Model created in COMSOL Multiphysics 6.4

Discharge and Self-Discharge of a Lead–Acid Battery

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Introduction

Lead–acid batteries are widely used as starter batteries for traction applications, such as for cars and trucks. The reason for this wide usage of lead–acid batteries is their low cost in combination with their performance robustness for a broad range of operating conditions. However, one drawback of this battery type is that the inherent thermodynamics of the battery chemistry causes the battery to self-discharge over time.

This example simulates a lead–acid battery at high (1200 A) and low (3 A) discharge rates, and the long-term self-discharge behavior with no applied external current (0 A).

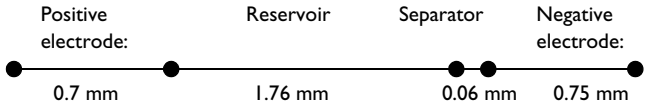

Figure 1: Modeled geometry. The model is in 1D in the x direction.

Model Definition

Figure 1 shows the 1D model geometry. There are four domains: the positive porous electrode, the reservoir, the separator, and the negative porous electrode.

The model uses the Lead–Acid Battery interface for solving for the following unknown variables:

- ϕ_s — the electronic potential
- ϕ_l — the ionic potential
- ε — the porosity (electrolyte volume fraction) of the porous electrodes
- c_l — the electrolyte concentration

ELECTROCHEMICAL REACTIONS

The main electrode reaction in the positive (PbO_2) electrode during discharge is

$$PbO_2(s) + HSO_4^-(aq) + 3H^+(aq) + 2e^- \rightarrow PbSO_4(s) + 2H_2O(l)$$

with an equilibrium potential that depends on the electrolyte concentration as shown in Figure 2.

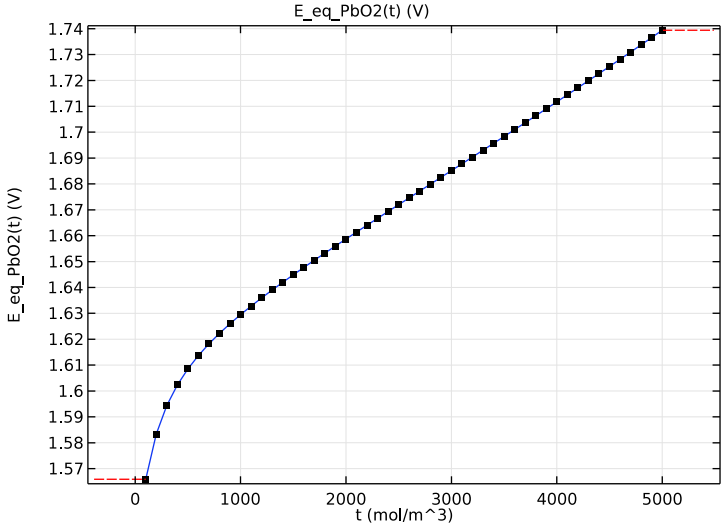

Figure 2: Equilibrium potential of the PbO_2 reaction as a function of electrolyte concentration in the positive electrode.

The combination of an aqueous solution and a high potential results in oxygen gas evolution at the positive electrode according to:

$$\mathrm{H_2O}(l) \rightarrow \frac{1}{2}\mathrm{O_2}(g) + 2\mathrm{H^+}(\mathrm{aq}) + 2e^- \qquad E_0 = 1.23\,\mathrm{V}$$

The main discharge reaction for the negative (Pb) electrode is:

$$\mathrm{Pb}(\mathrm{s}) + \mathrm{HSO_4^-}(\mathrm{aq}) \rightarrow \mathrm{PbSO_4}(s) + \mathrm{H^+}(\mathrm{aq}) + 2e^-$$

with an equilibrium potential that depends on the electrolyte concentration as shown in Figure 3.

