygen, gold completely corrodes with cyanide. This is primarily due to the gold complex: $Au(CN)_2^{-1}$.

You can download a worked example of this chapter from the OLI Wiki Page