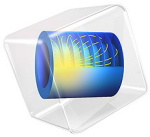


Two-Phase Flow Modeling of Copper Electrowinning Using Bubbly Flow

Introduction

Copper electrowinning is the process of copper extraction from an electrolyte solution, and its subsequent deposition at the cathode surface, by passing an external current through the electrolytic cell. In the cell, an insoluble anode is typically used. During the process, oxygen bubbles are generated at the anode surface leading to a large recirculation zone between the anode and cathode surfaces.

In the model example presented here, charge and mass transports of ionic species are modeled using the Tertiary Current Distribution, Nernst–Planck interface and the two-phase flow generated due to oxygen gas evolution at the anode surface is modeled using the Bubbly Flow, Laminar Flow interface.

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

Model Definition

The electrowinning cell model geometry is shown in Figure 1. The two vertical boundaries represent the anode and the cathode surfaces, respectively. Since the oxygen gas evolves at the anode surface, this boundary also acts a gas inlet. The top boundary

serves as an inlet for the liquid phase and an outlet for the gas phase. The outlet boundary for both the liquid and gas phases is as shown Figure 1.

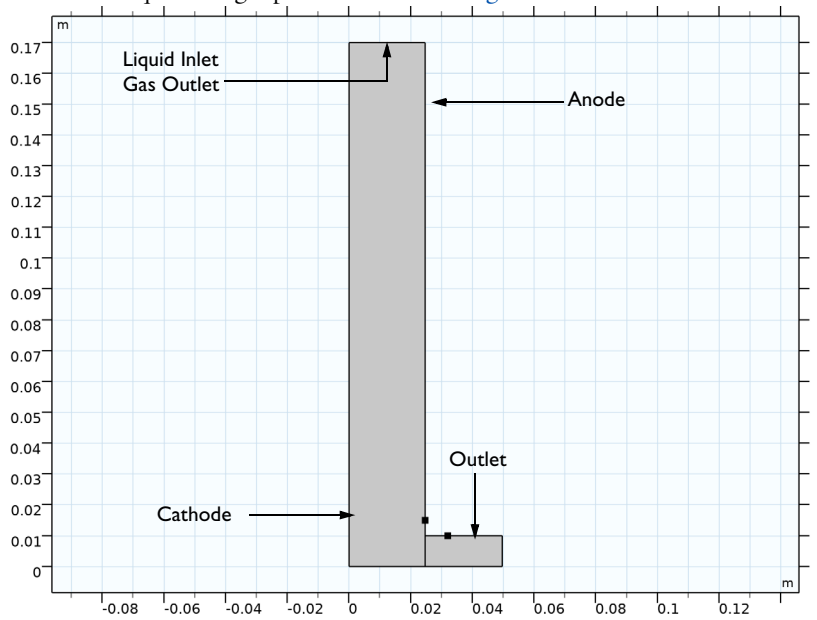


Figure 1: Model domain with boundaries corresponding to the anode, cathode, and vertical symmetry walls.

Mass transport by convection, diffusion and migration for three ionic species (copper, Cu^{2+}, hydrogen, $H^{+}$and bisulfate, HSO_4^{-}) is solved using the Tertiary Current Distribution, Nernst-Planck physics interface:

$$\frac{\partial \varepsilon_l c_i}{\partial t} + \nabla \cdot \mathbf{N}_i + \mathbf{u} \cdot \nabla c_i = 0$$

where ε_l is the electrolyte volume fraction. ε_l is defined in terms of the liquid phase fraction which is solved for in the Bubbly Flow, Laminar Flow interface, as discussed later in this section.

The flux for each of the ions in the electrolyte is given by the Nernst–Planck equation:

$$\mathbf{N}_i = -D_{i,\text{eff}} \nabla c_i - z_i u_{i,\text{eff}} F c_i \nabla \phi_l$$

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, $u_{i,\text{eff}}$ the mobility of the charged

species ($m^2/(s \cdot J \cdot mole)$), F Faraday's constant (As/mole), and ϕ_l the potential in the electrolyte (V).

The transport properties such as diffusion coefficients are defined using the electrolyte volume fraction:

$$D_{i,\,\mathrm{eff}} = \varepsilon_l^{1.5} D_i$$

The velocity field used in the mass transport equation comes from the Bubbly Flow, Laminar Flow interface and is corrected for the electrolyte volume fraction.

The electroneutrality condition is given by the following expression:

$$\sum_i z_i c_i = 0$$

ELECTROCHEMICAL REACTIONS

The copper reduction and the oxygen evolution due to water decomposition are the two electrochemical reactions considered in the copper electrowinning model presented here.

