Rotating Cylinder Hull Cell

Introduction

The rotating cylinder Hull (RCH) cell provides an effective experimental tool to investigate electrodeposition since a wide range of current densities and controllable hydrodynamic conditions can be achieved in a single experiment.

This model example simulates non-uniform current, potential and concentration distributions along the working electrode of the RCH cell. Primary, secondary and tertiary current distributions are compared, demonstrating how complexity can be gradually incorporated in the model. The example is based on a paper by C. T. J. Low and others (Ref. 1).

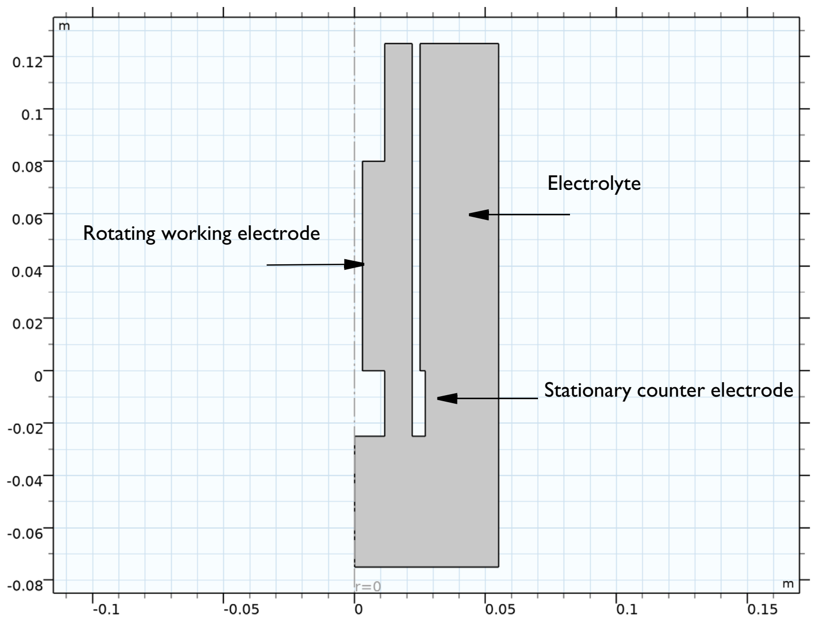


Figure 1: 2D axisymmetric geometry of the RCH cell. The Electrolyte, the rotating working electrode and the stationary counter electrode are highlighted.

Model Definition

Because of the symmetry of the RCH cell geometry, a 2D axisymmetric space dimension is used. Figure 1 shows the model geometry, where the rotating cylinder working electrode, the stationary concentric counter electrode and the electrolyte are highlighted.

ELECTROLYTE CHARGE TRANSPORT

First, use the Primary Current Distribution interface to solve for the electrolyte potential, ϕ_l(V), according to:

$$\mathbf{i}_l = -\sigma_l \nabla \phi_l$$
$$\nabla \cdot \mathbf{i}_l = 0$$

where $\mathbf{i}_l$ (A/m^2) is the electrolyte current density vector and σ_l (S/m) is the electrolyte conductivity, which is assumed to be a constant.

Use the default Insulation condition for all boundaries except the counter and working electrode surfaces:

$$\mathbf{n} \cdot \mathbf{i}_l = 0$$

where $\mathbf{n}$ is the normal vector, pointing out of the domain.

Use an Electrolyte Potential boundary condition to apply a 0 V electrolyte potential along the counter electrode boundary surfaces:

$$\phi_l = 0$$

Use the Electrode Surface boundary node at the working electrode surface, and set the average current density. This boundary condition yields a constant potential at the working electrode boundary that satisfies the average current density value.

$$\int (\mathbf{n} \cdot \mathbf{i}_l) dS = i_{\mathrm{avg}}$$

For the secondary current distribution, change the **Current Distribution Type** of the current distribution interface to **Secondary**. The Electrode Surface now sets the boundary condition for the electrode potential so that

$$\int \left(\sum_m i_{\mathrm{loc},\, m} \right) dS = i_{\mathrm{avg}}$$

is fulfilled, where $i_{\mathrm{loc},m}$ (A/m^2) is the local individual electrode reaction current density of the depositing electrode reaction.

Use a Cathodic Tafel Expression to model the electrode reaction, this sets the local current density to

$$i_{\text{loc}} = -i_0 10^{\frac{\eta}{A_c}}$$

where i_0 is the exchange current density, A_c (V) is the Tafel slope and the overpotential η (V) is calculated from

$$\eta = \phi_{s,\text{ext}} - \phi_l - E_{\text{eq}}$$

The $\phi_{s,ext}$ is computed in order to satisfy the average current density defined at the Electrode Surface.

