

Primary Current Distribution in a Lead—Acid Battery Grid Electrode

This example demonstrates the use of the Primary Current Distribution interface for modeling current distributions in electrochemical cells.

In primary current distribution, the potential losses due to electrode kinetics and mass transport are assumed to be negligible, and ohmic losses are govern the current distribution in the cell. Here you investigate primary current distribution in a positive lead-acid battery grid electrode during a high load (100 A) discharge.

In a traditional lead-acid electrode, the porous electrode is supported by a metal grid that also provides electronic conduction throughout the electrode. Optimizing the design of the grid leads to increased performance and lifetime as well as reduced weight (Ref. 1).

Model Definition

The half-cell geometry consists of a grid and a lug of the same metal material, a matrix of porous electrodes residing within the grid, and an electrolyte domain. The geometry is shown in Figure 1.

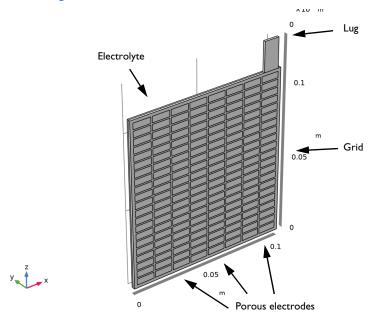


Figure 1: Modeled geometry.

The Primary Current Distribution interface is used to model the current distribution in the half cell. The potential in the electrolyte is set to zero at the external boundary that is parallel to the grid. A discharge current of 100 A is applied to the end of the lug. Isolation is used for all other boundaries.

The equilibrium potential for the positive electrode reaction versus a reversible hydrogen electrode (RHE) is used to relate the electrode to the electrolyte phase potential:

$$\phi_s + \phi_l = 1.7 \text{ V}$$

The above condition is applied as a constraint in the porous electrode domains.

The problem is solved using a Stationary study.

Results and Discussion

Figure 2 shows the electrolyte potential in the electrolyte and the porous electrode domains. The potential drop is highest, roughly 0.2 V, in the area close to the lug.

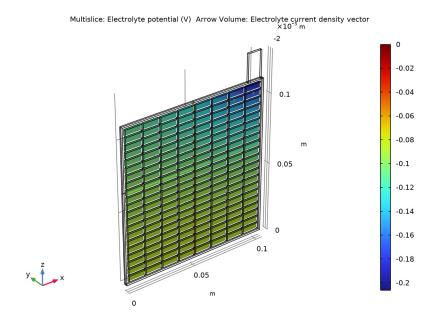


Figure 2: Electrolyte potential in the electrolyte and porous electrodes.

Figure 3 shows the potential in the grid and the lug. The potential difference between the corner of the grid closest to the lug and the far end corner is about 0.15 V.

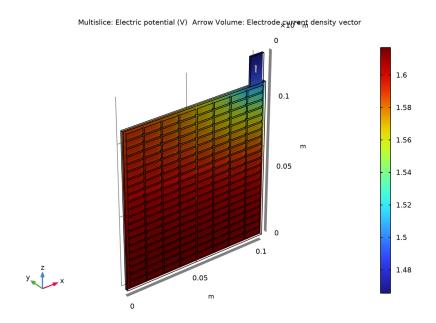


Figure 3: Electric potential in the grid and the lug.

Finally, the current density distribution in the electrolyte symmetry plane is plotted in Figure 4. The currents are about twice as high in the active region closest to the lug compared to the opposite corner of the cell.

In this case an improvement of the battery performance would be possible by making the frame of the grid thicker toward the lug corner, thereby achieving a more uniform current distribution.

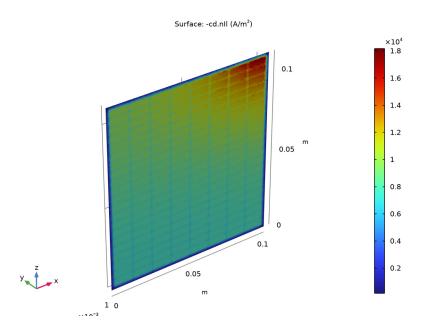


Figure 4: Electrolyte current density at the half-cell boundary.

Reference

1. K. Yamada, K.-I. Maeda, K. Sasaki, and T. Hirasawa "Computer-aided optimization of grid design for high-power lead-acid batteries," J. Power Sources, selected papers from the Ninth European Lead Battery Conference, vol. 144, no. 2, pp. 352-357, 2005.

