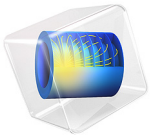


Pulse Reverse Plating

Introduction

This tutorial explores how pulse reverse plating can be used as an additive-free alternative to attenuate small protrusions during copper metal deposition. By adjusting the process parameters, including the length of the forward and reverse pulses (duty cycles), a bright mirror-like metal surface can be created. Pulse reverse plating may also be used for improved dimensional control of printed circuit board (PCB) plating (Ref. 1), for co-deposition of metal alloys.

The model assumes that a quasi-stationary current distribution establishes quickly during each pulse, so that an average of the forward and reverse deposition rates can be used in the time-dependent deforming geometry simulation.

Model Definition

Figure 1 shows the model geometry. The single domain consists of an electrolyte with a conductivity of 5 S/m. The electrode surface is located at $y = 0$ mm, with a small protrusion with a height of 40 mm, centered around $x = 0$. The local current density i_{loc} on electrode surface is modeled using Butler-Volmer kinetics.

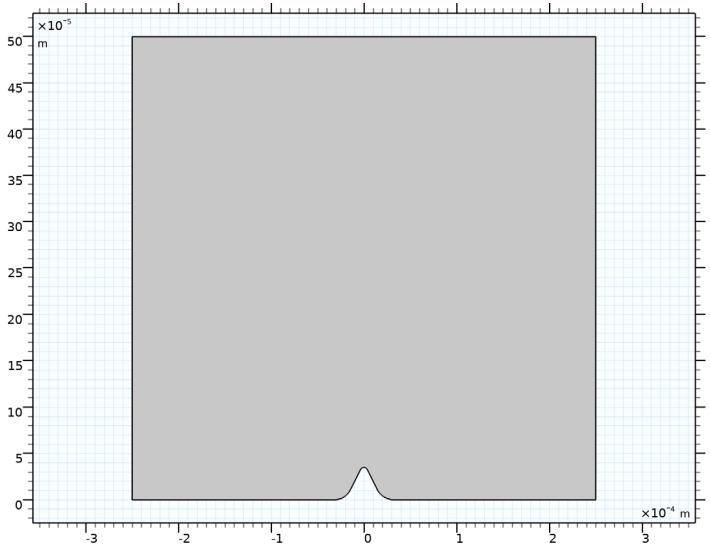


Figure 1: Model geometry.

On the electrode surface, copper is assumed to be deposited according to

$$Cu^{2+} + 2e^{-} \leftrightarrow Cu(s) \quad (1)$$

When modeling constant direct current (DC) plating, the average electrolyte current density of $i_{\text{avg, fwd}} = 5\ \text{A/dm}^2$ is applied on the top boundary, and the resulting growth velocity along the electrode surface is used as a boundary condition for the deformed geometry (ALE) time-dependent simulation.

For the pulse reverse simulations, the average current density for the reverse pulse on the top boundary is set to $i_{\text{avg, rev}} = -50\ \text{A/dm}^2$. Denoting the forward duty cycle (the relative time spent in forward mode) as t_{fwd} (dimensionless), the forward pulse average current density can be calculated as

$$i_{\text{avg, fwd}} = \frac{(i_{\text{avg}} - (1 - t_{\text{fwd}})i_{\text{avg, rev}})}{t_{\text{fwd}}} \quad (2)$$

The simulated plating time is 1 h, whereas the forward-to-reverse pulse switching is assumed to occur on a time scale significantly shorter (a few seconds), since concentration gradients due to the mass-transport limitations at the higher current densities during the reverse pulse must not be allowed to form.

The current distributions for the pulse reverse plating are assumed to be quasi-stationary within each pulse period, and the current distributions during the forward and the reverse pulse are solved simultaneously on the same time-dependent geometry, using different potential dependent variables. The local growth velocity on the electrode surface is then based on the time-averaged sum of the local current densities during the forward and reverse pulses:

$$v_n = \frac{M}{2F\rho}(i_{\text{loc, fwd}} - (1 - t_{\text{fwd}})i_{\text{loc, rev}}) \quad (3)$$

where ρ and M are the density and molar mass or copper, respectively, and $i_{\text{loc, fwd}}$ and $i_{\text{loc, rev}}$ are the local current density on the electrode surface during the forward and reverse pulses.

Solving the quasi-stationary current distributions separately for the forward and reverse pulses, using constant average current densities for each pulse period, saves computational time. The reason is that the time-dependent solver then does not need to resolve the explicit switching of the current density.

