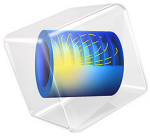

Alloy Deposition

Introduction

Electrochemical codeposition is a common low-cost method for producing metal alloys. This tutorial model demonstrates electrodeposition of a nickel (Ni)–phosphorous (P) alloy.

The model accounts for charge and mass transport of a multitude of species along with multiple electrode reactions such as Ni and P electrodeposition and hydrogen evolution. The model computes the steady state spatial distributions of the various species along the diffusion layer. The polarization plot along with deposition mole fraction plot reveal the desirable operating conditions for alloy preparation.

The model is based on a journal paper (Ref. 1).

Model Definition

The model is solved over a 1D computational domain that consists of a diffusion layer with an electrode surface at one end and a reference electrode at the other end, as shown in Figure 1. The electrolyte interval of length 0.02 cm is considered in the model.

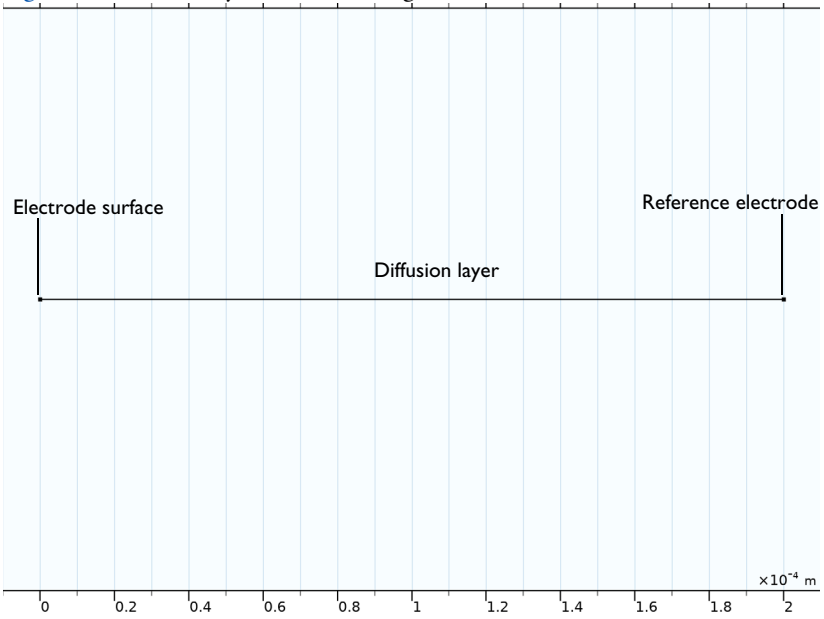

Figure 1: Description of the model geometry including diffusion layer adjacent to the electrode surface.

Mass transport by convection, diffusion and migration for six species: H^+, OH^-, Ni^{2+}, H_3PO_2, SO_4^{2-}, and Na^+, is solved using the **Tertiary Current Distribution, Nernst-Planck** interface:

$$\mathbf{N}_i = -D_i \nabla c_i - z_i u_i F c_i \nabla \phi_l$$

where $\mathbf{N}_i$ denotes the transport vector (mol/(m^2·s)), c_i the concentration in the electrolyte (mol/m^3), z_i the charge for the ionic species, u_i the mobility of the charged species (m^2/(s·J·mole)), F Faraday's constant (As/mole), and ϕ_l the potential in the electrolyte (V). The material balances are expressed through

$$\nabla \cdot \mathbf{N}_i + \mathbf{u} \cdot \nabla c_i = 0$$

where $\mathbf{u}$ denotes the velocity field.

The velocity in the normal direction to the electrode surface is defined by an analytical expression (originating from the von Karman and Cochran solution to the Navier-Stokes equations) as

$$v_x = -a\Omega\left(\frac{\Omega}{\nu}\right)^{\frac{1}{2}} x^2$$

where $a \approx 0.51$ is a numerical parameter related to the velocity profile close to the surface, Ω is the rotation speed (rad/s), ν is the kinematic viscosity (m^2/s), and x is the distance in the normal direction to the electrode surface (m).