For tertiary current distribution, in addition to the Secondary Current Distribution interface, solve for cupric ions concentration using a Transport of Diluted Species interface to model transport by Fickian diffusion in a 30 micrometer thick diffusion layer next to the working electrode surface:

$$\mathbf{N} = -D\nabla c$$
$$\nabla \cdot \mathbf{N} = 0$$

where c (mol/m^3) is the cupric ions concentration, $\mathbf{N}$ (mol/(m^2·s)) the flux vector, and D (m^2/s) the diffusion coefficient.

Use the default No Flux conditions for the top and bottom boundaries of the diffusion layer domain:

$$\mathbf{n} \cdot \mathbf{N} = 0$$

The concentration at the right boundary of the diffusion layer is set to the bulk concentration:

$$c = c_b$$

where c_b (mol/m^3) is the bulk cupric ions concentration.

On the working electrode surface, couple the cupric ions flux over the boundary to the local current density by using an Electrode-Electrolyte Interface Coupling boundary condition. This sets the flux to be proportional to the electrode current density according to Faraday's law:

$$\mathbf{n} \cdot \mathbf{N} = \frac{\nu i_{\text{loc, Cu}}}{nF}$$

where F is Faraday's constant (96485 C/mol), ν the stoichiometric coefficient for cupric ions in the reduction reaction and n the number of electrons in the reaction.

The sign convention for ν is that it should be negative for reactants and positive for products in a reduction reaction. A reduction reaction is one where the electrons participate as reactants. n is always positive. Set ν to -1 and n to 2 for this model.

Finally, set the electrode kinetics to be concentration dependent using the following expression:

$$i_{\mathrm{loc,\ Cu}} = -\left(\frac{c}{c_b}\right) i_0 10^{\frac{\eta}{A_c}}$$

Results and Discussion

Figure 2 shows the normalized primary current density distribution along the working electrode surface obtained from the numerical model as well as from an analytical expression reported in Ref. 1. The normalized current density is found to decrease with the distance away from the counter electrode surface indicating its dependence on the geometry of RCH cell.

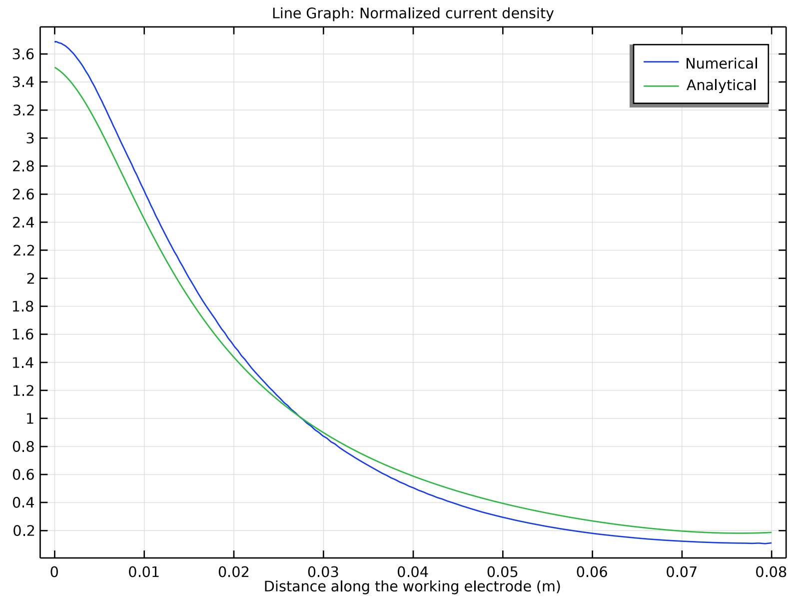


Figure 2: Normalized primary current density distribution obtained from the numerical model and the analytical expression.

Figure 3 shows the overpotential variation along the working electrode surface obtained from the model for the varied applied current densities for the secondary current distribution. For the lower applied current densities, the overpotential is found to be quite uniform along the working electrode surface and low in magnitude. For the higher applied current densities, however, the overpotential is found to be considerably non-uniform and high in magnitude, particularly in a region closer to the counter electrode surface.