In order to mitigate potential issues with inverted mesh elements, the upper boundary is moved using a velocity proportional to the average current density according to

$$v_{\mathrm{bnd}} = \frac{M}{2F\rho} i_{\mathrm{avg}} \tag{4}$$

Results and Discussion

Figure 2 shows the electrode profile evolution during pure DC plating. The initial protrusion grows in size and will result in a non-even surface.

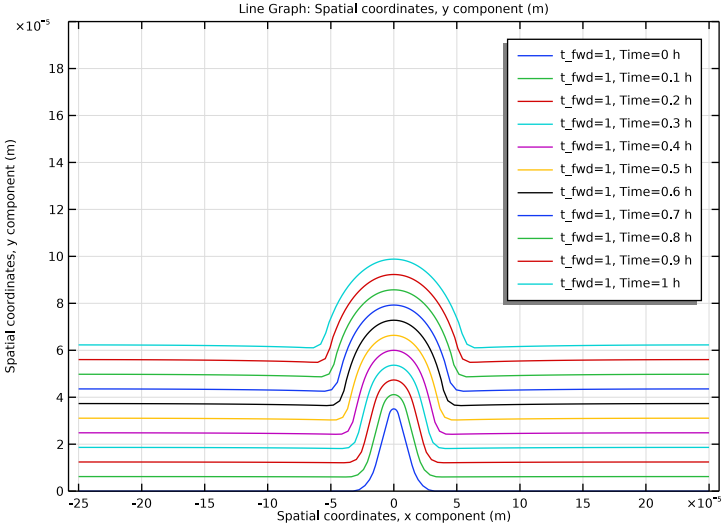


Figure 2: Profile evolution during DC plating.

Figure 3 shows the profile evolution for $t_{\mathrm{fwd}} = 0.85$. The initial protrusion is now attenuated, approaching a flat surface as the plating proceeds.

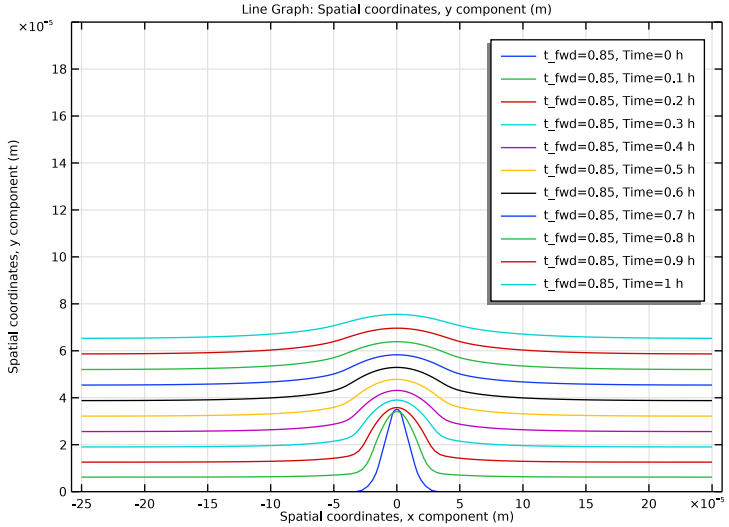


Figure 3: Profile evolution for $t_{\mathrm{fwd}} = 0.85$.

Finally, Figure 4 shows a comparison of the final profiles at t=1 h.

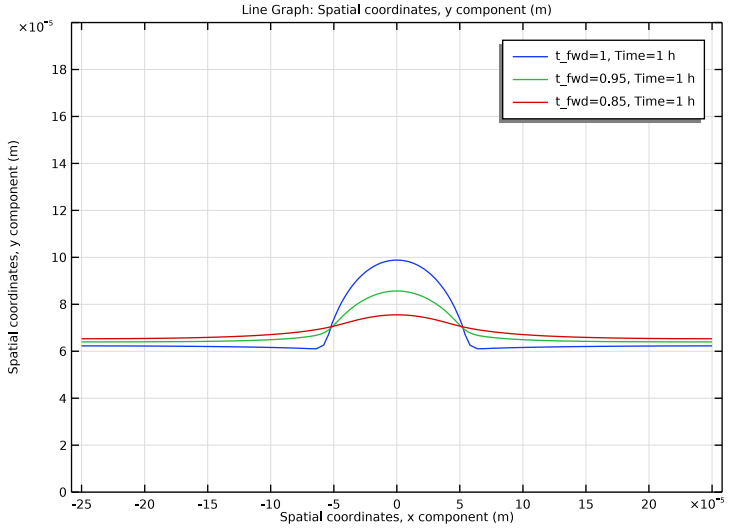


Figure 4: Comparison of final electrode surface profiles for different values of t_{fwd}.