The copper reduction at the cathode surface proceeds as:

$$\mathrm{Cu}^{2+} + 2e^- \rightarrow \mathrm{Cu}$$

The oxygen evolution at the anode surface proceeds as:

$$2\mathrm{H_2O} \rightarrow 4\mathrm{H}^+ + \mathrm{O_2} + 4\mathrm{e}^-$$

Concentration dependent kinetics is used to model the copper reduction and oxygen evolution oxidation reactions, which will set the local current density according to:

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

where $i_{0,\mathrm{m}}$ is the exchange current density, $C_{\mathrm{R,m}}$ is the reduced species expression, $C_{\mathrm{O,m}}$ is the oxidized species expression, $\alpha_{\mathrm{a,m}}$ is the anodic transfer coefficient, $\alpha_{\mathrm{c,m}}$ is the cathodic transfer coefficient, and η_{m} is the overpotential for species m (Cu and H, respectively).

The overpotential η_{m} (V) is calculated from:

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

The total current of 5.14 A is applied at the anode surface which is used to calculate the external electric potential, $\phi_{s,\,\mathrm{ext}}$.

The equilibrium potentials for the copper reduction and oxygen evolution oxidation reactions are calculated using the Nernst equation:

$$E_{\mathrm{eq,Cu}} = E^0_{\mathrm{eq,\,Cu}} + \frac{RT}{nF}\ln\left(\frac{c_{\mathrm{Cu}}}{c_{\mathrm{Cu,ref}}}\right)$$

$$E_{\mathrm{eq,H}} = E^0_{\mathrm{eq,H}} + \frac{RT}{nF}\ln\left(\frac{c_{\mathrm{H}}}{c_{\mathrm{H,ref}}}\right)^4$$

where $E^0_{\mathrm{eq,\,Cu}}$ and $E^0_{\mathrm{eq,H}}$ are the standard equilibrium potentials for the copper reduction and oxygen evolution oxidation reactions and are considered to be 0.34 V and 1.23 V, respectively. Moreover, $c_{\mathrm{Cu,ref}}$ and $c_{\mathrm{H,ref}}$ are the reference concentrations for copper and hydrogen ions, respectively.

At the anode and cathode surface boundaries, fluxes of ionic species are defined in terms of the electrochemical reactions as:

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

where ν_{m} is the stoichiometric coefficient, $i_{\mathrm{loc,m}}$ is the local current density, n_{m} is the number of electrons, and F is Faraday's constant (96,485 C/mol). This will set the flux to be proportional to the electrode current density according to Faraday's law.

The electrode kinetics parameters: $i_{0,\mathrm{Cu}}$=100 A/m^2 and $i_{0,\mathrm{H}}$= 3×10^7 A/m^2 are taken from Ref. 1.

BUBBLY FLOW INTERFACE

The Bubbly Flow interface sets up a two-phase flow model for oxygen gas bubbles in a liquid electrolyte. The physics interface tracks the averaged gas-phase concentration rather than each bubble in detail. The physics interface solves for the liquid velocity, the pressure, and the volume fraction of the gas phase. Details of the governing equations are presented in the theory section for the Bubbly Flow interfaces in the *CFD Module User's Guide*.

The Physical Model settings for the Bubbly Flow interface provides a low gas concentration option which is active per default. This option is applicable if the gas concentration is about 1%, in which case the transport equations can be simplified compared to cases with higher gas concentrations. Considering the possibility of higher

gas phase faction, particularly near the anode surface, the low gas concentration option is disabled in this model.

For demonstration purpose, density and viscosity of the liquid phase are assumed to be uniform and are considered to be 1200 kg/m^3 and 0.835×10^{-3} kg/m/s, respectively. However, they can be set to be dependent upon the copper concentration.

For laminar flow the gas velocity $\mathbf{u}_g$ is calculated from:

$$\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{slip}$$

where $\mathbf{u}_l$ stands for the liquid-phase velocity, and $\mathbf{u}_{slip}$ stands for the relative velocity between gas and liquid, the so-called slip velocity.

The slip velocity is calculated from a slip model. The Bubbly Flow interface provides several slip models. The most appropriate slip model for this electrowinning cell is a pressure-drag balance slip model with a drag coefficient tuned for small spherical bubbles using Hadamard—Rybczynski model. The gas bubbles diameter is considered to be 50 μm.

The top boundary of the electrowinning cell acts as an inlet for the liquid phase and as an outlet for the gas phase. The Inlet boundary feature is used here to set the normal inflow velocity to 0.0001 m/s and to set the gas outlet boundary condition.

The Outlet boundary feature is used to set zero pressure for the liquid phase and to set gas outlet boundary condition for the gas phase for the boundary shown in Figure 1.

The Wall boundary feature is used to set no slip boundary condition for the liquid phase and to set the gas mass flux at the anode surface as

$$-\mathbf{n} \cdot \mathbf{N}_{O_2} = \frac{Mw_{O_2} i_{loc,H}}{4F}$$

where $\mathbf{N}_{O_2}$ is the gas mass flux for oxygen bubbles; Mw_{O_2} is the molar mass of oxygen; $i_{loc,H}$ is the local current density of oxygen evolution reaction evaluated at the Tertiary Current Distribution, Nernst–Planck physics interface; and F is Faraday's constant.

Results and Discussion

Figure 2 shows surface plot of the liquid phase velocity magnitude along with arrow plot of the liquid phase velocity field after 60 s of deposition operation. A large vortex can be seen at the top of the electrowinning cell in Figure 2. The higher magnitude of liquid phase velocity at the anode surface indicates the generation of oxygen bubbles due to water

decomposition electrochemical reaction and their rise to the top of the cell due to buoyancy effects.