All species along with their diffusion coefficients and reference concentrations are tabulated in Table 1.

TABLE 1: MODELED SPECIES WITH THEIR RESPECTIVE DIFFUSION COEFFICIENTS (Ref. 1).

Species	D (m^2/s)·10^9	c_{ref} (mol/m^3)
Ni^{+2}	0.71	380
H_3PO_2	1.54	380
SO_4^{-2}	1.065	580
Na^+	1.334	300
H^+	9.312	100
OH^-	5.26	1e-10

The concentration at the reference electrode boundary is set to the reference concentration for all species as tabulated in Table 1:

$$c_i = c_{i,\,\mathrm{ref}}$$

At the electrode surface boundary, an **Electric potential** boundary condition is used wherein the external electric potential, $\phi_{s,ext}$, is set to the applied potential, which is varied from –0.5 V/SHE to –1.1 V/SHE in the interval of –0.025 V/SHE.

The water dissociation equilibrium reaction is built-in for the Tertiary Current Distribution, Nernst–Planck interface when using a water-based with electroneutrality charge conservation model:

$$H_2O \leftrightarrow H^+ + OH^-$$

ELECTROCHEMICAL REACTIONS

The following electrochemical reactions occur at the electrode surface:

Nickel electrodeposition

$$Ni^{+2} + 2e^- \rightarrow Ni \qquad E^0_{\mathrm{eq,\,Ni}} = -0.23\,V$$

Phosphorous electrodeposition

$$H_3PO_2 + H^+ + e^- \rightarrow P + 2H_2O \qquad E^0_{\mathrm{eq,\,P}} = -0.51\,V$$

Hydrogen evolution

$$2H^+ + 2e^- \rightarrow H_2 \qquad E^0_{\mathrm{eq,\,H}} = 0\,V$$

Butler-Volmer kinetics is used to model all electrochemical reactions, which will set the local current density according to

$$i_{\mathrm{loc,\,m}} = i_{0,\,\mathrm{m}}\left(\exp\left(\frac{\alpha_{a,\,\mathrm{m}} F \eta_{\mathrm{m}}}{RT}\right) - \exp\left(-\frac{\alpha_{c,\,\mathrm{m}} F \eta_{\mathrm{m}}}{RT}\right)\right)$$

where $i_{0,m}$ is the exchange current density (A/m^2), $\alpha_{a,m}$ is the anodic transfer coefficient, $\alpha_{c,m}$ is the cathodic transfer coefficient, F is the Faraday's constant (96,485 C/mol), $\eta_{,m}$ is the overpotential (V), R is the Ideal gas constant (8.314 J/mol/K) and T is the temperature (K). The subscript m signifies the m^{th} electrochemical reaction.

The $\eta_{,m}$ is calculated from

$$\eta_{\mathrm{m}} = \phi_{s,\,\mathrm{ext}} - \phi_l - E_{\mathrm{eq,\,m}}$$

The equilibrium potentials for the electrochemical reactions are calculated using the Nernst equation accounting for its dependence on the ionic species concentration and relative activity of deposited species:

$$E_{\mathrm{eq,m}} = E^0_{\mathrm{eq,m}} - \frac{RT}{n_{\mathrm{m}}F}\ln\prod_i\left(\frac{c_{i,\,\mathrm{ref}}}{1[M]}\right)^{\nu_i} - \frac{RT}{n_{\mathrm{m}}F}\ln\prod_j\left(\frac{x_j}{a_{j,\,\mathrm{ref}}}\right)^{\nu_i} - \frac{RT}{n_{\mathrm{m}}F}\ln\prod_i\left(\frac{c_i}{c_{i,\,\mathrm{ref}}}\right)^{\nu_i}$$

where $E^0_{\mathrm{eq,\,m}}$ is the standard electrode potential (V), n_{m} is the number of electrons, $c_{i,\mathrm{ref}}$ is the reference concentration of ionic species i ($\mathrm{mol/m^3}$), x_j is the mole fraction of deposited species j, and $a_{j,\mathrm{ref}}$ is the reference relative activity of deposited species j.