Reference

1. P. Leisner, P. Møller, M. Fredenberg, and I. Belov, "Recent progress in pulse reversal plating of copper for electronics applications," *Transactions of the IMF*, vol. 85, no. 1, pp. 40–45, 2007.

Application Library path: `Electrodeposition_Module/Tutorials/pulse_reverse_plating`

Modeling Instructions

This tutorial consists of two parts. In the first part you will set up a direct current (DC) plating model to simulate how a small protrusion grows during the plating process.

In the second part you will add a current distribution model also for a reverse plating pulse, and examine how the protrusion is attenuated depending on the length of the reverse pulse.

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>Electrodeposition, Deformed Geometry>Electrodeposition, Secondary**.
3. Click **Add**.
4. Click **Study**.
5. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Secondary Current Distribution>Time Dependent with Initialization**.
6. Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

Load the model parameters from a text file.

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 `pulse_reverse_plating_parameters.txt`.

GEOMETRY 1

Polygon 1 (pol1)

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

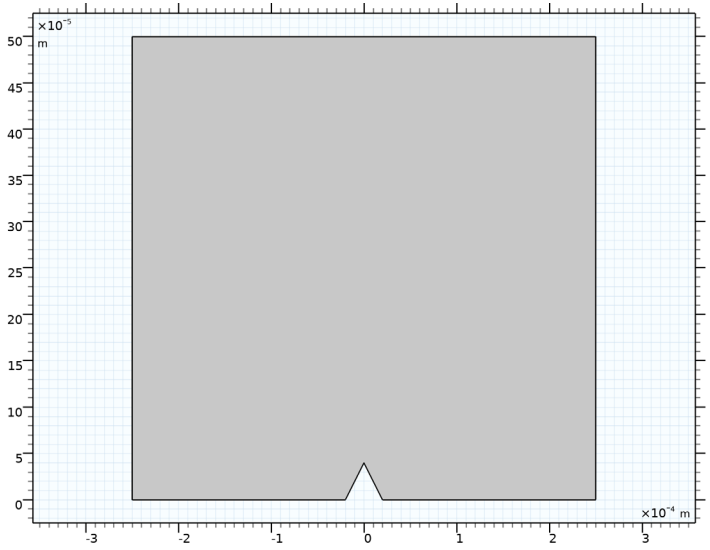
Load the coordinates of corners of the geometry from a text file.

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 `pulse_reverse_plating_coordinates.txt`.

5 Click **Build Selected**.



Fillet 1 (fil1)

Round the corners by adding fillets.

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

2 On the object **pol1**, select Point 4 only.

3 In the **Settings** window for **Fillet**, locate the **Radius** section.

4 In the **Radius** text field, type `H_prot/10`.

5 Click **Build Selected**.

Fillet 2 (fil2)

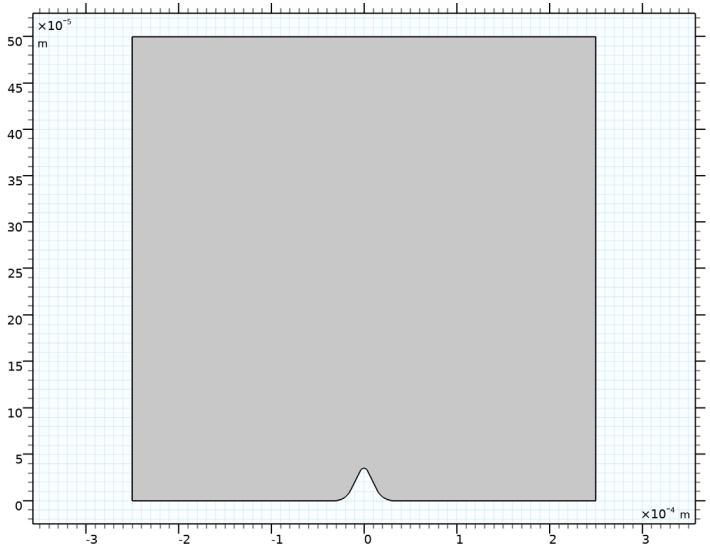
1 In the **Geometry** toolbar, click **Fillet**.