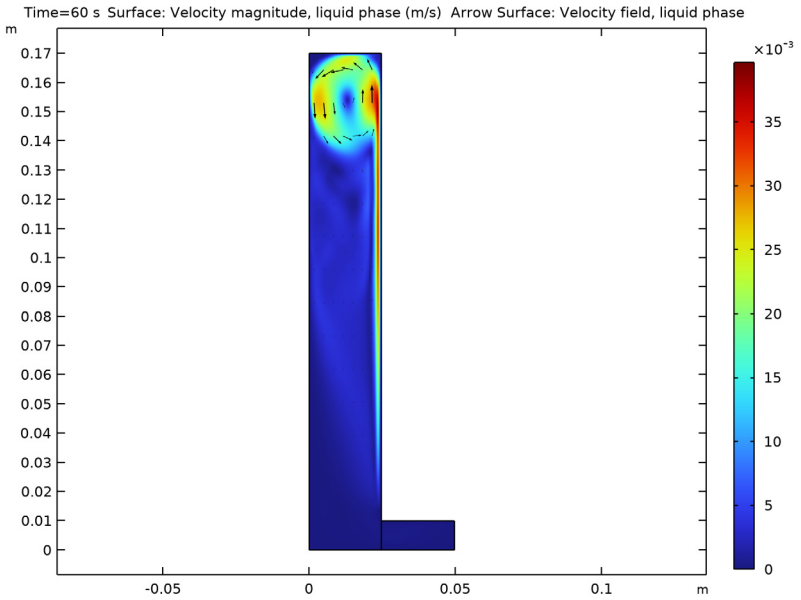


Figure 2: Surface plot of the liquid phase velocity magnitude along with arrow plot of the liquid phase velocity field after 60 seconds of deposition operation.

Figure 3 shows surface plot of the gas phase volume fraction along with streamline plot of the liquid phase velocity field after 60 s of deposition operation. The gas phase volume fraction is seen to be higher near anode surface in Figure 3, similar to the liquid phase velocity shown in Figure 2. The buoyancy force of oxygen bubbles generated at the anode

surface is a strong driving force for the fluid flow in the electrowinning cell. The highest magnitude of the gas phase volume fraction is found to be just over 0.02.

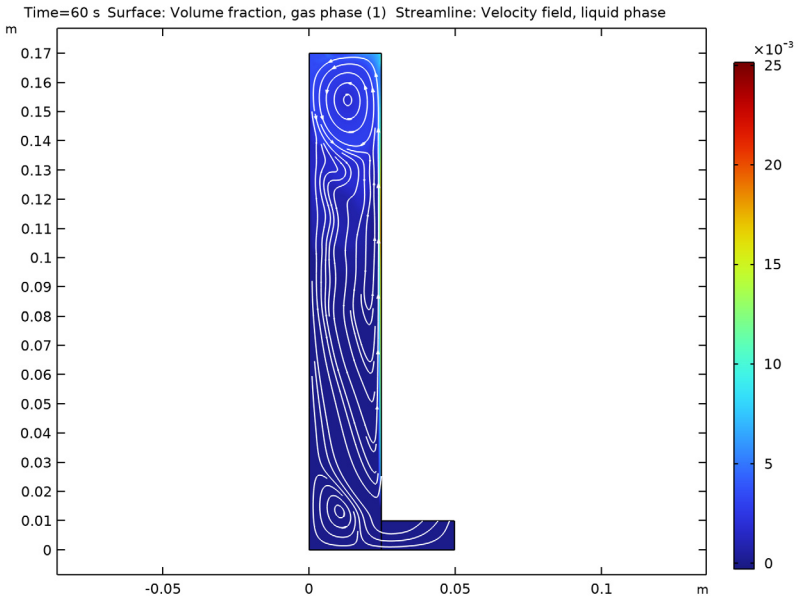


Figure 3: Surface plot of the gas phase volume fraction along with streamline plot of the liquid phase velocity field after 60 seconds of deposition operation.

Figure 4 shows surface plot of the copper concentration along with streamline plot of the total flux after 60 s of deposition operation. It can be seen that the copper concentration is quite uniform throughout the electrowinning cell due to a strong stirring effect of oxygen bubbles. The lowest copper concentration is observed at the cathode surface

(which is not clearly visible in Figure 4) since copper ions are consumed here during deposition.

