

22. Modeling the Effects of Acidity & Alkalinity on Corrosion

Overview

In this section we take a brief look at the effects of acidity and alkalinity on corrosion. You should already be familiar with many of the features and controls of the Corrosion Analyzer; thus we will not dwell on the intricate details.

In this section we will generate a stability diagram for iron in water at high temperature, simulating a high temperature boiler. We then create a stability diagram for alkaline neutralization in an oil refinery.

High Temperature Iron in Water

Using the skills you already know, create a stream and stability diagram definition for the following condition:

Table 22-1 High Temperature Iron Example Parameters

Parameter	Value	Comment
Stream Amount (mol)	55.5082	Default value
Temperature (°C)	300	
Pressure (atm)	150	
H2O (mol)	55.5082	Default Value
Base Titrant	NaOH	No initial value
Acid Titrant	HCl	No Initial Value
Contact Surface	Fe	

As with the previous tour, the contact surface will be iron (Fe). The titrants will be hydrochloric acid (HCl) for the acid and sodium hydroxide (NaOH) for the base. Allow for only the iron subsystem to be displayed.

The input grid should look like the following figure:

Description
Definition
Report

Variable	Value
Stream Parameters	
Stream Amount (mol)	55.5082
Temperature (°C)	300.000
Pressure (atm)	150.000
Inflows (mol)	
H2O	55.5082
Fe	0.0
NaOH	0.0
HCl	0.0

Special Conditions
 Solids Only

Summary

Unit Set: [Metric \(moles\)](#)

Automatic Chemistry Model
[A.Q \(H+ ion\) Databanks:](#)
[Corrosion](#)
[Public](#)

Figure 22-1 The stream definition.

Description Definition **Stability Diagram** Report

Variable	Value
Stream Parameters	
Stream Amount (mol)	55.5082
Temperature (°C)	300.000
Pressure (atm)	150.000
Calculation Parameters	
Use Single Titrant	No
pH Acid Titrant	HCl
pH Base Titrant	NaOH
Inflows (mol)	
H2O	55.5082
NaOH	0.0
HCl	0.0
Fe	0.0
Contact Surface (mol)	
Fe	

Type of diagram: Pourbaix Diagram Specs...

Summary
 Unit Set: Metric (moles)
 Automatic Chemistry Model
 AQ (H+ ion) Databanks:
 Corrosion
 Public
 Redox selected
 Stability diagram: E vs pH
 Auto-selected titrants
 Acid: HCl
 Base: NaOH
 Range on E:
 -2.00000 to 2.00000 V (SHE)
 Range on pH:
 0.0 to 14.0000
 Subsystems
 Iron
 Water
 Alloy Activity Module:
 Activated
 Calculation not done

Figure 22-2: The definition grid prior to calculation.

Click the **Calculate** button. When the calculation has finished, click the **Stability Diagram** tab.