2 On the object **fil1**, select Points 3 and 6 only.

3 In the **Settings** window for **Fillet**, locate the **Radius** section.

4 In the **Radius** text field, type `W_prot/2`.

5 Click **Build Selected**.



SECONDARY CURRENT DISTRIBUTION (CD)

Now start setting up the DC plating current distribution model.

Electrolyte 1

1 In the **Model Builder** window, under **Component 1 (comp1)>** **Secondary 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 Current 1

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

2 Select Boundary 3 only.

3 In the **Settings** window for **Electrolyte Current**, locate the **Electrolyte Current** section.

4 From the list, choose **Average current density**.

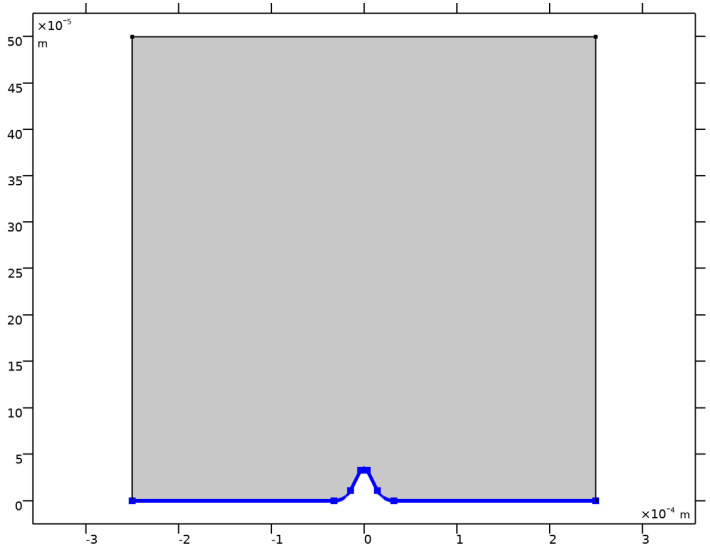
5 In the $i_{l,average}$ text field, type `i_avg`.

Electrode Surface 1

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

Use a box selection to select all the (lower) boundaries pertaining to the electrode surface, including the protrusion.

2 Select Boundaries 2, 4–6, and 8–10 only.



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

4 Click **Create Selection**.

By creating a selection in this way you can conveniently select the same set of boundaries again later on.

5 In the **Create Selection** dialog box, type `Electrode Surface` in the **Selection name** text field.

6 Click **OK**.

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

Use a **Dissolving-Depositing** Species to define the growth velocity of the electrode surface.

8 Click + **Add**.

9 In the table, enter the following settings:

Species	Density (kg/m^3)	Molar mass (kg/mol)
Cu	rho	M

10 Clear the **Solve for surface concentration variables** check box.

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Electrode Surface 1** node, then click **Electrode Reaction 1**.

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

3 In the n text field, type 2.

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

Species	Stoichiometric coefficient (1)
Cu	1

5 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Butler-Volmer**.

6 In the i_0 text field, type i0.

7 In the α_a text field, type alpha_a.

8 In the α_c text field, type alpha_c.

MULTIPHYSICS

Nondeforming Boundary 1 (ndb1)

Modify the default selection of the **Nondeforming Boundary** node to only include the vertical boundaries.

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Nondeforming Boundary 1 (ndb1)**.

2 Select Boundaries 1 and 7 only.

3 In the **Settings** window for **Nondeforming Boundary**, locate the **Nondeforming Boundary** section.

4 From the **Boundary condition** list, choose **Zero normal displacement**.

DEFINITIONS

We will now set up the boundary velocity of the upper boundary to a user-defined expression. First, load some variable expressions from a text file.

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **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 `pulse_reverse_plating_variables.txt`.

The `vn_avg` variable is marked in orange indicating a missing definition. This is expected. We will properly define and make use of this variable in the second part of the tutorial.

The `vn_bnd` variable will next be used now to set up the upper boundary velocity.

DEFORMED GEOMETRY (DG)

In the **Model Builder** window, under **Component 1 (comp1)** click **Deformed Geometry (dg)**.

Prescribed Normal Mesh Velocity 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Prescribed Normal Mesh Velocity**.