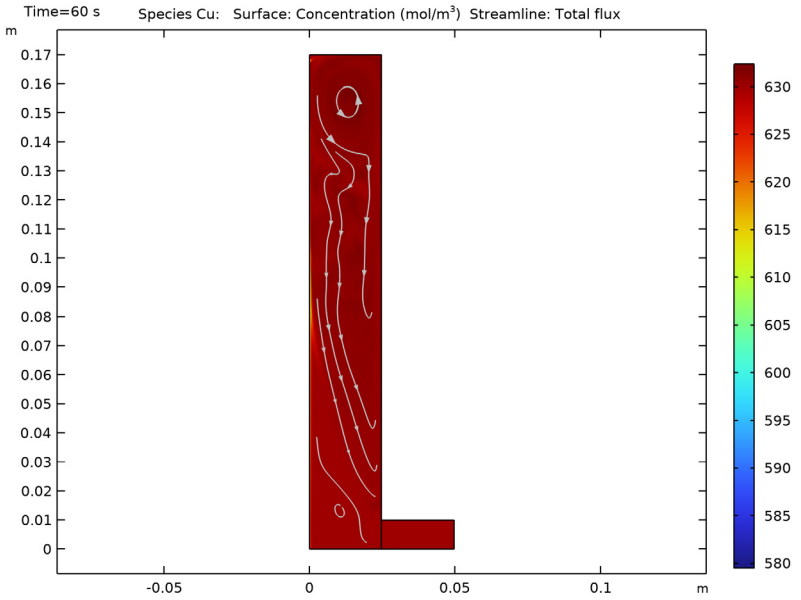


Figure 4: Surface plot of the copper concentration along with streamline plot of the total flux after 60 seconds of deposition operation.

To bring out the depletion of copper ions at the cathode surface, several line plots are plotted next for the copper concentration.

Figure 5 shows line plot of the copper concentration along the cathode surface after 60 s of deposition operation. It can be seen that the copper concentration varies considerably with distance from the bottom of the cathode surface. The peak in the copper

concentration at the top of the cathode surface corresponds to a vortex in the liquid phase velocity magnitude observed in Figure 2.

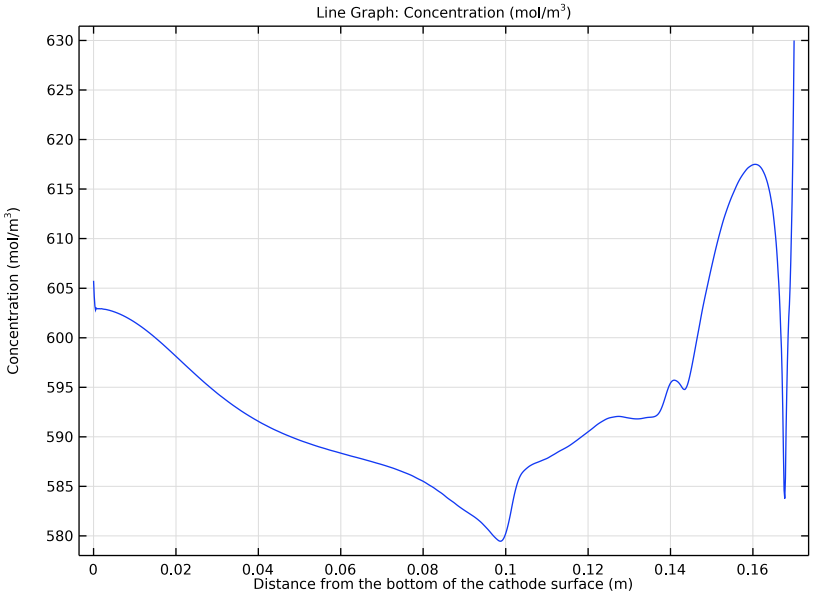


Figure 5: Line plot of the copper concentration along the cathode surface after 60 seconds of deposition operation.

Figure 6 shows line plot of the change in copper concentration with time for 60 s of deposition operation at three different locations on the cathode surface. It can be seen that

the copper concentration attained a steady state at the top and middle of the cathode surface whereas it decreased continuously at the bottom of the cathode surface.

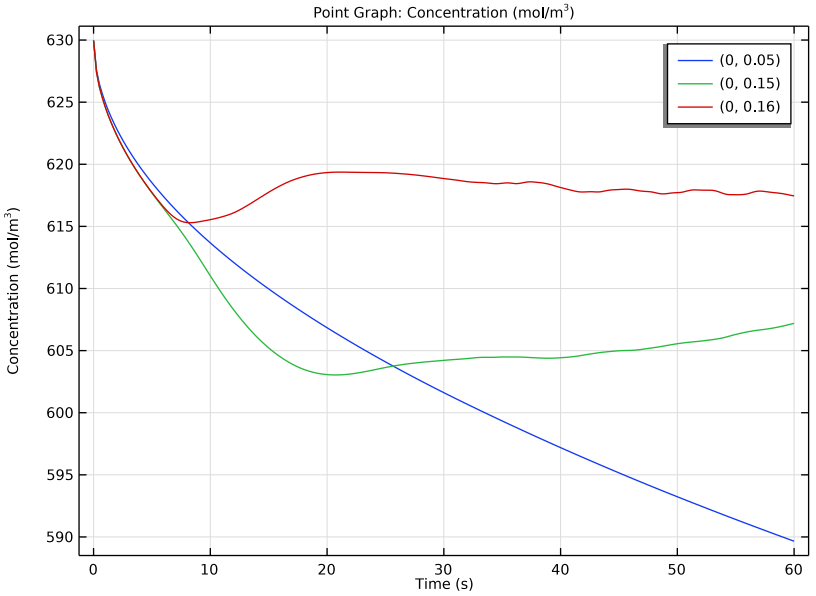


Figure 6: Line plot of the change in copper concentration with time at different locations on the cathode surface.