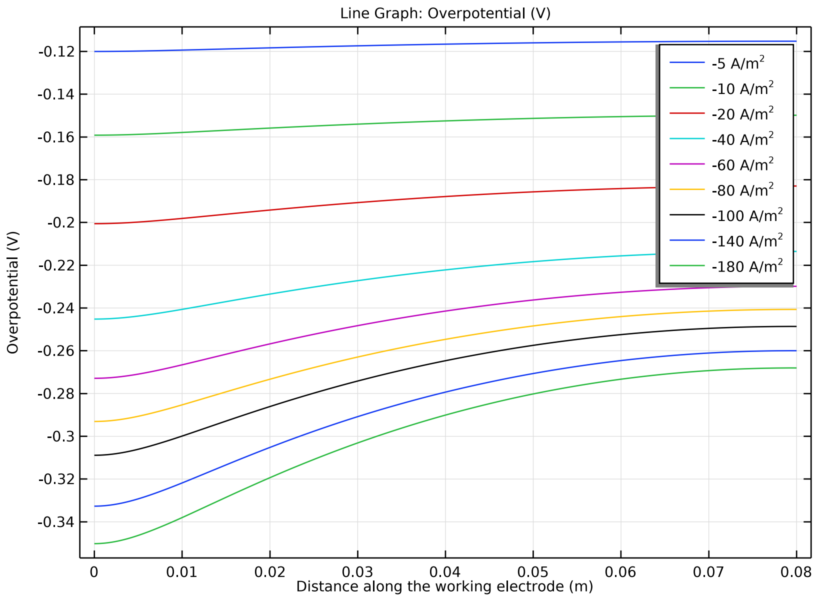


Figure 3: Overpotential variation for the varied applied current densities in the case of secondary current distribution.

Figure 4 shows the normalized current density variation along the working electrode surface obtained from the model for the varied applied current densities in the case of secondary current distribution. The normalized current density variation is quite uniform for the lower applied current densities and non-uniform for the higher applied current densities, in correspondence to the overpotential variation.

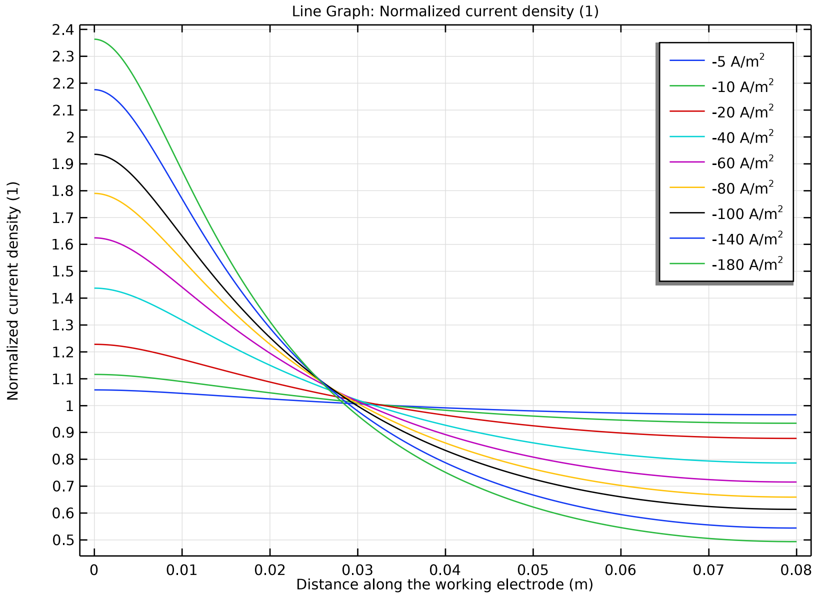


Figure 4: Normalized current density variation for the varied applied current densities in the case of secondary current distribution.

Figure 5 shows the overpotential variation along the working electrode surface obtained from the model for the varied applied current densities in the case of tertiary current distribution. The shape of overpotential variation obtained for tertiary current distribution is found to be similar to secondary current distribution. However, the magnitude of overpotential is generally higher in the former case, particularly in a region closer to the counter electrode surface.

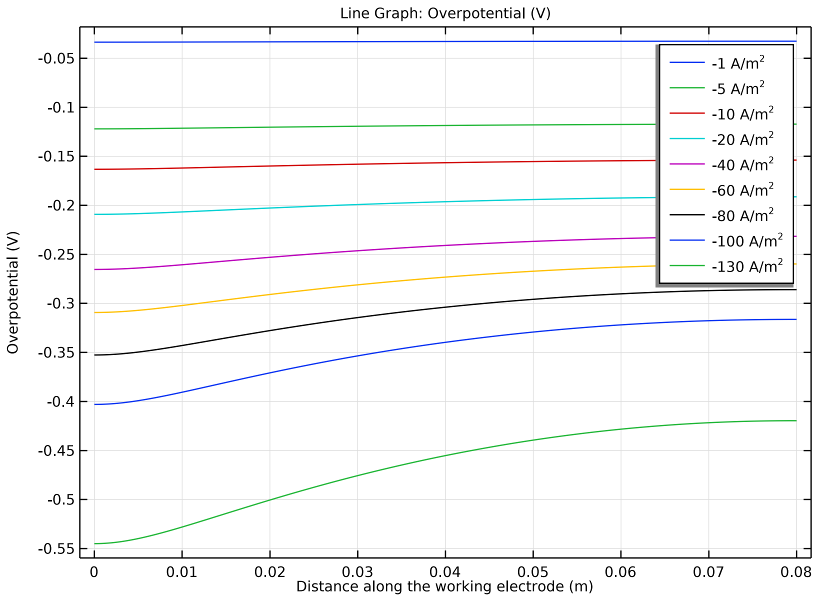


Figure 5: Overpotential variation for the varied applied current densities in the case of tertiary current distribution.