2 Select Boundary 3 only.

3 In the **Settings** window for **Prescribed Normal Mesh Velocity**, locate the **Normal Mesh Velocity** section.

4 In the v_n text field, type `-vn_bnd`.

MESH 1

Modify the mesh as follows to get more mesh elements along 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 **Mesh Settings** section.

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

Size 1

1 In the **Model Builder** window, right-click **Free Triangular 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 **Boundary**.

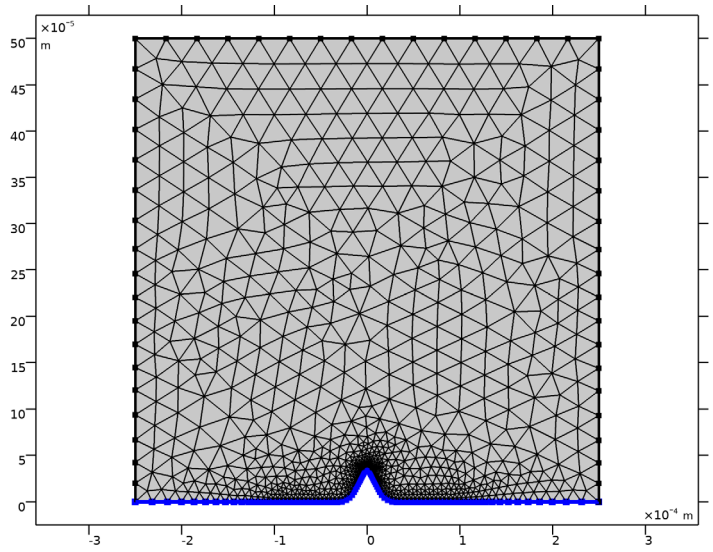
4 From the **Selection** list, choose **Electrode Surface**.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section. Select the **Maximum element growth rate** check box.

7 In the associated text field, type `1.1`.

8 Click **Build All**.



STUDY 1

The DC problem is now ready for solving. Change the simulation time to 1 hour.

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 2: Time Dependent**.

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

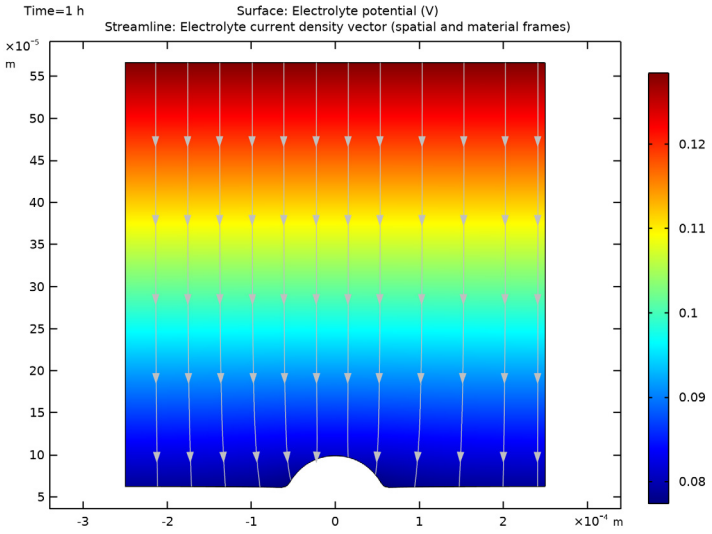
3 From the **Time unit** list, choose **h**.

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

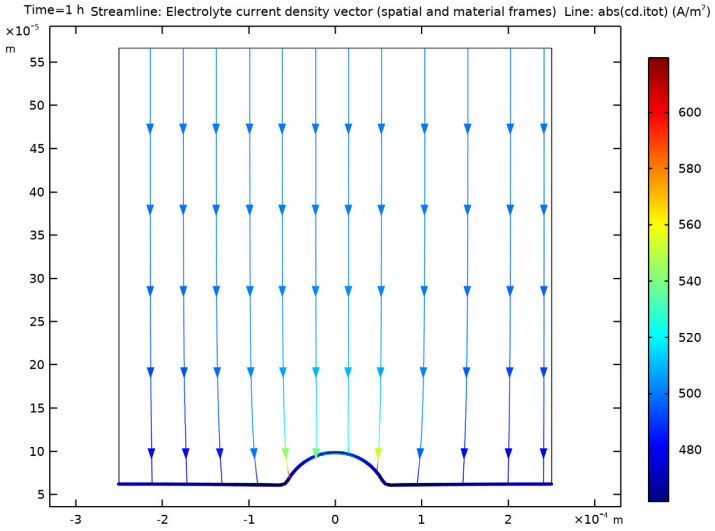
RESULTS

Electrolyte Potential (cd)