Figure 7 shows line plot of the change in copper concentration across the boundary layer thickness at a specific position on the cathode surface after 60 s of deposition operation. It can be seen that the copper concentration varies considerably across boundary layer thickness and it remains uniform toward the bulk of the electrolyte solution. This result

confirms that the mesh used in the model is fine enough to resolve the change in copper concentration across the boundary layer at the cathode surface.

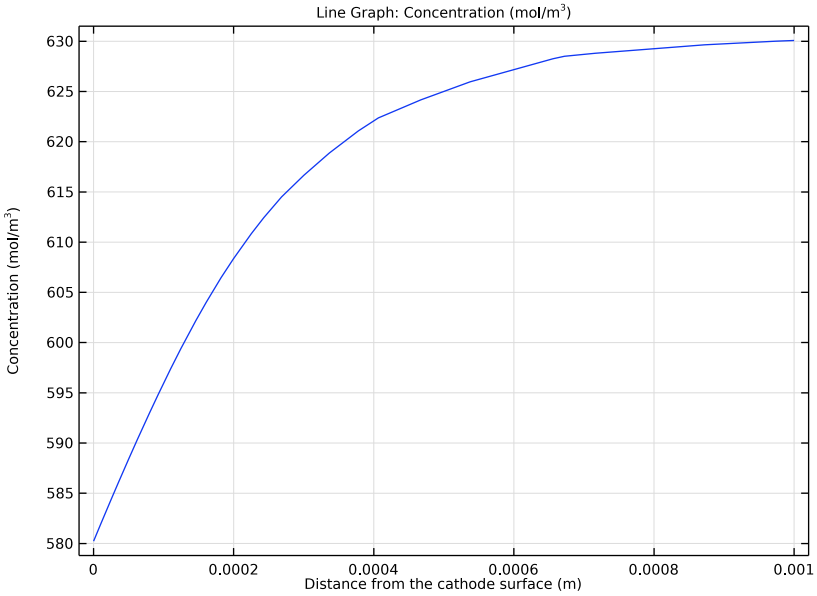


Figure 7: Line plot of the change in copper concentration within the boundary layer at a specific position on the cathode surface after 60 seconds of deposition operation.

Figure 8 shows line plot of the change in copper deposition thickness along the cathode surface after 60 s of deposition operation. It can be seen that the copper deposition is considerably higher at the top half of the cathode surface when compared to the bottom

half. The peak in the copper deposition thickness at the top of the cathode surface corresponds to a vortex in the liquid phase velocity magnitude observed in Figure 2.

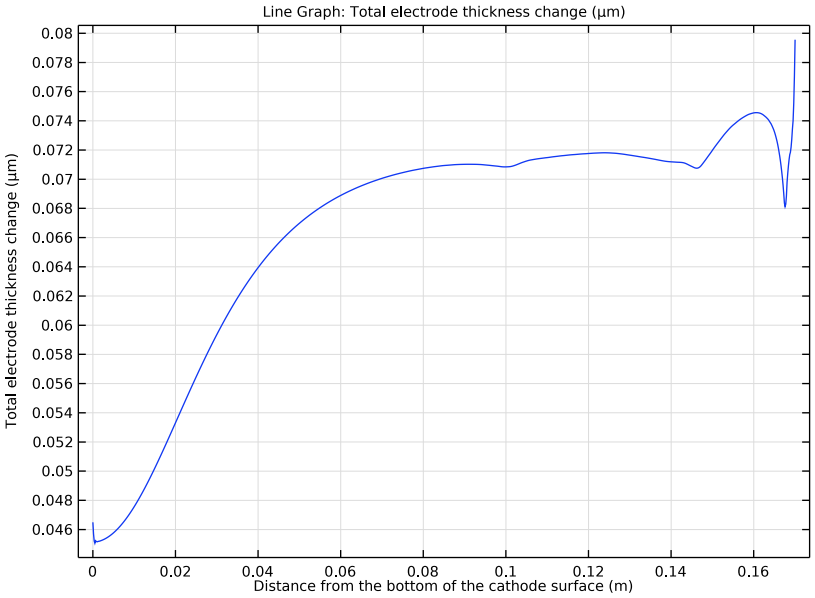


Figure 8: Line plot of the copper deposition thickness along the cathode surface after 60 seconds of deposition operation.

Reference

1. J.M. Werner, W. Zeng, M.L. Free, Z. Zhang, and J. Cho, "Modeling and Validation of Local Electrowinning Electrode Current Density Using Two Phase Flow and Nernst-Planck Equations," *Journal of The Electrochemical Society*, vol. 165, p. E190, 2018.

Application Library path: `Electrodeposition_Module/Tutorials/cu_electrowinning_bubbly_flow`

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 **2D**.