Figure 6 shows the local current density variation along the working electrode surface obtained from the model for the varied applied current densities in the case of tertiary current distribution. The local current density variation is found to be non-uniform with the increase in the applied current density, eventually approaching the limiting current density in a region closer to the counter electrode surface.

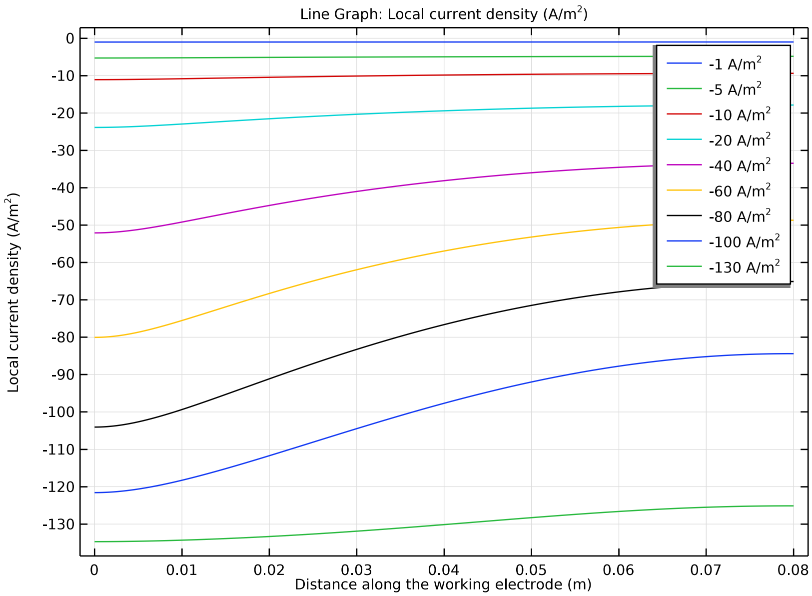


Figure 6: Local current density variation for the varied applied current densities in the case of tertiary current distribution.

Figure 7 shows the normalized concentration variation along the working electrode surface obtained from the model for the varied applied current densities in the case of tertiary current distribution. For the lower applied current densities, the normalized concentration is close to 1 indicating that the reaction is kinetically limited and hence, secondary current distribution is good enough in this range. For the higher applied current densities, however, the normalized concentration variation is significant. For the highest applied current density, the normalized concentration is 0 in a region closer to the counter electrode surface, confirming that the electrodeposition reaction is mass transport limited. This shows that a tertiary current distribution model is required for the larger applied current densities.

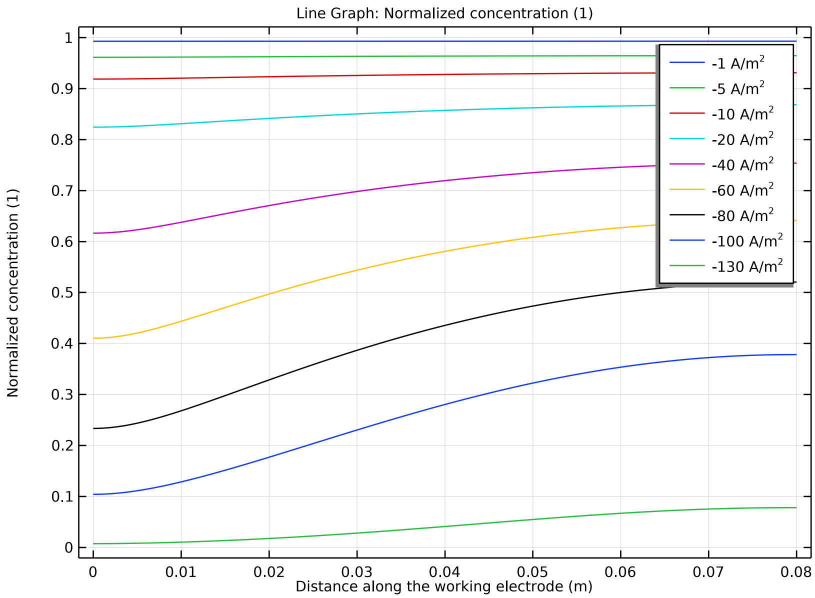


Figure 7: Normalized concentration variation for varied applied current densities in the case of tertiary current distribution.

Figure 8 shows the normalized current density variation along the working electrode surface obtained from the model for primary, secondary and tertiary current distributions at the representative applied current density of 100 A/m^2. The primary current distribution is the most non-uniform, followed by the secondary and then the tertiary current distribution. The primary current distribution model is not adequate for capturing the electrodeposition process under non-equilibrium conditions. The secondary current distribution is applicable for the lower applied current densities, where the electrodeposition reaction is kinetic limited. The tertiary current distribution is valid when concentration gradients cannot be neglected, which is the case for the higher applied current densities.