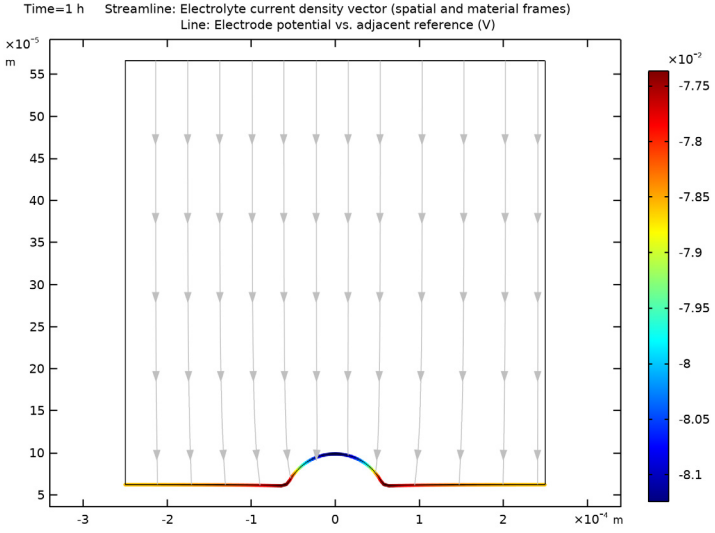
Explore the plots that were created by default.



Electrolyte Current Density (cd)



Electrode Potential vs. Adjacent Reference (cd)



SECONDARY CURRENT DISTRIBUTION - FORWARD (PLATING)

You have now completed the first DC part of this tutorial. We will now modify the DC current distribution model to represent the current distribution during the forward pulse.

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

2 In the **Settings** window for **Secondary Current Distribution**, type `Secondary Current Distribution - Forward (Plating)` in the **Label** text field.

Electrolyte Current 1

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

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

3 In the $i_{l,average}$ text field, type `i_fwd`.

COMPONENT 1 (COMP1)

Now add a second current distribution interface to represent the current distribution during the reverse pulse.

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 **Electrochemistry>Primary and Secondary Current Distribution>Secondary Current Distribution (cd)**.

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

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

SECONDARY CURRENT DISTRIBUTION - REVERSE (DISSOLUTION)

In the **Settings** window for **Secondary Current Distribution**, type `Secondary Current Distribution - Reverse (Dissolution)` in the **Label** text field.

Electrolyte 1

Set up the physics for the reverse pulse in a similar way as for the forward pulse.

1 In the **Model Builder** window, under **Component 1 (comp1)>Secondary Current Distribution - Reverse (Dissolution) (cd2)** 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 Current 1

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

2 Select Boundary 3 only.

3 In the **Settings** window for **Electrolyte Current**, locate the **Electrolyte Current** section.

4 From the list, choose **Average current density**.

5 In the $i_{l,average}$ text field, type `i_rev`.

Electrode Surface 1

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 **Electrode Surface**.

4 Locate 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	M

6 Clear the **Solve for surface concentration variables** check box.

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Electrode Surface 1** node, then click **Electrode Reaction 1**.

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

3 In the n text field, type 2.

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

Species	Stoichiometric coefficient (1)
Cu	1

5 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Butler-Volmer**.

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

7 In the α_a text field, type `alpha_a`.

8 In the α_c text field, type `alpha_c`.

DEFINITIONS

Variables 1

The `vn_avg` variable should now be marked in black.

MULTIPHYSICS

Deforming Electrode Surface 1 (des1)

Disable the **Deforming Electrode Surface** node and set up the boundary velocity for the electrode surface manually using the `vn_avg` variable.

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** right-click **Deforming Electrode Surface 1 (des1)** and choose **Disable**.

DEFORMED GEOMETRY (DG)

In the **Model Builder** window, under **Component 1 (comp1)** click **Deformed Geometry (dg)**.

Prescribed Normal Mesh Velocity 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Prescribed Normal Mesh Velocity**.

2 In the **Settings** window for **Prescribed Normal Mesh Velocity**, locate the **Boundary Selection** section.

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

4 Locate the **Normal Mesh Velocity** section. In the v_n text field, type `-vn_avg`.

5 Click to expand the **Moving Boundary Smoothing** section. Select the **Enable moving boundary smoothing** check box.

STUDY 1

Solver Configurations

The reverse pulse plating model is now ready for solving. Use a Parametric Sweep to simulate different lengths of the forward plating duty cycle.