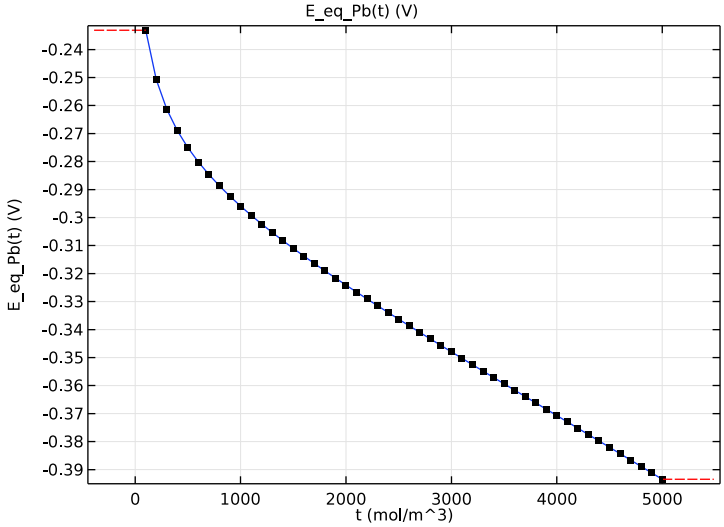

Figure 3: Equilibrium potential of the Pb reaction as a function of electrolyte concentration in the negative electrode.

This dependence of the equilibrium potential on the electrolyte concentration, for both discharge reactions, is present in the Materials Library for the Battery Design Module.

The low operating potential of the negative electrode results in hydrogen evolution according to:

$$2\mathrm{H}^{+}(\mathrm{aq}) + 2e^{-} \rightarrow \mathrm{H}_2(g) \qquad E_0 = 0\,\mathrm{V}$$

For the gas evolution reaction, Butler–Volmer type kinetic expressions are used. For the main discharge reactions the default discharge reactions of the Lead–Acid Battery interface are used.

ELECTROLYTE TRANSPORT PARAMETERS

The electrolyte diffusion coefficient and the electrolyte conductivity vary with the concentration according to Figure 4 and Figure 5, respectively. This data is also present in the Materials Library for the Battery Design Module.

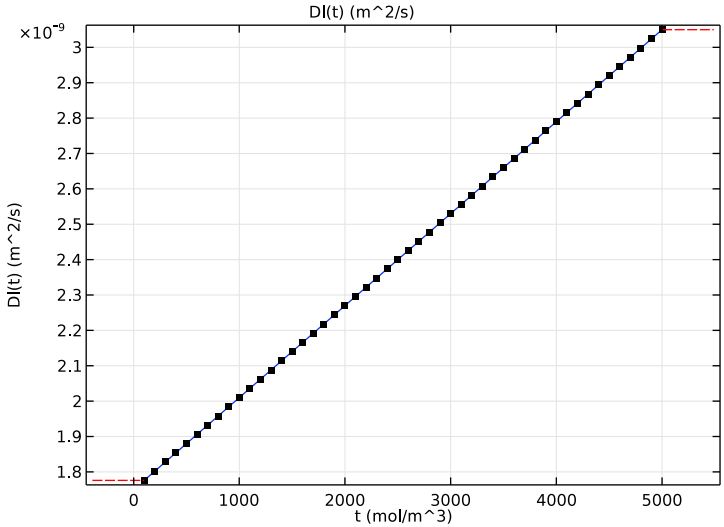

Figure 4: Electrolyte diffusion coefficient as a function of electrolyte concentration.

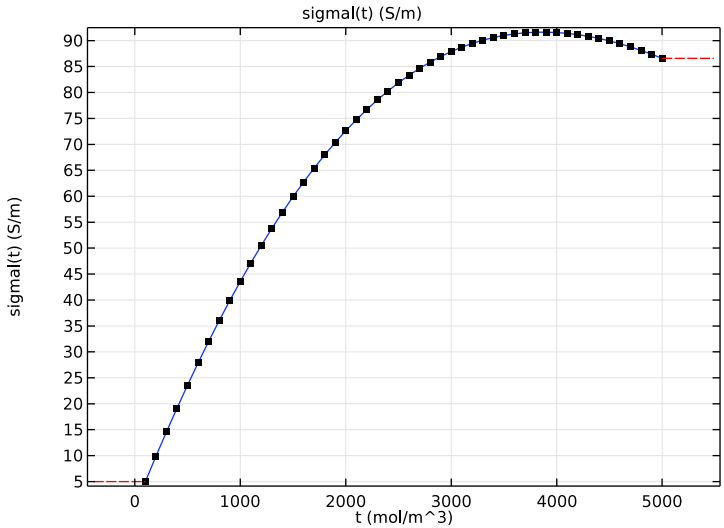

Figure 5: Electrolyte conductivity as a function of electrolyte concentration.

BOUNDARY AND INITIAL CONDITIONS

The outer boundary of the negative electrode is grounded and a discharge current is applied to the positive end terminal.