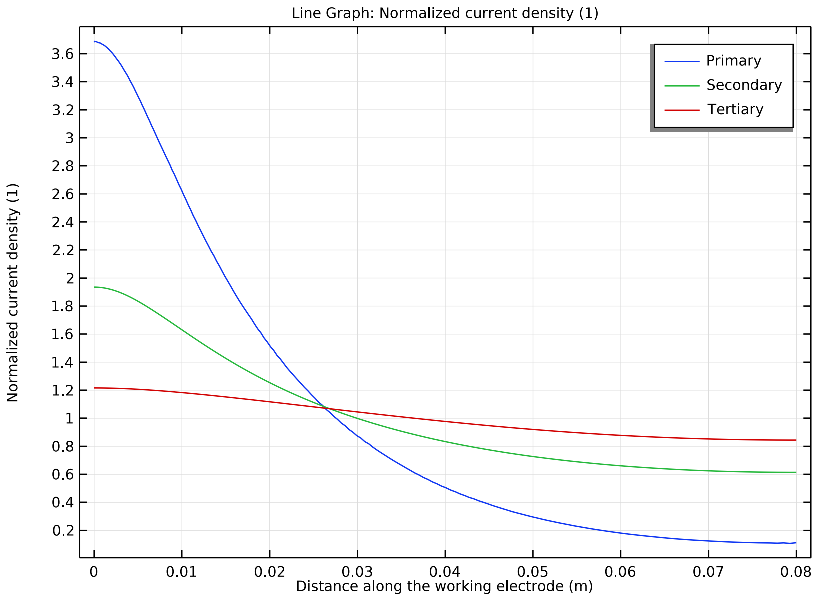


Figure 8: Normalized current density variation for primary, secondary and tertiary current distributions at the representative applied current density of 100 A/m^2.

Notes About the COMSOL Implementation

The primary current distribution is first implemented using the Primary Current Distribution interface and the Electrode Surface node for the working electrode surface.

The secondary current distribution is then implemented by introducing the electrode kinetics for the working electrode surface using the Electrode Surface node.

Finally, the tertiary current distribution is implemented by coupling the Transport of Diluted Species interface with the Secondary Current Distribution interface.

A parametric sweep study type is used to vary the current density applied at the working electrode surface for the secondary and tertiary current distributions.

Reference

1. C.T.J. Low, E.P.L. Roberts, and F.C. Walsh, "Numerical simulation of the current, potential and concentration distributions along the cathode of a rotating cylinder Hull cell," *Electrochimica Acta*, vol. 52, pp 3831–3840, 2007.

Application Library path: `Electrodeposition_Module/Verification_Examples/rotating_cylinder_hull_cell`

Modeling Instructions

The current distribution in the rotating cylinder Hull (RCH) cell is modeled in three steps to demonstrate how complexity can be gradually introduced in the model. In the first and second steps, the primary and secondary current distributions are modeled using the Primary or Secondary Current Distribution interface, respectively. In the third step, the tertiary current distribution is modeled by adding a Transport of Diluted Species interface. Make use of the symmetry of the system by modeling the RCH cell using a 2D axisymmetric geometry.

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

NEW

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

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.
2 In the **Select Physics** tree, select **Electrochemistry> Primary and Secondary Current Distribution>Primary Current Distribution (cd)**.
3 Click **Add**.
4 Click **Study**.
5 In the **Select Study** tree, select **General Studies>Stationary**.
6 Click **Done**.

GEOMETRY 1

Load the model parameters from a text file.

GLOBAL DEFINITIONS

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 `rotating_cylinder_hull_cell_parameters.txt`.

GEOMETRY 1

Draw the cell as a polygon, insert the polygon coordinates in the table from a text file.

Polygon 1 (pol1)

1. In the **Geometry** toolbar, click **Polygon**.
2. In the **Settings** window for **Polygon**, locate the **Coordinates** section.
3. Click **Load from File**.
4. Browse to the model's Application Libraries folder and double-click the file `rotating_cylinder_hull_cell_polygon.txt`.
5. Click **Build Selected**.

Boundary Layer

Draw the boundary layer as a rectangle.

1. In the **Geometry** toolbar, click **Rectangle**.
2. In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3. In the **Width** text field, type `30e-6`.
4. In the **Height** text field, type `H`.
5. Locate the **Position** section. In the **r** text field, type `0.003`.
6. In the **Label** text field, type `Boundary Layer`.
7. Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.
8. Click **Build Selected**.
9. Click the **Zoom Extents** button in the **Graphics** toolbar.

GLOBAL DEFINITIONS

Load the model variables from a text file.

DEFINITIONS

Variables 1

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 `rotating_cylinder_hull_cell_variables.txt`.