The exchange current density for the electrochemical reactions are described to account for its dependence on the ionic species concentration and relative activity of deposited species as,

$$i_{0,\mathrm{m}} = i_{0,\,\mathrm{reff,m}}\prod_j\left(\frac{x_j}{a_{j,\,\mathrm{ref}}}\right)^{\frac{\alpha_{c,\,\mathrm{m}}\nu_i}{n_{\mathrm{m}}}}\prod_{i:\nu_i>0}\left(\frac{c_i}{c_{i,\,\mathrm{ref}}}\right)^{\frac{\alpha_{c,\,\mathrm{m}}\nu_i}{n_{\mathrm{m}}}}\prod_{i:\nu_i<0}\left(\frac{c_i}{c_{i,\,\mathrm{ref}}}\right)^{-\frac{\alpha_{a,\,\mathrm{m}}\nu_i}{n_{\mathrm{m}}}}$$

where $i_{0,\mathrm{ref,m}}$ is the reference exchange current density ($\mathrm{A/m^2}$).

At the electrode surface boundary, fluxes of ionic species are defined in terms of the electrochemical reactions as

$$\mathbf{n}\cdot\mathbf{N}_i = \frac{\nu_i i_{\mathrm{loc,\,m}}}{n_{\mathrm{m}}F}$$

where ν_i is the stoichiometric coefficient of ionic species i. This will set the flux to be proportional to the electrode current density according to Faraday's law.

At the electrode surface boundary, the rate of deposition of deposited species is defined in terms of the electrochemical reactions as

$$R_j = -\frac{\nu_{\mathrm{d},j} i_{\mathrm{loc,\,m}}}{n_{\mathrm{m}}F}$$

where $\nu_{\mathrm{d},j}$ is the stoichiometric coefficient of deposited species j.

The mole fraction of deposited species is defined in terms of the rate of deposition as

$$x_j = \frac{R_j}{\sum_j R_j}$$

Figure 2 shows the change in concentration for all species along the diffusion layer at applied potential of –0.8 V/SHE. It can be seen that the concentration gradient is the highest for Ni^{2+} at the electrode surface.

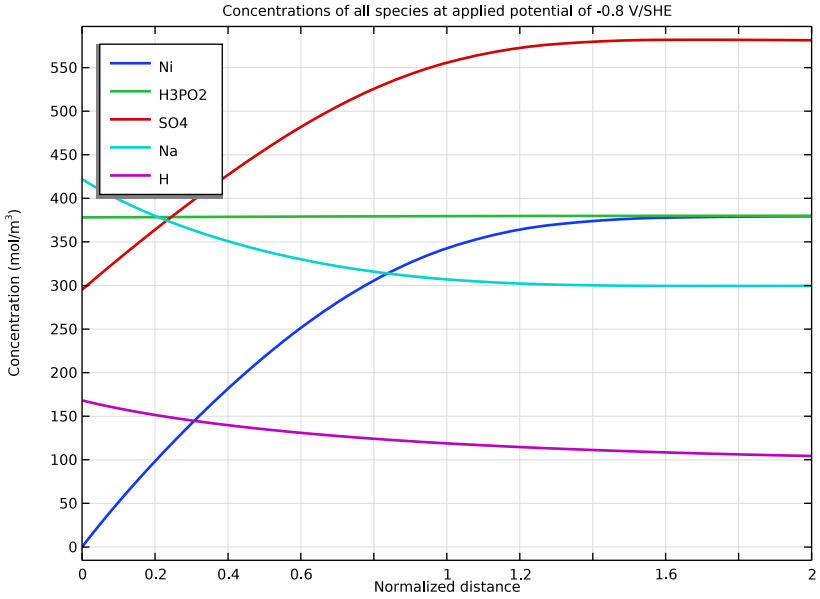

Figure 2: The change in concentration for all species along the diffusion layer at applied potential –0.8 V/SHE.