Three different discharge currents are simulated in three separate studies. The first study performs a C/20-discharge — a constant current in order to obtain a full discharge in 20 hours, followed by a one-hour relaxation period at zero external load. The second study simulates a high load 20C-discharge during 1 minute. In the third study the external load is set to zero and the simulation time is extended to one year to study the self-discharge behavior.

Results and Discussion

Figure 6 shows the polarization plot of the cell. At the shut-off of the current the cell voltage first rises swiftly due to the sudden absence of activation and resistive losses, but after this the potential continues to rise slightly during a relaxation period.

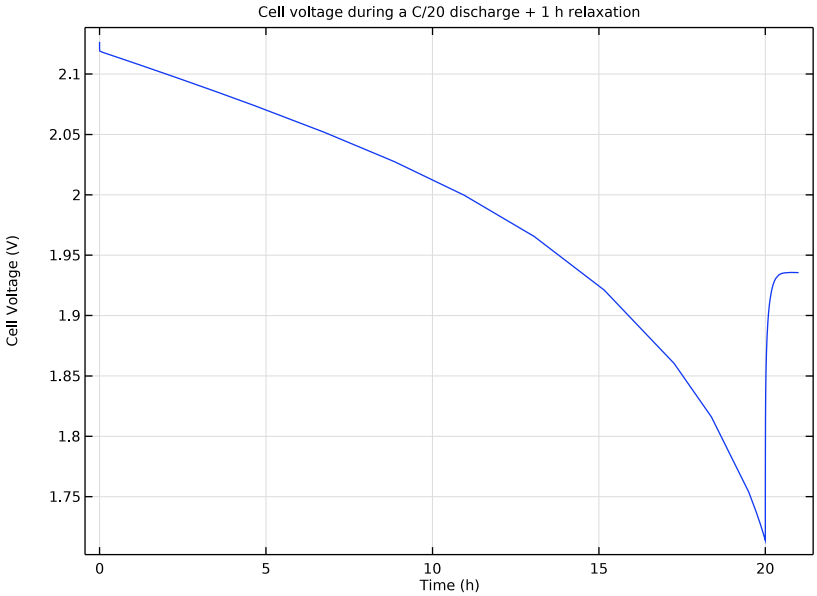

Figure 6: Cell voltage versus time for a C/20 discharge + 1-hour resting period.

Figure 7 depicts the reason for the slow rise in potential during the resting period. When the current is cut off at 20 h there is an electrolyte concentration gradient in the cell, but

as electrolyte diffuses into the electrodes during the resting period the cell potential rises slightly.

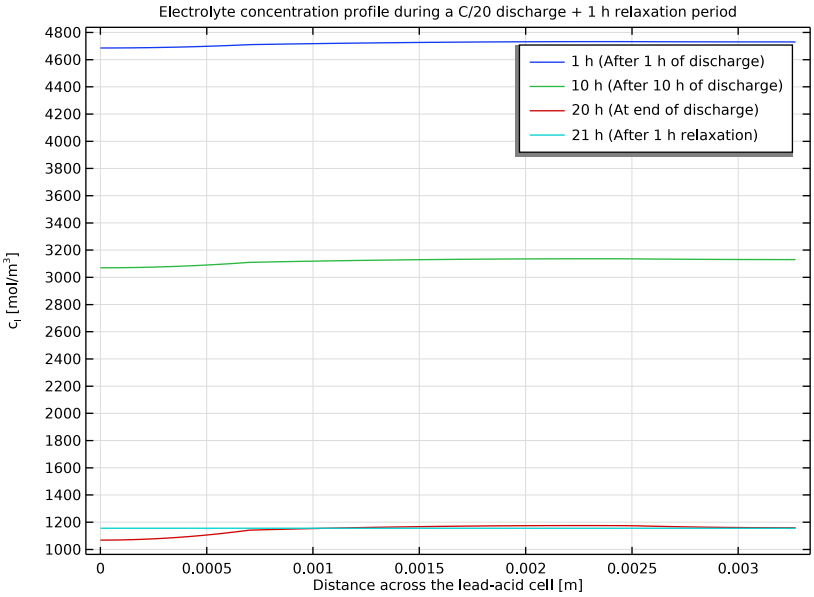

Figure 7: Electrolyte concentration profile at certain times during the C/20 discharge + 1-hour relaxation simulation.

Figure 8 shows the state-of-charge variation in the electrodes during the C/20 simulation. At this relatively low discharge current the electrodes are discharged quite uniformly.