Working Electrode

Add selections to the model for the working and counter electrode boundaries.

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 4 only.

5 In the **Label** text field, type `Working Electrode`.

Counter Electrode

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

3 From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundaries 18–20 only.

5 In the **Label** text field, type `Counter Electrode`.

PRIMARY CURRENT DISTRIBUTION (CD)

Now specify the physics for the primary current distribution model.

Electrolyte 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Primary Current Distribution (cd)** click **Electrolyte 1**.

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

3 From the σ_l list, choose **User defined**. In the associated text field, type `sigma`.

Electrolyte Potential 1

Set the electrolyte potential to zero (default value) for the counter electrode surface.

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

2 In the **Settings** window for **Electrolyte Potential**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Counter Electrode**.

Electrode Surface 1

Use an Electrode Surface feature to prescribe an average current density on the working electrode surface. The boundary condition yields a constant electrode potential, along the given boundary, that satisfies the given value of the average current density.

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

2 In the **Settings** window for **Electrode Surface**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Working Electrode**.

4 Locate the **Electrode Phase Potential Condition** section. From the **Electrode phase potential condition** list, choose **Average current density**.

5 In the $i_{\mathrm{l,average}}$ text field, type `i_app`.

MESH 1

Create a mesh consisting of a mapped mesh in the boundary layer close to the working electrode, and a triangular mesh for the rest of the geometry.

Mapped 1

1 In the **Mesh** toolbar, click **Mapped**.

2 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Boundary Layer**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 5 and 6 only.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 4 and 7 only.

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

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 200.

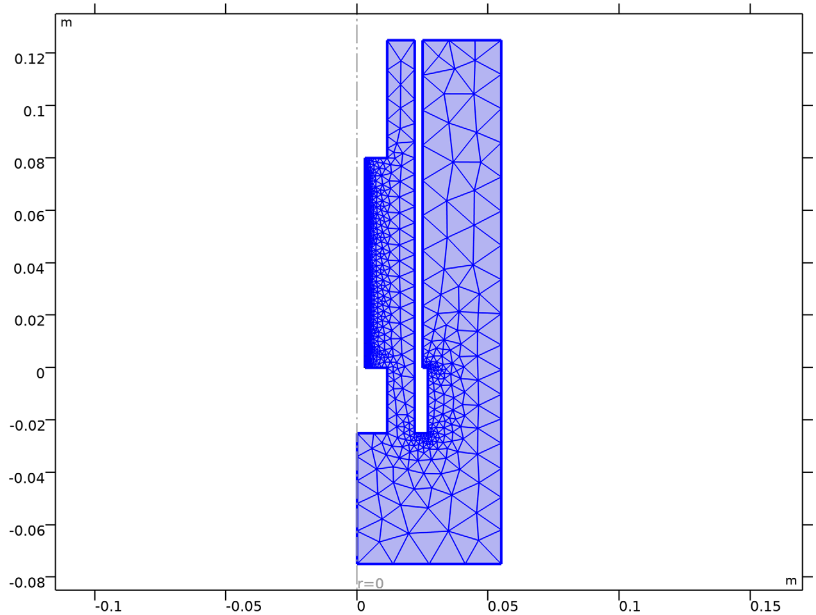
6 In the **Element ratio** text field, type 10.

Free Triangular 1

1 In the **Mesh** toolbar, click **Free Triangular**.

2 In the **Settings** window for **Free Triangular**, click **Build All**.

Your finished mesh should now look like this:



STUDY 1

Now solve the primary current distribution model.

1 In the **Home** toolbar, click **Compute**.

Store the solution for primary current density distribution in order to compare the results with later simulations.

Solution 1 (sol1)

1 In the **Model Builder** window, expand the **Study 1>Solver Configurations** node.

2 Right-click **Solution 1 (sol1)** and choose **Solution>Copy**.

Primary

1 In the **Model Builder** window, right-click **Solution 1 - Copy 1 (sol2)** and choose **Rename**.

2 In the **Rename Solution** dialog box, type `Primary` in the **New label** text field.

3 Click **OK**.

RESULTS

Plot the normalized current density and compare it with the analytical solution in the following way:

1D Plot Group 9

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.
3 From the **Dataset** list, choose **Study 1/Primary (sol2)**.

Line Graph 1

1 Right-click **1D Plot Group 9** and choose **Line Graph**.
2 In the **Settings** window for **Line Graph**, locate the **Selection** section.
3 From the **Selection** list, choose **Working Electrode**.
4 Locate the **y-Axis Data** section. In the **Expression** text field, type `cd.iloc_er1/i_app`.
5 Select the **Description** check box. In the associated text field, type `Normalized current density`.
6 In the **Unit** field, type .
7 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
8 In the **Expression** text field, type `z`.
9 Select the **Description** check box. In the associated text field, type `Distance along the working electrode`.
10 Click to expand the **Legends** section. Select the **Show legends** check box.
11 From the **Legends** list, choose **Manual**.
12 In the table, enter the following settings:

Legends
Numerical

13 In the **1D Plot Group 9** toolbar, click **Plot**.

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.
2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3 In the **Expression** text field, type `i_analytical`.
4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

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

Legends
Analytical

6 In the **1D Plot Group 9** toolbar, click **Plot**.

Normalized current density, Primary

1 In the **Model Builder** window, right-click **1D Plot Group 9** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Normalized current density, Primary` in the **New label** text field.