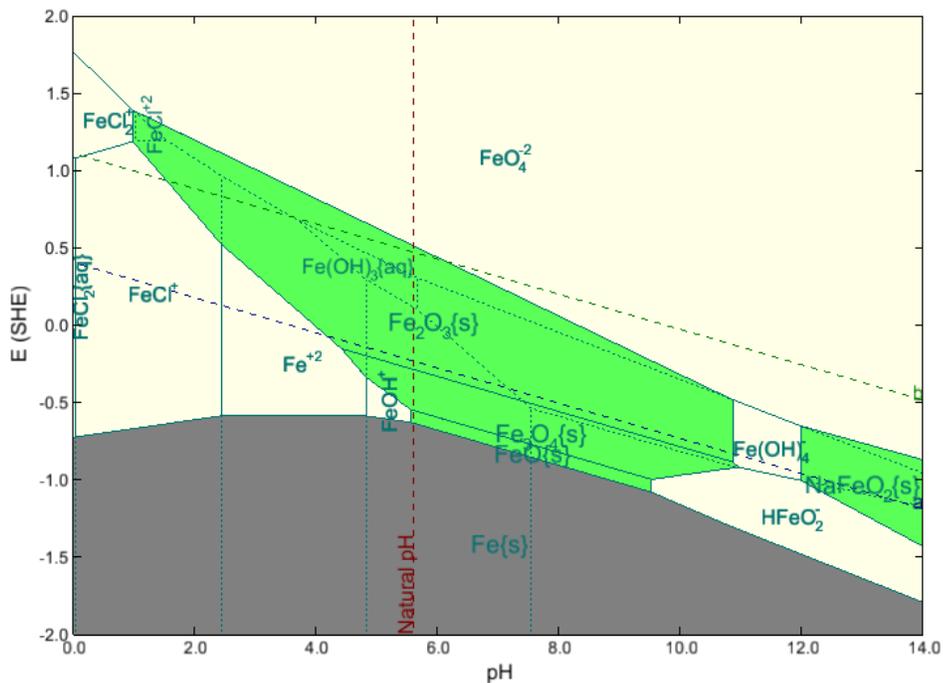


Figure 22-3 Iron in water at 300 °C and 150 atmospheres.

We can see from the diagram that passivation is only possible at moderate pH's.

How does the prediction of passivation relate to corrosion rate data?⁴³

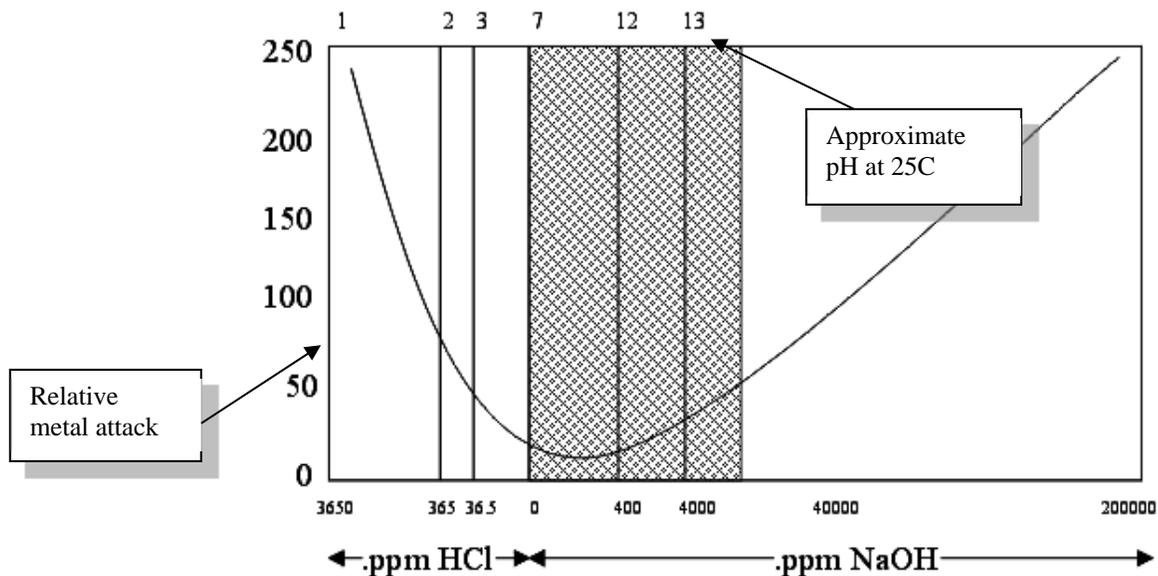


Figure 22-4 Relative metal attack v. pH and titrant concentration

The hatched area corresponds to the stability of a passivation layer. The corrosion rate is greatly reduced when a passivation layer is present.

Neutralization of Refinery Streams with Alkanolamines

Create a Stream Definition for the following conditions

Table 22-2 Alkanolamine Example

Parameter	Value	Comment
Stream Amount (mol)	55.5082	Default value
Temperature (°C)	50	
Pressure (atm)	1	
H ₂ O (mol)	55.5082	Default Value
Acid Titrant	HCl	No initial value
Base Titrant	DEA ⁴⁴	No Initial Value
C ₈ H ₁₈ (mol)	2E-07	

⁴³ Relative corrosion rate data as a function of HCl and NaOH added to Solution (Partridge and Hall, Trans. Am. Soc. Mech. Eng. 1939, 61, 597)