Figure 3 shows the polarization plot describing the change in cathodic (negative) total current density for different cathodic (negative) applied potentials at the electrode surface.

The polarization plot shows larger cathodic current densities for larger cathodically applied potentials, with a plateau around -0.8 V/SHE.

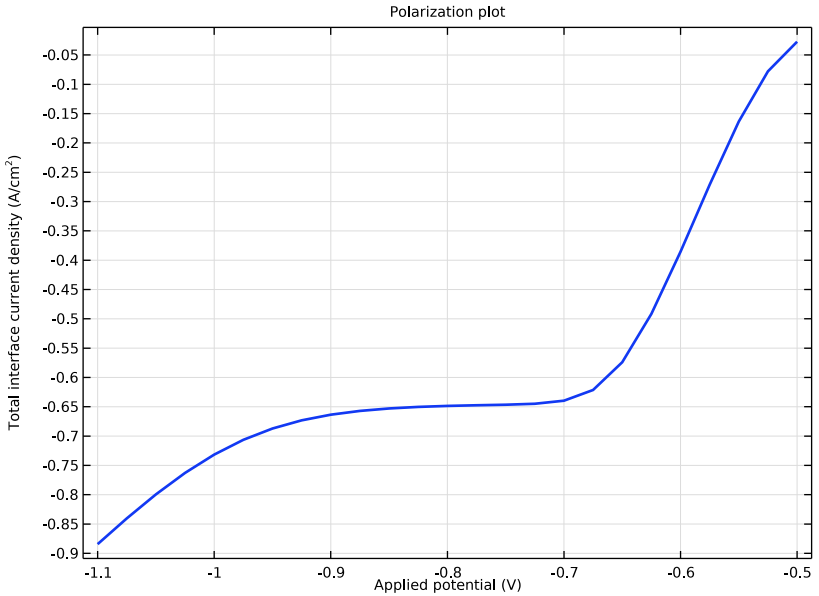

Figure 3: The polarization plot showing the change in the cathodic (negative) current density for different cathodic (negative) applied potentials at the electrode surface.

Figure 4 shows the change in the deposition mole fraction for Ni and P for different cathodic (negative) applied potentials at the electrode surface. It can be seen that at potentials above the -0.8 V/SHE plateu, Ni is predominantly deposited at the electrode

surface, whereas at potentials below the -0.8 V/SHE plataeu, P starts getting deposited at the electrode surface, providing the desirable operating conditions for alloy deposition.

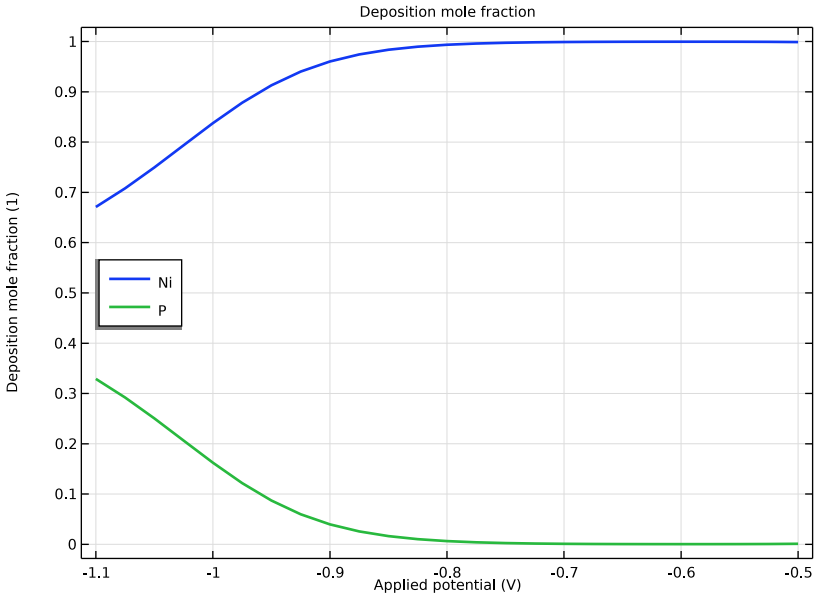

Figure 4: The change in deposition mole fraction for Ni and P for different cathodic (negative) applied potentials at the electrode surface.