Application Library path: Battery_Design_Module/Batteries,_General/ primary_cd_grid

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 📋 3D.
- 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 M Done.

GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 primary_cd_grid_parameters.txt.

GEOMETRY I

Start building the geometry using a work plane representing the electrode grid plane.

Work Plane I (wbl)

- I In the Geometry toolbar, click 🔁 Work Plane.
- ${\bf 2}\;$ In the Settings window for Work Plane, locate the Plane Definition section.
- 3 From the Plane list, choose xz-plane.
- 4 Click A Go to Plane Geometry.

Work Plane I (wpl)>Rectangle I (rl)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type W.
- 4 In the **Height** text field, type H.
- 5 Click Pauld Selected.

Work Plane I (wp I)>Plane Geometry

Draw one porous electrode section, then use it to create an array of porous electrodes.

Work Plane I (wp I)>Rectangle 2 (r2)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type W_porous.
- 4 In the **Height** text field, type H_porous.
- **5** Locate the **Position** section. In the **xw** text field, type **s_frame**.
- 6 In the yw text field, type s_frame.

Work Plane I (wpl)>Array I (arrl)

- I In the Work Plane toolbar, click Transforms and choose Array.
- **2** Select the object **r2** only.
- 3 In the Settings window for Array, locate the Size section.
- 4 In the xw size text field, type N_x.
- 5 In the yw size text field, type N_z.
- 6 Locate the Displacement section. In the xw text field, type W_porous+s_grid.
- 7 In the **yw** text field, type H_porous+s_grid.
- 8 Click Pauld Selected.

Work Plane I (wp I)>Plane Geometry

Draw the lug as an additional rectangle. It has the same thickness as the electrode.

Work Plane I (wp I)>Rectangle 3 (r3)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- 3 In the Width text field, type W_lug.
- 4 In the **Height** text field, type H_lug.
- 5 Locate the **Position** section. In the xw text field, type W-s frame-W lug.
- 6 In the yw text field, type H.
- 7 Click | Build Selected.
- 8 Click the Zoom Extents button in the Graphics toolbar.

Extrude I (extI)

- I In the Model Builder window, under Component I (compl)>Geometry I right-click Work Plane I (wpl) and choose Extrude.
- 2 In the Settings window for Extrude, locate the Distances section.

3 In the table, enter the following settings:

Distances (m) d_electrode

4 Click Pauld Selected.

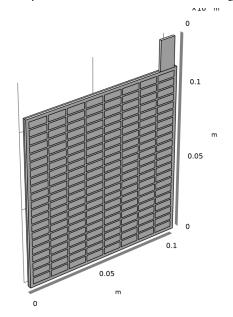
Electrolyte

Finalize the geometry by drawing the electrolyte domain.

- I In the Geometry toolbar, click Block.
- 2 In the Settings window for Block, locate the Size and Shape section.
- 3 In the Width text field, type W.
- 4 In the **Depth** text field, type d_electrolyte.
- 5 In the **Height** text field, type H.
- 6 Locate the Selections of Resulting Entities section. Select the Resulting objects selection check box.
- 7 In the Label text field, type Electrolyte.
- 8 Click Build All Objects.

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

The completed geometry should look as shown in the following figure:





DEFINITIONS

Create a selection for the union of the grid and lug domains to facilitate setting up the model.

Grid + Lug

- I In the **Definitions** toolbar, click **\(\big|_{\text{a}} \) Explicit**.
- 2 Select Domains 1 and 171 only.
- 3 In the Settings window for Explicit, type Grid + Lug in the Label text field.

Use a Complement selection to select the porous electrodes.

Porous Electrodes

- I In the **Definitions** toolbar, click **\(\) Complement**.
- 2 In the Settings window for Complement, locate the Input Entities section.
- 3 Under Selections to invert, click + Add.
- 4 In the Add dialog box, in the Selections to invert list, choose Grid + Lug and Electrolyte.
- 5 Click OK.

6 In the Settings window for Complement, type Porous Electrodes in the Label text field.

PRIMARY CURRENT DISTRIBUTION (CD)

Current Conductor I

- I In the Model Builder window, under Component I (compl) right-click Primary Current Distribution (cd) and choose Current Conductor.
- 2 In the Settings window for Current Conductor, locate the Domain Selection section.
- 3 From the Selection list, choose Grid + Lug.
- 4 Locate the **Electrode** section. From the σ_s list, choose **User defined**. In the associated text field, type sigma_metal.