⁴⁴ The “ESP” name for this species is DEXH, which can be used as an input to make your life easier. The formula name is: HN(C₂H₄OH)₂

C7H16 (mol)	8E-07	
C3H8 (mol)	1.2E-04	
C4H10 (mol)	2E-05	
C5H12 (mol)	7E-6	
C6H14 (mol)	2E-6	
H2S	0.01	
Contact Surface	Fe	

The input grid should look approximately like this:

Variable	Value
Stream Parameters	
Stream Amount (mol)	55.5183
Temperature (°C)	50.0000
Pressure (atm)	1.00000
Inflows (mol)	
H2O	55.5082
HCl	0.0
HN(C2H4OH)2	0.0
C8H18	2.00000e-7
C7H16	8.00000e-7
n-C4H10	2.00000e-5
C5H12	7.00000e-6
C6H14	2.00000e-6
H2S	0.0100000
Fe	0.0

This species is DEA

Figure 22-5 Stream input grid.

Create a stability diagram as in previous chapters

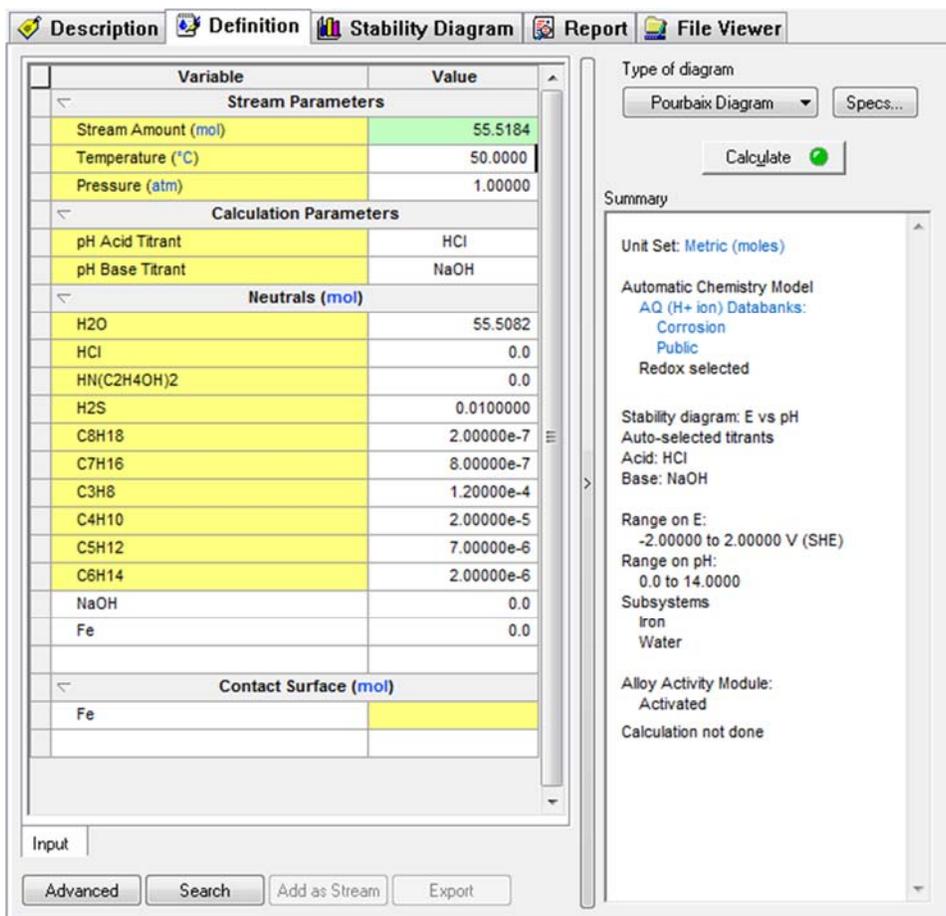
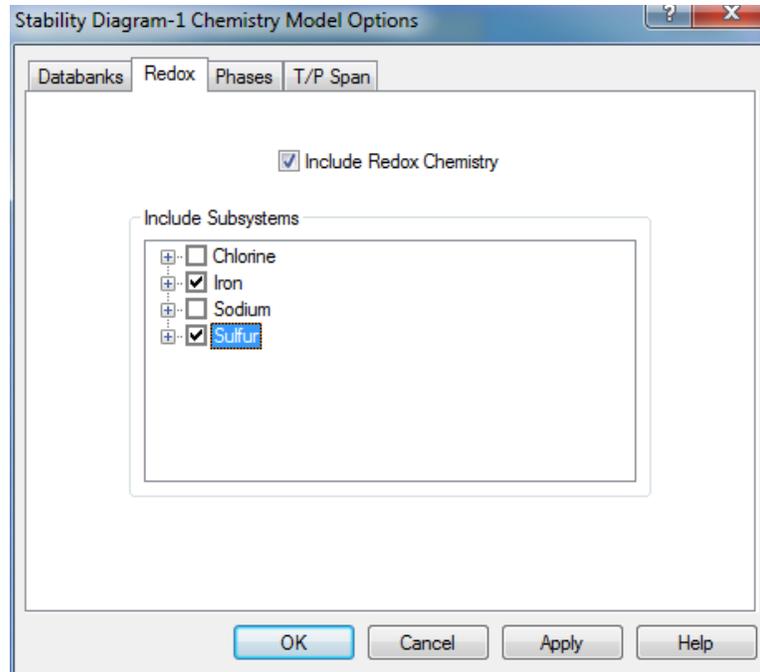