3 Click **OK**.

PRIMARY CURRENT DISTRIBUTION (CD)

Now, solve the secondary current distribution model by changing the Current Distribution Type setting on the physics node.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Primary Current Distribution (cd)**.

2 In the **Settings** window for **Primary Current Distribution**, locate the **Current Distribution Type** section.

3 From the **Current distribution type** list, choose **Secondary**.

The secondary current distribution model includes activation losses on the electrodes. Add the parameter settings for the electrode kinetics.

Electrode Reaction 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Secondary Current Distribution (cd)>Electrode Surface 1** click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Electrode Kinetics** section.

3 From the **Kinetics expression type** list, choose **Cathodic Tafel equation**.

4 In the i_0 text field, type `i0`.

5 In the A_c text field, type `Ac`.

STUDY 1

Add an auxiliary continuation sweep to vary the applied current density.

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
i_app (Applied current density)	-5, -10, -20, -40, -60, -80, -100, -140, -180	A/m^2

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

Store the solution for the secondary current distribution model. It will be used for comparison later.

Solution 1 (sol1)

In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Solution 1 (sol1)** and choose **Solution>Copy**.

Secondary

1 In the **Model Builder** window, right-click **Solution 1 - Copy 1 (sol3)** and choose **Rename**.

2 In the **Rename Solution** dialog box, type `Secondary` in the **New label** text field.

3 Click **OK**.

RESULTS

Plot the overpotential and the normalized current density for different values of the applied current density as follows:

1D Plot Group 10

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

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

3 From the **Dataset** list, choose **Study 1/Secondary (sol3)**.

Line Graph 1

1 Right-click **1D Plot Group 10** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **Working Electrode**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Secondary Current Distribution>Electrode kinetics>cd.eta_er1 - Overpotential - V**.

5 Locate the **y-Axis Data** section. Select the **Description** check box.

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

7 In the **Expression** text field, type `z`.

8 Select the **Description** check box. In the associated text field, type `Distance along the working electrode`.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 In the **1D Plot Group 10** toolbar, click **Plot**.

Overpotential, Secondary

1 In the **Model Builder** window, under **Results** click **1D Plot Group 10**.

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

Overpotential, Secondary 1

Right-click **Overpotential, Secondary** and choose **Duplicate**.

Line Graph 1

1 In the **Model Builder** window, expand the **Overpotential, Secondary 1** node, then click **Line Graph 1**.

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

3 In the **Expression** text field, type `cd.iloc_er1/i_app`.

4 In the **Description** text field, type `Normalized current density`.

5 In the **Overpotential, Secondary 1** toolbar, click **Plot**.

Normalized current density, Secondary

1 In the **Model Builder** window, right-click **Overpotential, Secondary 1** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Normalized current density, Secondary` in the **New label** text field.

3 Click **OK**.

COMPONENT 1 (COMP1)

Now, set up the tertiary current distribution model by including a Transport of Diluted Species interface, and by coupling it with the Secondary Current Distribution interface. Transport of Diluted Species is active in a very small domain (30 micrometer thick) next to the working electrode.

ADD PHYSICS

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

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

3 In the tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

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

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

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Settings** window for **Transport of Diluted Species**, locate the **Domain Selection** section.

2 From the **Selection** list, choose **Boundary Layer**.

3 Locate the **Transport Mechanisms** section. Clear the **Convection** check box.

Transport Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species (tds)** click **Transport Properties 1**.

2 In the **Settings** window for **Transport Properties**, locate the **Diffusion** section.

3 In the D_c text field, type `D`.

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 c text field, type `cb`.

Concentration 1

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

2 Select Boundary 7 only.

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

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

5 In the $c_{0,c}$ text field, type `cb`.

Electrode Surface Coupling 1

Use an Electrode Surface Coupling node to couple the reaction term with the local current density obtained from the Secondary Current Distribution interface.

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

2 In the **Settings** window for **Electrode Surface Coupling**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Working Electrode**.

Reaction Coefficients 1

1 In the **Model Builder** window, expand the **Electrode Surface Coupling 1** node, then click **Reaction Coefficients 1**.
2 In the **Settings** window for **Reaction Coefficients**, locate the **Model Inputs** section.
3 From the i_{loc} list, choose **Local current density, Electrode Reaction 1 (cd/es1/er1)**.
4 Locate the **Stoichiometric Coefficients** section. In the n text field, type `2`.
5 In the ν_c text field, type `-1`.