Reference

1. S. Chen, K.-M. Yin, and R. E. White, "A Mathematical Model for the Electrodeposition of Alloys on a Rotating Disk Electrode," *J. Electrochem. Soc.*, vol. 135, no. 9, pp. 2193–2200, 1988.

Application Library path: `Electrodeposition_Module/Tutorials/alloy_deposition`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

2 In the **Select Physics** tree, select **Electrochemistry>Tertiary Current Distribution, Nernst-Planck>Tertiary, Water-Based with Electroneutrality (tcd)**.

3 Click **Add**.

4 In the **Number of species** text field, type 4.

5 In the **Concentrations (mol/m³)** table, enter the following settings:

cNi
cH3PO2
cSO4
cNa

6 Click **Study**.

7 In the **Select Study** tree, select **General Studies>Stationary**.

8 Click **Done**.

GLOBAL DEFINITIONS

Load the model parameters from a text file.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `alloy_deposition_parameters.txt`.

GEOMETRY 1

The geometry consists of a linear segment describing the diffusion layer.

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 In the table, enter the following settings:

Coordinates (m)
0
0.02[cm]

4 Click **Build All Objects**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

DEFINITIONS

Variables 1

Load the model variables from a text file.

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `alloy_deposition_variables.txt`.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

Start by defining the physics.

Species Charges 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)** click **Species Charges 1**.

2 In the **Settings** window for **Species Charges**, locate the **Charge** section.

3 In the z_{cNi} text field, type `2`.

4 In the z_{cSO4} text field, type `-2`.

5 In the z_{cNa} text field, type `1`.

Electrolyte 1

1 In the **Model Builder** window, click **Electrolyte 1**.

2 In the **Settings** window for **Electrolyte**, locate the **Convection** section.

3 Specify the $\mathbf{u}$ vector as

vx	x

4 Locate the **Diffusion** section. In the D_{cNi} text field, type `DNi`.

5 In the D_{cH3PO2} text field, type `DH3PO2`.

6 In the D_{cSO4} text field, type `DSO4`.

7 In the D_{cNa} text field, type `DNa`.

8 In the D_{cH} text field, type `DH`.

9 In the D_{cOH} text field, type `DOH`.

Initial Values 1

Set the initial values to the concentration of the species in the bulk.

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *cNi* text field, type `cNi0`.

4 In the *cH3PO2* text field, type `cH3PO20`.

5 In the *cSO4* text field, type `cSO40`.

6 In the *cNa* text field, type `cNa0`.

Electrode Surface 1

Set the electrode kinetics for multiple electrode reactions using the **Electrode Surface** node. Use the Dissolving-Depositing Species section to evaluate the rate of deposition for Nickel and Phosphorous at the electrode surface.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Surface**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Electrode Surface**, click to expand the **Dissolving-Depositing Species** section.

4 Click **Add**.

5 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
Ni	rho_Ni	M_Ni

6 Click **Add**.

7 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
P	rho_P	M_P

8 Locate the **Electrode Phase Potential Condition** section. In the $\phi_{s,ext}$ text field, type `E_app`.

Electrode Reaction: Ni Deposition

1 In the **Model Builder** window, under **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (tcd)>Electrode Surface 1** click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction: Ni Deposition` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the n text field, type `2`.

