

# 24. Modeling the Effect of Oxidizing Inhibitors on Corrosion

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## Overview

In this chapter we will look at the effect of modeling corrosion inhibitors. We will do this by superimposing two stability diagrams over one another. If one solid field overlaps the corrosion range of the other system, then passivation is likely.

### Iron in the presence of chromates

Create a stream with the following composition:

Table 24-1 Inhibition using chromates

Parameter	Value	Comment
Stream Amount (mol)	55.5082	Default value
Temperature (°C)	25	
Pressure (atm)	1	
H2O (mol)	55.5082	Default Value
Acid Titrant	HCl	No initial value
Base Titrant	NaOH	No Initial Value
K2CrO4 (mol)	0.001	Used as an corrosion inhibitor
Contact Surface	Fe	
Contact Surface	Cr	

Create a stability diagram using the above stream. Select both *Fe* and *Cr* oxidation and reduction subsystems. In this case, the two metals will be used in addition to water in the redox subsystems.

Use the **Chemistry** model item and **Model Options > Redox** to ensure that Chromium and Iron are selected in the **Included Subsystems** list.

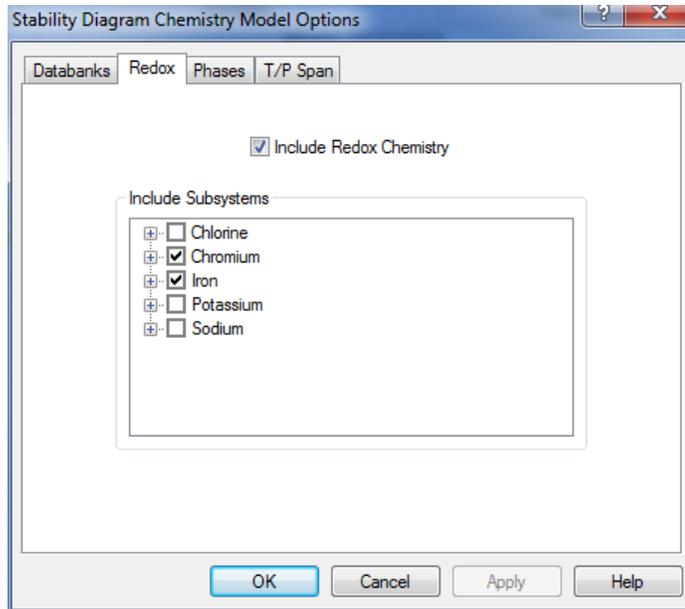


Figure 24-1 Selecting subsystems.

The filled out definition for the stability diagram should look like the following figure:

Variable	Value
<b>Stream Parameters</b>	
Stream Amount (mol)	55.5092
Temperature (°C)	25.0000
Pressure (atm)	1.00000
<b>Calculation Parameters</b>	
Use Single Titrant	No
pH Acid Titrant	HCl
pH Base Titrant	NaOH
<b>Inflows (mol)</b>	
H2O	55.5082
HCl	0.0
NaOH	0.0
K2CrO4	1.00000e-3
Fe	0.0
Cr	0.0
<b>Contact Surface (mol)</b>	
Fe	
Cr	

**Summary**

Type of diagram: Pourbaix Diagram

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: Chromium, Iron, Water

Alloy Activity Module: Activated

Calculation not done

Figure 24-2 The filled out grid. Note that two metals are used.

We want to shade the chromium subsystem instead of the default iron subsystem. Click the **Specs...** button and then select the **Display** category.



## Iron in the presence of arsenates

Create a stream with the following composition:

Table 24-2 Inhibition using arsenates

Parameter	Value	Comment
Stream Amount (mol)	55.5082	Default value
Temperature (°C)	25	
Pressure (atm)	1	
H <sub>2</sub> O (mol)	55.5082	Default Value
Acid Titrant	HCl	No initial value
Base Titrant	NaOH	No Initial Value
Na <sub>3</sub> AsO <sub>4</sub> (mol)	0.001	Used as an corrosion inhibitor
Contact Surface	Fe	
Contact Surface	As	

Create a stability diagram using the above stream. Select both *Fe* and *As* oxidation and reduction subsystems. In this case, the two metals will be used in addition to water in the subsystems.

The stability diagram definition should look similar to this:

The screenshot shows the 'Stability Diagram' tab in the OLI Analyzer software. The main window is divided into a table for defining input parameters and a summary panel on the right.

Variable	Value
<b>Stream Parameters</b>	
Stream Amount (mol)	55.5092
Temperature (°C)	25.0000
Pressure (atm)	1.00000
<b>Calculation Parameters</b>	
Use Single Titrant	No
pH Acid Titrant	HCl
pH Base Titrant	NaOH
<b>Inflows (mol)</b>	
H2O	55.5082
HCl	0.0
NaOH	0.0
Na3AsO4	1.00000e-3
Fe	0.0
As	0.0
<b>Contact Surface (mol)</b>	
Fe	
As	

Summary Panel:

- Type of diagram: Pourbaix Diagram
- 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: Arsenic, Iron, Water
- Alloy Activity Module: Activated
- Calculation not done

Figure 24-5 Input for Iron/Arsenate diagram

Use the **Specs...** button and select the **Display** category to select **Arsenic** as the subsystem to shade.

Click the **Calculate** button when ready. Click on the **Stability Diagram** tab when finished.