Porous Electrode I

- I In the Physics toolbar, click **Domains** and choose **Porous Electrode**.
- 2 In the Settings window for Porous Electrode, locate the Domain Selection section.
- 3 From the Selection list, choose Porous Electrodes.
- 4 Locate the Electrolyte Current Conduction section. From the σ_l list, choose User defined. In the associated text field, type sigma_electrolyte.
- 5 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**. In the associated text field, type sigma_porous.

Porous Electrode Reaction 1

- I In the Model Builder window, click Porous Electrode Reaction I.
- 2 In the Settings window for Porous Electrode Reaction, locate the Equilibrium Potential section.
- **3** In the E_{eq} text field, type 1.7.

Electrolyte I

- I In the Model Builder window, under Component I (compl)>
 Primary Current Distribution (cd) click Electrolyte I.
- 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.

Electrolyte Potential I

- I In the Physics toolbar, click **Boundaries** and choose **Electrolyte Potential**.
- 2 Select Boundary 9 only.

Electrode Current I

- I In the Physics toolbar, click **Boundaries** and choose **Electrode Current**.
- 2 Select Boundary 1000 only.
- 3 In the Settings window for Electrode Current, locate the Electrode Current section.
- 4 In the $I_{\rm s total}$ text field, type -100.

DEFINITIONS

The highest gradients in the model are to be expected at the edges between the porous electrode and the electrolyte. Create a selection of these edges to use later when setting up the mesh.

Adjacent I

- I In the **Definitions** toolbar, click **\bigcip_a Adjacent**.
- 2 In the Settings window for Adjacent, locate the Input Entities section.
- 3 Under Input selections, click + Add.
- 4 In the Add dialog box, select Porous Electrodes in the Input selections list.
- 5 Click OK.
- 6 In the Settings window for Adjacent, locate the Output Entities section.
- 7 From the Geometric entity level list, choose Adjacent edges.

Adjacent 2

- I In the **Definitions** toolbar, click **Adjacent**.
- 2 In the Settings window for Adjacent, locate the Input Entities section.
- 3 Under Input selections, click + Add.
- 4 In the Add dialog box, select Electrolyte in the Input selections list.
- 5 Click OK.
- 6 In the Settings window for Adjacent, locate the Output Entities section.
- 7 From the Geometric entity level list, choose Adjacent edges.

Intersection I

- I In the **Definitions** toolbar, click intersection.
- 2 In the Settings window for Intersection, locate the Geometric Entity Level section.
- 3 From the Level list, choose Edge.
- **4** Locate the **Input Entities** section. Under **Selections to intersect**, click + **Add**.
- 5 In the Add dialog box, in the Selections to intersect list, choose Adjacent 1 and Adjacent 2.

6 Click OK.

MESH I

Edge I

- I In the Mesh toolbar, click A More Generators and choose Edge.
- 2 In the Settings window for Edge, locate the Edge Selection section.
- **3** From the **Selection** list, choose **Intersection I**.

Size 1

- I Right-click **Edge** I and choose **Size**.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Element Size Parameters section.
- **5** Select the **Maximum element size** check box. In the associated text field, type **s_grid/2**.

Free Tetrahedral I

- I In the Mesh toolbar, click A Free Tetrahedral.
- 2 In the Model Builder window, right-click Mesh I and choose Build All.

STUDY I

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

RESULTS

The electrolyte potential (Figure 2) and electrode potential versus ground (Figure 3) are plotted by default.

Electrolyte Current Density at the Half-cell Boundary

To create Figure 4, do the following steps.

- I In the Home toolbar, click **Add Plot Group** and choose 3D Plot Group.
- 2 In the Settings window for 3D Plot Group, type Electrolyte Current Density at the Half-cell Boundary in the Label text field.
- 3 Locate the Plot Settings section. Clear the Plot dataset edges check box.

Surface 1

- I Right-click Electrolyte Current Density at the Half-cell Boundary and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- 3 In the Expression text field, type -cd.nIl.

Selection I

- I Right-click Surface I and choose Selection.
- **2** Select Boundary 9 only.
- 3 In the Electrolyte Current Density at the Half-cell Boundary toolbar, click Plot.