SECONDARY CURRENT DISTRIBUTION (CD)

The electrode kinetics is made concentration dependent by changing the exchange current density term as follows:

Electrode Reaction 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Secondary Current Distribution (cd)>Electrode Surface 1** click **Electrode Reaction 1**.
2 In the **Settings** window for **Electrode Reaction**, locate the **Electrode Kinetics** section.
3 In the i_0 text field, type `i0*(c/cb)`.

Change the applied current density values for the tertiary current distribution model.

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**, locate the **Study Extensions** section.
3 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
i_app (Applied current density)	-1, -5, -10, -20, -40, -60, -80, -100, -130	A/m^2

The model is now ready to be solved.

4 In the **Home** toolbar, click **Compute**.

RESULTS

Electrolyte Potential (cd)

Plot the overpotential, the local current density and the normalized concentration for the tertiary current density distribution as follows:

1D Plot Group 12

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

Line Graph 1

1 Right-click **1D Plot Group 12** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **Working Electrode**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Secondary Current Distribution>Electrode kinetics>cd.eta_er1 - Overpotential - V**.

5 Locate the **y-Axis Data** section. Select the **Description** check box.

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

7 In the **Expression** text field, type `z`.

8 Select the **Description** check box. In the associated text field, type `Distance along the working electrode`.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 In the **1D Plot Group 12** toolbar, click **Plot**.

Overpotential, Tertiary

1 In the **Model Builder** window, under **Results** click **1D Plot Group 12**.

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

Overpotential, Tertiary 1

Right-click **Overpotential, Tertiary** and choose **Duplicate**.

Line Graph 1

1 In the **Model Builder** window, expand the **Overpotential, Tertiary 1** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Secondary Current Distribution>Electrode kinetics>cd.iloc_er1 - Local current density - A/m²**.

3 Locate the **y-Axis Data** section. In the **Description** text field, type `Local current density`.

4 In the **Overpotential, Tertiary 1** toolbar, click **Plot**.

Local current density, Tertiary

1 In the **Model Builder** window, under **Results** click **Overpotential, Tertiary 1**.
2 In the **Settings** window for **1D Plot Group**, type `Local current density, Tertiary` in the **Label** text field.

Local current density, Tertiary 1

Right-click **Local current density, Tertiary** and choose **Duplicate**.

Line Graph 1

1 In the **Model Builder** window, expand the **Local current density, Tertiary 1** node, then click **Line Graph 1**.
2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
3 In the **Expression** text field, type `c/cb`.
4 In the **Description** text field, type `Normalized concentration`.
5 In the **Local current density, Tertiary 1** toolbar, click **Plot**.

Normalized concentration, Tertiary

1 In the **Model Builder** window, right-click **Local current density, Tertiary 1** and choose **Rename**.
2 In the **Rename 1D Plot Group** dialog box, type `Normalized concentration, Tertiary` in the **New label** text field.
3 Click **OK**.

1D Plot Group 15

Now compare the primary, secondary and tertiary current distributions by plotting the normalized current density for a representative value of applied current density.

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.
2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.
3 From the **Dataset** list, choose **None**.

Line Graph 1

1 Right-click **1D Plot Group 15** and choose **Line Graph**.
2 In the **Settings** window for **Line Graph**, locate the **Data** section.
3 From the **Dataset** list, choose **Study 1/Primary (sol2)**.
4 Locate the **Selection** section. From the **Selection** list, choose **Working Electrode**.
5 Locate the **y-Axis Data** section. In the **Expression** text field, type `cd.iloc_er1/i_app`.

6 Select the **Description** check box. In the associated text field, type `Normalized current density`.

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

8 In the **Expression** text field, type `z`.

9 Select the **Description** check box. In the associated text field, type `Distance along the working electrode`.

10 Locate the **Legends** section. Select the **Show legends** check box.

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

12 In the table, enter the following settings:

Legends
`Primary`

13 In the **1D Plot Group 15** toolbar, click **Plot**.

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 1/Secondary (sol3)**.

4 From the **Parameter selection (i_app)** list, choose **From list**.

5 In the **Parameter values (i_app (A/m^2))** list, select **-100**.

6 Locate the **Title** section. From the **Title type** list, choose **None**.

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

Legends
`Secondary`

8 In the **1D Plot Group 15** toolbar, click **Plot**.

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

4 In the **Parameter values (i_app (A/m^2))** list, select **-100**.

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

Legends
`Tertiary`

6 In the **1D Plot Group 15** toolbar, click **Plot**.

Current density comparison

1 In the **Model Builder** window, right-click **1D Plot Group 15** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Current density comparison` in the **New label** text field.

3 Click **OK**.

Electrolyte Potential, 3D (cd)

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