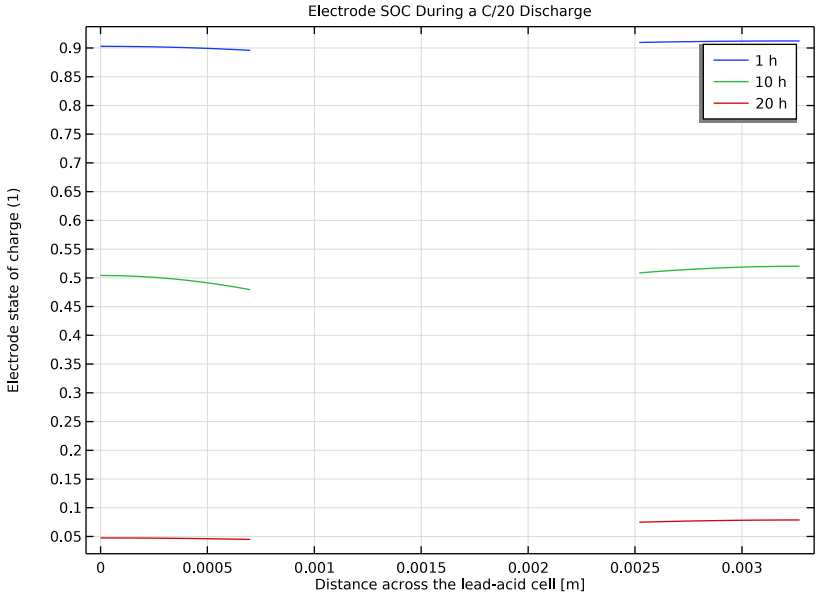

Figure 8: State-of-charge in the electrodes at 1, 10, and 20 h during the C/20 simulation.

When performing the 20C simulation the concentration (Figure 9) and state-of-charge gradients (Figure 10) are much higher. These very high currents causes the battery voltage

to drop significantly already after one minute due to electrolyte depletion in the positive electrode (even though two-thirds of the active electrode material is left in the electrodes).

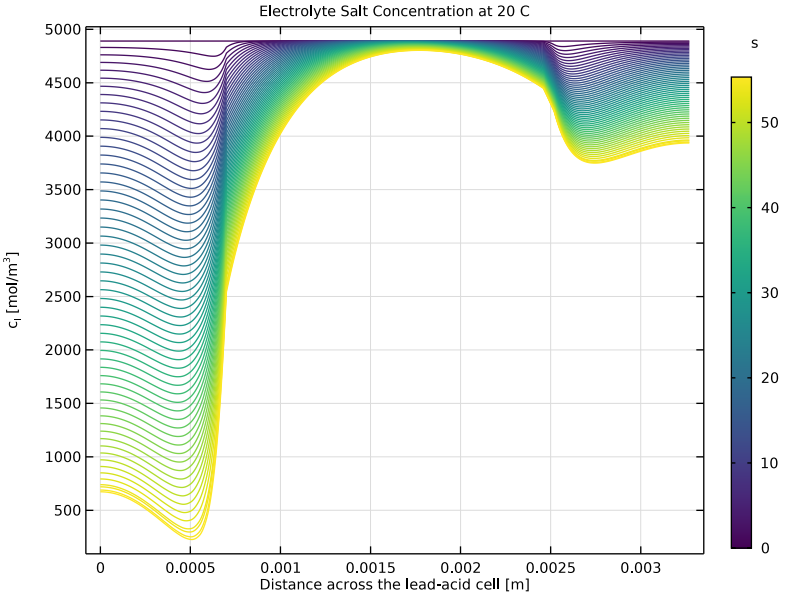

Figure 9: Electrolyte concentration profile (one profile curve per second) during a 20C discharge until cell voltage falls below 1.5 V.