4 In the ν_{cNi} text field, type `-1`.

5 In the **Stoichiometric coefficients for dissolving-depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (1)
Ni	1

6 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq_ref_Ni-R_const*T/(2*F_const)*log(max(xNi,eps^2)/aNi_ref)`.

7 Click to expand the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
cNi	`cNi_ref`

8 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0_ref_Ni*(max(xNi,eps)/aNi_ref)^0.75`.

Electrode Surface 1

In the **Model Builder** window, click **Electrode Surface 1**.

Electrode Reaction: P Deposition

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction: P Deposition` in the **Label** text field.

3 Locate the **Stoichiometric Coefficients** section. In the ν_{cH3PO2} text field, type `-1`.

4 In the **Stoichiometric coefficients for dissolving-depositing species:** table, enter the following settings:

Species	Stoichiometric coefficient (1)
P	1

5 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `Eeq_ref_P-R_const*T/(F_const)*log(max(xP,eps)/aP_ref)`.

6 Click to expand the **Reference Concentrations** section. In the table, enter the following settings:

Electrolyte species	Reference concentrations (mol/m^3)
cH3PO2	`cH3PO2_ref`

7 In the $c_{\mathrm{H,ref}}$ text field, type `cH_ref`.

8 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_P*(max(xP,eps^2)/aP_ref)^0.5`.

Electrode Surface 1

In the **Model Builder** window, click **Electrode Surface 1**.

Electrode Reaction: Hydrogen Evolution

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, type `Electrode Reaction: Hydrogen Evolution` in the **Label** text field.

3 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `Eeq_ref_H`.

4 Click to expand the **Reference Concentrations** section. In the $c_{\mathrm{H,ref}}$ text field, type `cH_ref`.

5 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_H`.

Concentration 1

Set concentrations of the species at the reference electrode boundary.

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species cNi** check box.

5 Select the **Species cH3PO2** check box.

6 Select the **Species cSO4** check box.

7 Select the **Species cNa** check box.

8 In the $c_{0,cNi}$ text field, type `cNi0`.

9 In the $c_{0,cH3PO2}$ text field, type `cH3PO20`.

10 In the $c_{0,cSO4}$ text field, type `cSO40`.

11 In the $c_{0,cNa}$ text field, type `cNa0`.

Electrolyte Potential 1

Set electrolyte potential at the reference electrode boundary to 0.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrolyte Potential**.

2 Select Boundary 2 only.

COMPONENT 1 (COMP1)

Now add a **General Form Boundary PDE** interface to solve for deposition mole fraction of Nickel.

ADD PHYSICS

1 In the **Physics** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Mathematics>PDE Interfaces>Lower Dimensions>General Form Boundary PDE (gb)**.

4 Click to expand the **Dependent Variables** section. In the **Dependent variables (1)** table, enter the following settings:

xNi

5 Click **Add to Component 1** in the window toolbar.

6 In the **Physics** toolbar, click **Add Physics** to close the **Add Physics** window.

GENERAL FORM BOUNDARY PDE (GB)

1 In the **Settings** window for **General Form Boundary PDE**, locate the **Boundary Selection** section.

2 In the list, select **2**.

3 Click **Remove from Selection**.

4 Select Boundary 1 only.

5 Locate the **Units** section. In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	1

General Form PDE 1

1 In the **Model Builder** window, under **Component 1 (comp1)> General Form Boundary PDE (gb)** click **General Form PDE 1**.

2 In the **Settings** window for **General Form PDE**, locate the **Source Term** section.

3 In the *f* text field, type `xNi-xNi_expr`.

4 Locate the **Damping or Mass Coefficient** section. In the d_a text field, type `0`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the *xNi* text field, type `1`.

GLOBAL DEFINITIONS

Default Model Inputs

Set the default model input temperature to `T`.

1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General>Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T`.

MESH 1

Build a mesh using a finer resolution at the electrode surface.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra fine**.

Size 1

1 In the **Model Builder** window, click **Size 1**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section.

5 Select the **Maximum element size** check box. In the associated text field, type `1.0E-6`.

Edge 1

In the **Model Builder** window, right-click **Edge 1** and choose **Build All**.