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

3 Click **Add**.

4 In the **Number of species** text field, type 3.

5 In the **Concentrations** table, enter the following settings:

cCu
cH
cHSO4

6 In the **Select Physics** tree, select **Fluid Flow>Multiphase Flow>Bubbly Flow>Bubbly Flow, Laminar Flow (bf)**.

7 Click **Add**.

8 Click **Study**.

9 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Tertiary Current Distribution, Nernst-Planck>Time Dependent with Initialization**.

10 Click **Done**.

GEOMETRY 1

Draw the geometry by making a union of two rectangles.

Rectangle 1 (r1)

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 `0.02467`.

4 In the **Height** text field, type `0.17`.

Rectangle 2 (r2)

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 `0.025`.

4 In the **Height** text field, type `0.01`.

5 Locate the **Position** section. In the **x** text field, type `0.02467`.

Point 1 (pt1)

1 In the **Geometry** toolbar, click **Point**.

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

3 In the **x** text field, type `0.032`.

4 In the **y** text field, type `0.01`.

Point 2 (pt2)

1 In the **Geometry** toolbar, click **Point**.

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

3 In the **x** text field, type `0.02467`.

4 In the **y** text field, type `0.015`.

5 Click **Build Selected**.

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 `cu_electrowinning_bubbly_flow_parameters.txt`.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (TCD)

First set the species for the electroneutrality condition and then set up the electrochemical model, consisting of species properties and separator domains, and boundaries comprising of an anode surface, a cathode surface, an inflow and an outflow.

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

2 In the **Settings** window for **Tertiary Current Distribution, Nernst-Planck**, locate the **Electrolyte Charge Conservation** section.

3 From the **From electroneutrality** list, choose **cHSO4**.

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_{cCu} text field, type `2`.

4 In the z_{cH} text field, type `1`.

5 In the z_{cHSO4} text field, type `-1`.

Separator 1

1 In the **Physics** toolbar, click **Domains** and choose **Separator**.

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

3 From the **Selection** list, choose **All domains**.

4 Locate the **Convection** section. Specify the $\mathbf{u}$ vector as

`bf.phil*u`	`x`
`bf.phil*v`	`y`

5 Locate the **Diffusion** section. In the D_{cCu} text field, type `DCu`.

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

7 In the D_{cHSO4} text field, type `DHSO4`.

8 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `bf.phil`.

Anode Surface

Set the electrode kinetics at the anode surface.

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

2 In the **Settings** window for **Electrode Surface**, type `Anode Surface` in the **Label** text field.

3 Select Boundary 8 only.

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

5 In the $I_{l,total}$ text field, type `Itot`.

Oxygen Evolution Reaction

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

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

3 Locate the **Stoichiometric Coefficients** section. In the n text field, type `4`.

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

5 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq0_O2`.

6 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0a_O2`.

Cathode Surface

Next, define the electrode kinetics at the cathode 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**, type `Cathode Surface` in the **Label** text field.

4 Click to expand the **Dissolving-Depositing Species** section. Click **Add**.

5 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
Cu	rho_Cu	Mw_Cu

Copper Deposition Reaction

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

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

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

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

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

Species	Stoichiometric coefficient (1)
Cu	1

6 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `Eeq0_Cu`.

7 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0c_Cu`.

8 In the α_a text field, type `alphaa_Cu`.

Inflow 1

Now, set the concentration of species at the Inflow boundary.

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

2 Select Boundary 3 only.

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

4 In the $c_{0,cCu}$ text field, type `cOCu`.

5 In the $c_{0,cH}$ text field, type `cOH`.

Outflow 1

Set the Outflow boundary.

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

2 Select Boundary 9 only.

Initial Values 1

Set the initial values for concentration.

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 cCu text field, type `cOCu`.

4 In the cH text field, type `cOH`.

BUBBLY FLOW, LAMINAR FLOW (BF)

Next, set up physics for the Bubbly Flow. The low gas concentration formulation is typically valid for gas phase fraction of 0.01. Considering that we may get higher gas phase fraction, particularly near the anode surface, clear the Low gas concentration check box under Physical Model.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Bubbly Flow, Laminar Flow (bf)**.

2 In the **Settings** window for **Bubbly Flow, Laminar Flow**, locate the **Physical Model** section.

3 Clear the **Low gas concentration** check box.

Fluid Properties 1

Now, set the physical properties for the liquid and gas phases. For simplicity, density and viscosity of the liquid phase are assumed to be constant. Set Calculate from ideal gas law option for density of the gas phase and Pressure-drag balance option for slip model.

1 In the **Model Builder** window, under **Component 1 (comp1)>Bubbly Flow, Laminar Flow (bf)** click **Fluid Properties 1**.

2 In the **Settings** window for **Fluid Properties**, locate the **Liquid Properties** section.

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

4 From the μ_l list, choose **User defined**. In the associated text field, type `nu`.

5 Locate the **Gas Properties** section. From the ρ_g list, choose **Calculate from ideal gas law**.

6 In the M_g text field, type `Mw_O2`.

7 In the d_b text field, type `d_b`.

8 Locate the **Slip Model** section. From the **Slip model** list, choose **Pressure-drag balance**.

Initial Values 1

Set the initial value for pressure.