Parametric Sweep

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

2 Right-click **Study 1** and choose **Parametric Sweep**.

3 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
t_fwd (Forward current duty cycle)	`1 0.95 0.85`	

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

RESULTS

Create a line plot to compare the shapes of the electrode surface at different times and values for the duty cycle values as follows:

Electrode Shape Comparison

1. In the **Home** toolbar, click  **Add Plot Group** and choose **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Electrode Shape Comparison` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.
4. From the **Time selection** list, choose **Last**.

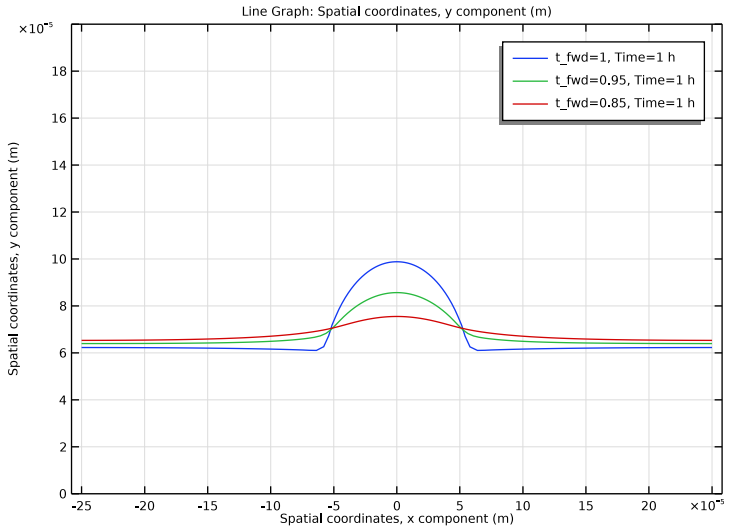
Line Graph 1

1. Right-click **Electrode Shape Comparison** and choose **Line Graph**.
2. In the **Settings** window for **Line Graph**, locate the **Selection** section.
3. From the **Selection** list, choose **Electrode Surface**.
4. Locate the **y-Axis Data** section. In the **Expression** text field, type `y`.
5. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
6. In the **Expression** text field, type `x`.
7. Click to expand the **Legends** section. Select the **Show legends** check box.

Electrode Shape Comparison

1. In the **Model Builder** window, click **Electrode Shape Comparison**.
2. In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
3. Locate the **Axis** section. Select the **Manual axis limits** check box.
4. In the **y minimum** text field, type `0`.
5. In the **y maximum** text field, type `2e-4`.

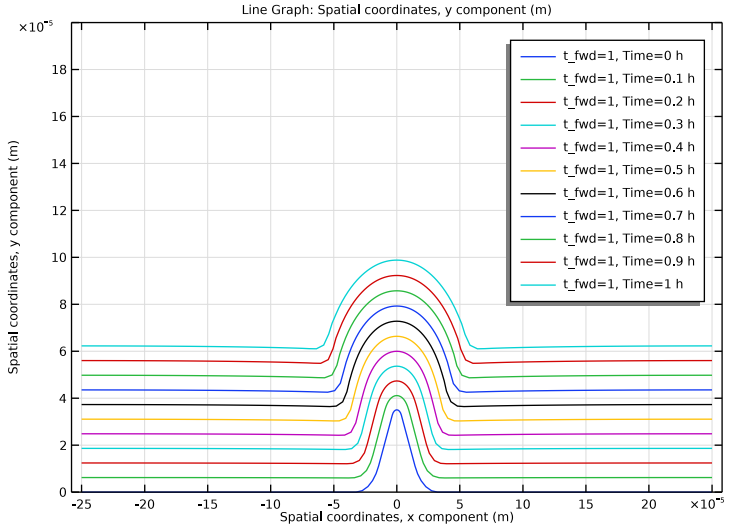
6 In the **Electrode Shape Comparison** toolbar, click **Plot**.



7 Locate the **Data** section. From the **Parameter selection (t_fwd)** list, choose **First**.

8 From the **Time selection** list, choose **All**.

9 In the **Electrode Shape Comparison** toolbar, click **Plot**.



10 From the **Parameter selection (t_fwd)** list, choose **Last**.

11 In the **Electrode Shape Comparison** toolbar, click **Plot**.