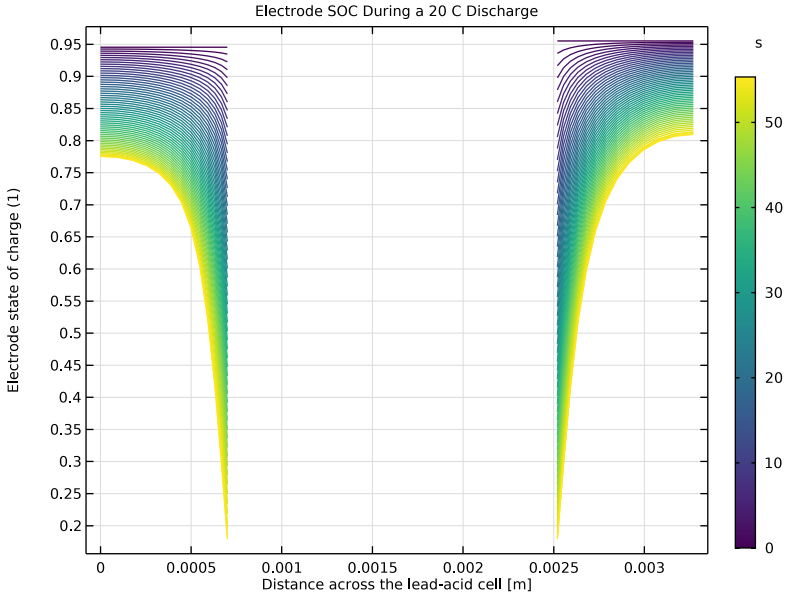

Figure 10: State-of-charge decrease during the 20C discharge simulation.

Figure 11 compares the discharge curves of the three simulations on a log t scale. The 20C cell voltage is much lower than the C/20 curve due to higher internal resistive and activation losses. The self-discharge curve indicates a moderate cell voltage drop after a year. Figure 12 shows that the state-of-charge of the positive electrode has decreased by over 25% during the same period.

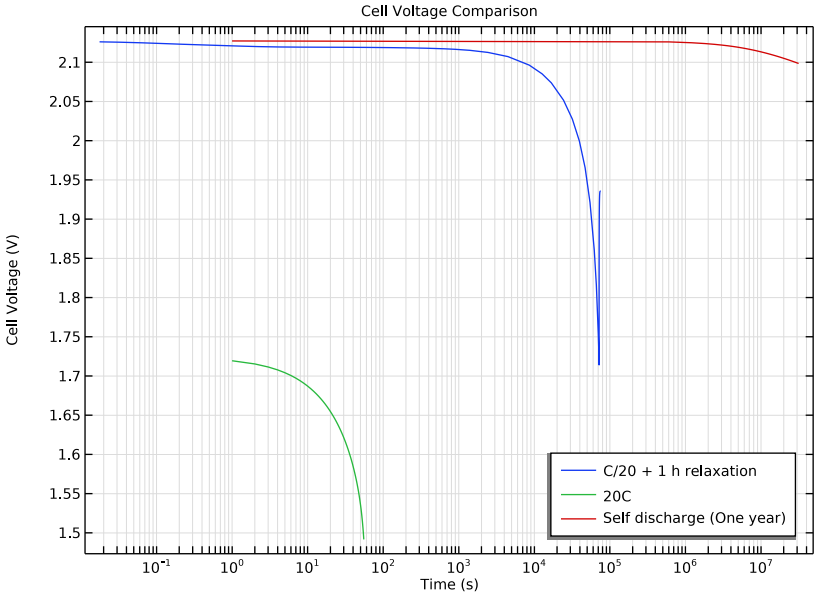

Figure 11: Discharge curves (cell voltage versus time) for the three simulations.

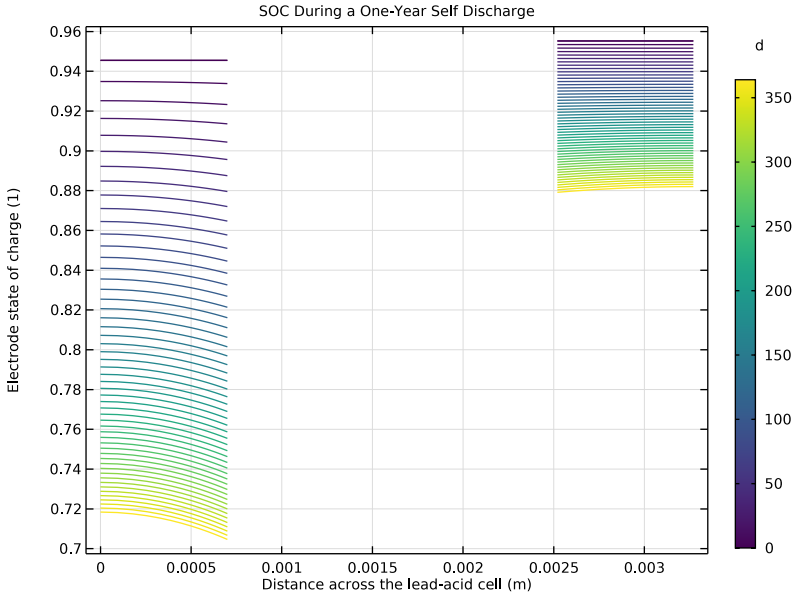

Figure 12: State-of-charge during the one-year self-discharge simulation.