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

2 In the **Settings** window for **Initial Values**, type `rho*g_const*(0.17-y)` in the p text field.

Gravity 1

Next, add gravitation force using Gravity feature.

1 In the **Physics** toolbar, click **Domains** and choose **Gravity**.

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

3 From the **Selection** list, choose **All domains**.

Wall (Gas Inlet)

Next, set the gas mass influx at the anode surface.

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

2 In the **Settings** window for **Wall**, type `Wall (Gas Inlet)` in the **Label** text field.

3 Select Boundary 8 only.

4 Locate the **Gas Boundary Condition** section. From the **Gas boundary condition** list, choose **Gas flux**.

5 In the $N_{\rho g \phi g}$ text field, type `(tcd.iloc_er1)*Mw_O2/(4*F_const)`.

Liquid Inlet and Gas Outlet

Set the liquid inlet velocity and gas outlet using Inlet feature.

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

2 In the **Settings** window for **Inlet**, type `Liquid Inlet and Gas Outlet` in the **Label** text field.

3 Select Boundary 3 only.

4 Locate the **Velocity** section. In the U_0 text field, type `Vb`.

5 Locate the **Gas Boundary Condition** section. From the **Gas boundary condition** list, choose **Gas outlet**.

Outlet 1

Set the liquid and gas outlet using Outlet feature.

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

2 Select Boundary 9 only.

GLOBAL DEFINITIONS

Default Model Inputs

Set up the temperature value used in the entire model.

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

Set the extra fine mesh near the cathode surface and set the boundary layers at the Wall features.

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

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Finer**.

4 Locate the **Sequence Type** section. 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 **Finer**.

Size 1

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

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 In the list, choose **2**, **5**, **6**, **7**, **8**, and **10**.

4 Click — **Remove from Selection**.

5 Select Boundary 1 only.

6 In the list, select **1**.

Size 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

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

4 Select Point 6 only.

5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.

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

7 Drag and drop below **Size 1**.

Boundary Layer Properties 1

Since it is usually a good idea to not have boundary layers on a boundary through which a significant gas flux is expected, anode boundary is excluded from boundary layers.

1 In the **Model Builder** window, expand the **Boundary Layers 1** node, then click **Boundary Layer Properties 1**.

2 Select Boundaries 1, 2, 5–7, and 10 only.

3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.

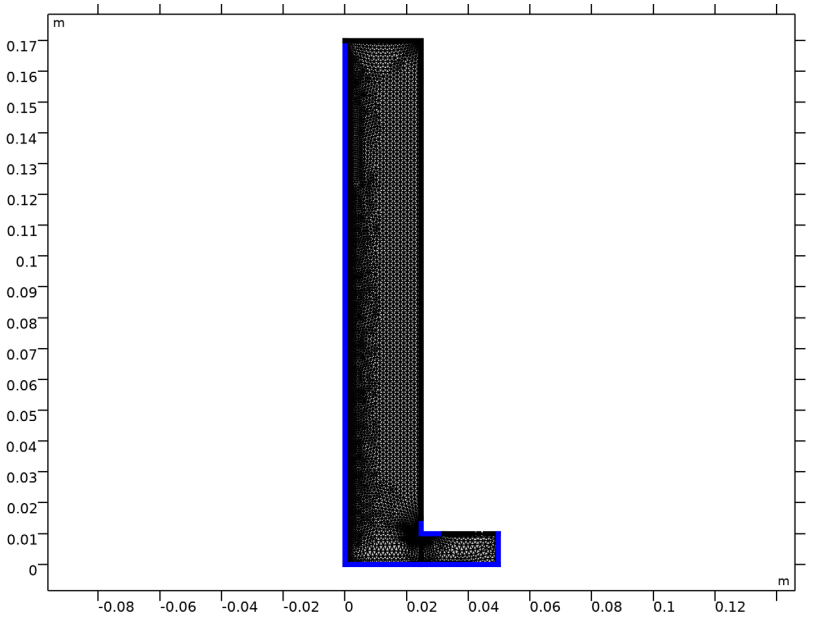
4 In the **Number of layers** text field, type `4`.

5 From the **Thickness specification** list, choose **First layer**.

6 In the **Thickness** text field, type `0.00005`.

7 Click **Build All**.

The mesh should look like this:



STUDY 1

Finally, update the study settings. Since we have not set the initial values for electrolyte potential, we will make use of Current Distribution Initialization study nodes. Add another Current Distribution Initialization study node and set current distribution type to Secondary. Disable Bubbly Flow interface from Current Distribution Initialization study nodes. Set the time range at the Time Dependent study node. Update the default solver setting by adding a Fully Coupled study node and then the model is ready to be solved.

Current Distribution Initialization 2

1 In the **Study** toolbar, click **Study Steps** and choose **Other> Current Distribution Initialization**.

2 In the **Settings** window for **Current Distribution Initialization**, locate the **Study Settings** section.

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

4 Right-click **Study 1>Step 3: Current Distribution Initialization 2** and choose **Move Up**.

Step 3: Time Dependent

1 In the **Model Builder** window, click **Step 3: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,0.25,60)`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Fully Coupled**.