STUDY 1

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_app (Applied potential)	`range(-0.5, -0.025, -1.1)`	V

6 In the **Home** toolbar, click = **Compute**.

RESULTS

Several plots are added by default. The following steps reproduce the plots from the Results and Discussion section:

Concentrations, All Species (tcd)

1 In the **Model Builder** window, under **Results** click **Concentrations, All Species (tcd)**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Parameter selection (E_app)** list, choose **From list**.

4 In the **Parameter values (E_app (V))** list, select **-0.8**.

5 Click to expand the **Title** section. In the **Title** text area, type `Concentrations of all species at applied potential of -0.8 V/SHE`.

6 Locate the **Plot Settings** section.

7 Select the **x-axis label** check box. In the associated text field, type `Normalized distance`.

8 Select the **y-axis label** check box.

9 Locate the **Axis** section. Select the **Manual axis limits** check box.

10 In the **x minimum** text field, type `0`.

11 In the **x maximum** text field, type `2`.

12 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Species Ni

1 In the **Model Builder** window, expand the **Concentrations, All Species (tcd)** node, then click **Species Ni**.

2 In the **Settings** window for **Line Graph**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `x/1.1517e-3[cm]`.

4 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

Species H3PO2

1 In the **Model Builder** window, click **Species H3PO2**.

2 In the **Settings** window for **Line Graph**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `x/1.1517e-3[cm]`.

4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

Species SO4

1 In the **Model Builder** window, click **Species SO4**.

2 In the **Settings** window for **Line Graph**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `x/1.1517e-3[cm]`.

4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

Species Na

1 In the **Model Builder** window, click **Species Na**.

2 In the **Settings** window for **Line Graph**, locate the **x-Axis Data** section.

3 In the **Expression** text field, type `x/1.1517e-3[cm]`.

4 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

5 In the **Model Builder** window, right-click **Species Na** and choose **Duplicate**.

Species H

1 In the **Model Builder** window, under **Results>Concentrations, All Species (tcd)** click **Species Na 1**.

2 In the **Settings** window for **Line Graph**, type `Species H` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `tcd.cH`.

4 Click to expand the **Legends** section. Find the **Prefix and suffix** subsection. In the **Prefix** text field, type `H`.

5 In the **Concentrations, All Species (tcd)** toolbar, click **Plot**.

The plot should look like Figure 2.

Polarization Plot

Next, plot the polarization plot.

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Polarization Plot` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Polarization plot`.

Point Graph 1

1 In the **Polarization Plot** toolbar, click **Point Graph**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Tertiary Current Distribution, Nernst-Planck>Electrode kinetics>tcd.itot - Total interface current density - A/m²**.

4 Locate the **y-Axis Data** section. In the **Unit** field, type `A/cm^2`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `E_app`.

7 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

8 In the **Polarization Plot** toolbar, click **Plot**.

The plot should look like Figure 3.

Deposition Mole Fraction

Finally, plot deposition mole fraction against the applied potential.

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Deposition Mole Fraction` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Deposition mole fraction`.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `Applied potential (V)`.

7 Select the **y-axis label** check box. In the associated text field, type `Deposition mole fraction (1)`.

8 Locate the **Legend** section. From the **Position** list, choose **Middle left**.

Point Graph 1

1 In the **Deposition Mole Fraction** toolbar, click **Point Graph**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `xNi`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `E_app`.

7 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

8 Click to expand the **Legends** section. Select the **Show legends** check box.

9 From the **Legends** list, choose **Manual**.

10 In the table, enter the following settings:

Legends
Ni

11 Right-click **Point Graph 1** and choose **Duplicate**.

Point Graph 2

1 In the **Model Builder** window, click **Point Graph 2**.

2 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `xP`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
P

5 In the **Deposition Mole Fraction** toolbar, click **Plot**.

The plot should look like Figure 4.