Figure 22-6: The stability diagram definition.

Remember to use the **Specs...** button to select the pH titrants. You are using HCL and DEA as the titrants.

Let's review the redox subsystems via Chemistry | Model Options | Redox

Make sure **Sodium** is not checked in the list of included subsystems and that Sulfur is checked in the **Redox** section of the chemistry model options.



22-7: Selecting the redox subsystems from the chemistry model options.

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

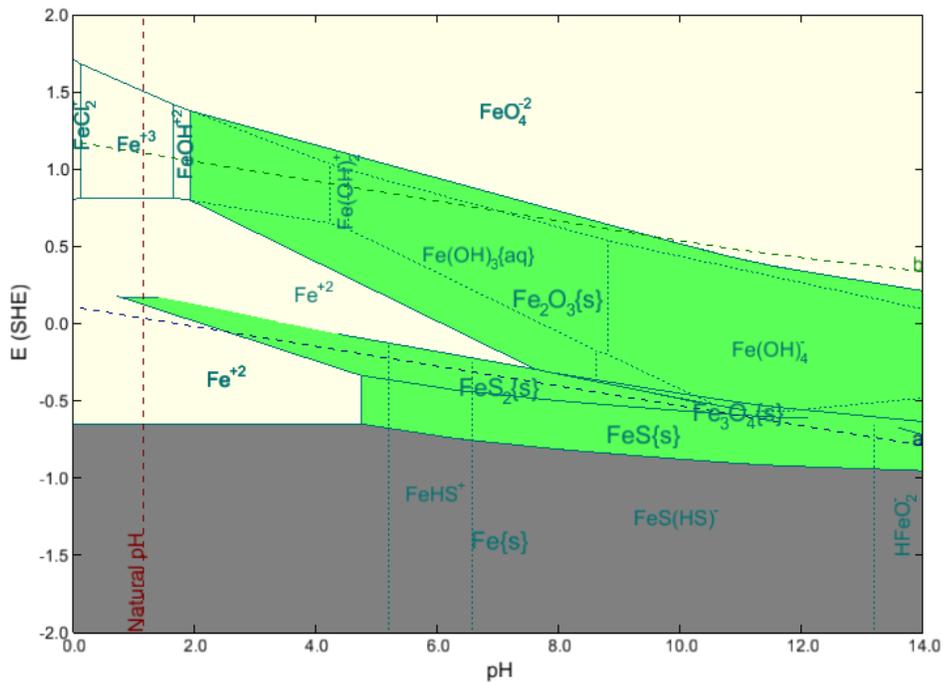


Figure 22-8 The stability of iron in DEA solutions.

You can download a worked example for this chapter from the [OLI Wiki Page](#)