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

RESULTS

Liquid (bf)

Update the default plot for the liquid velocity by adding arrow surface.

In the **Model Builder** window, under **Results** click **Liquid (bf)**.

Arrow Surface 1

1 In the **Liquid (bf)** toolbar, click **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)> Bubbly Flow, Laminar Flow>Velocity and pressure>u,v - Velocity field, liquid phase**.

3 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

4 In the **Liquid (bf)** toolbar, click **Plot**.

Surface plot for the liquid phase velocity should look like Figure 2.

Gas Phase (bf)

Next, update surface plot of the gas phase fraction by adding velocity streamlines.

In the **Model Builder** window, under **Results** click **Gas Phase (bf)**.

Streamline 1

1 In the **Gas Phase (bf)** toolbar, click **Streamline**.

2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Bubbly Flow, Laminar Flow>Velocity and pressure>u,v - Velocity field, liquid phase**.

3 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.

4 In the **Separating distance** text field, type `0.02`.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

6 From the **Arrow length** list, choose **Logarithmic**.

7 From the **Color** list, choose **White**.

Surface plot of the gas phase fraction should look like Figure 3.

Concentration, Cu (tcd)

The copper concentration at time t = 60 s should look like Figure 4.

Copper concentration along cathode surface

Next, plot the copper concentration line plot along the cathode surface.

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

2 In the **Settings** window for **1D Plot Group**, type `Copper concentration along cathode surface` in the **Label** text field.

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

Line Graph 1

1 In the **Copper concentration along cathode surface** toolbar, click **Line Graph**.

2 Select Boundary 1 only.

3 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)> Tertiary Current Distribution, Nernst-Planck>Species cCu>cCu - Concentration - mol/m³**.

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

5 In the **Expression** text field, type `y`.

6 In the **Copper concentration along cathode surface** toolbar, click **Plot**.

7 Select the **Description** check box. In the associated text field, type `Distance from the bottom of the cathode surface`.

8 In the **Copper concentration along cathode surface** toolbar, click **Plot**.

Line plot of the copper concentration along the cathode surface at time t = 60 s should look like Figure 5.

Now, to plot the change in copper concentration with time at three different locations of the cathode surface, follow the below instructions.

Cut Point 2D 1

1 In the **Results** toolbar, click **Cut Point 2D**.

2 In the **Settings** window for **Cut Point 2D**, locate the **Point Data** section.

3 In the **x** text field, type `0 0 0`.

4 In the **y** text field, type `0.05 0.15 0.16`.

Copper Concentration (Point Graph)

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

2 In the **Settings** window for **1D Plot Group**, type `Copper Concentration (Point Graph)` in the **Label** text field.

Point Graph 1

1 In the **Copper Concentration (Point Graph)** toolbar, click **Point Graph**.

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

3 From the **Dataset** list, choose **Cut Point 2D 1**.

4 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> Species cCu>cCu - Concentration - mol/m³**.

5 In the **Copper Concentration (Point Graph)** toolbar, click **Plot**.

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

Point graph of the copper concentration should look like Figure 6.

Now, to plot concentration variation within the boundary layer at a specific position on the cathode surface, follow the below instructions.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

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

3 In row **Point 1**, set **y** to `0.1`.

4 In row **Point 2**, set **y** to `0.1`.

5 In row **Point 2**, set **x** to `0.001`.

Copper Concentration (Boundary Layer)

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

2 In the **Settings** window for **1D Plot Group**, type `Copper Concentration (Boundary Layer)` in the **Label** text field.

Line Graph 1

1 In the **Copper Concentration (Boundary Layer)** toolbar, click **Line Graph**.

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

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Time selection** list, choose **Last**.

5 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> Species cCu>cCu - Concentration - mol/m³**.

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

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

8 Select the **Description** check box. In the associated text field, type `Distance from the cathode surface`.

9 In the **Copper Concentration (Boundary Layer)** toolbar, click **Plot**.

The copper concentration plot in boundary layer should look like Figure 7.

Copper Deposition Thickness

Finally, plot the copper deposition thickness along the cathode surface at time t = 60 s.

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

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

3 Locate the **Data** section. From the **Time selection** list, choose **Last**.

Line Graph 1

1 In the **Copper Deposition Thickness** toolbar, click **Line Graph**.

2 Select Boundary 1 only.

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

4 Click to select the **Activate Selection** toggle button.

5 Select Boundary 1 only.

6 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> Dissolving-depositing species>tcd.sbtot - Total electrode thickness change - m**.

7 Locate the **y-Axis Data** section. From the **Unit** list, choose **µm**.

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

9 In the **Expression** text field, type `y`.

10 Select the **Description** check box. In the associated text field, type `Distance from the bottom of the cathode surface`.

11 In the **Copper Deposition Thickness** toolbar, click  **Plot**.

The copper deposition thickness plot should look like Figure 8.