Reference

1. M. Cugnet, S. Laruelle, S. Grugeon, B. Sahut, J. Sabatier, J.M. Tarascon, and A. Oustaloup, "A Mathematical Model for the Simulation of New and Aged Automotive Lead–Acid Batteries," *J. Electrochem. Soc.*, vol. 156, pp. A974–A985, 2009.

Application Library path: `Battery_Design_Module/Batteries,_General/pb_acid_battery_1d`

Modeling Instructions

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

NEW

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

MODEL WIZARD

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

2 In the **Select Physics** tree, select **Electrochemistry** > **Batteries** > **Lead-Acid Battery (leadbat)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Time Dependent with Initialization**.

6 Click **Done**.

GLOBAL DEFINITIONS

Load the parameter values to be used in the model from a 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 `pb_acid_battery_1d_parameters.txt`.

Step 1 (step1)

Use a step function to switch off the applied discharge current at 20 h.

1 In the **Home** toolbar, click **Functions** and choose **Global** > **Step**.

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

3 In the **Location** text field, type `20*3600`.

4 In the **From** text field, type `1`.

5 In the **To** text field, type `0`.

GEOMETRY 1

Interval 1 (i1)

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

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

3 From the **Specify** list, choose **Interval lengths**.

4 In the table, enter the following settings:

Lengths (m)
L_pos
L_res
L_sep
L_neg

5 Click **Build All Objects**.

GEOMETRY 1

In the **Model Builder** window, collapse the **Component 1 (comp1)** > **Geometry 1** node.

ADD MATERIAL

Next, add the materials data for the sulfuric acid electrolyte, the positive lead oxide electrode and the negative lead electrode.

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

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

3 In the tree, select **Battery** > **Electrolytes** > **Sulfuric Acid (Lead-Acid Battery)**.

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

5 In the tree, select **Battery** > **Electrodes** > **Pb (Negative, Lead-Acid Battery)**.

6 Click the **Add to Component** button in the window toolbar.

7 In the tree, select **Battery** > **Electrodes** > **PbO2 (Positive, Lead-Acid Battery)**.

8 Click the **Add to Component** button in the window toolbar.

9 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Pb (Negative, Lead-Acid Battery) (mat2)

Select Domain 4 only.

PbO2 (Positive, Lead-Acid Battery) (mat3)

1 In the **Model Builder** window, click **PbO2 (Positive, Lead-Acid Battery) (mat3)**.

2 Select Domain 1 only.

LEAD-ACID BATTERY (LEADBAT)

Positive Porous Electrode 1

1 In the **Physics** toolbar, click **Domains** and choose **Positive Porous Electrode**.

2 Select Domain 1 only.

3 In the **Settings** window for **Positive Porous Electrode**, locate the **Electrolyte Properties** section.

4 From the **Electrolyte material** list, choose **Sulfuric Acid (Lead-Acid Battery) (mat1)**.

5 In the ex text field, type `ex`.

6 Locate the **Electrode Properties** section. In the ε_0 text field, type `eps_pos_min`.

7 In the ε_{max} text field, type `eps_pos_max`.

8 In the exm text field, type `exm`.

9 Click the **Show More Options** button in the **Model Builder** toolbar.

10 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

11 Click **OK**.

12 In the **Settings** window for **Positive Porous Electrode**, click to expand the **Equilibrium Potential Handling (Primary Condition)** section.

13 From the **Equilibrium potential based on** list, choose **First reaction**.

Separator 1

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

2 Select Domain 3 only.

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

4 In the ε_{sep} text field, type `eps_sep`.

5 In the ex text field, type `ex_sep`.

Negative Porous Electrode 1

1 In the **Physics** toolbar, click **Domains** and choose **Negative Porous Electrode**.

2 Select Domain 4 only.

3 In the **Settings** window for **Negative Porous Electrode**, locate the **Electrolyte Properties** section.

4 From the **Electrolyte material** list, choose **Sulfuric Acid (Lead-Acid Battery) (mat1)**.

5 In the ex text field, type `ex`.

6 Locate the **Electrode Properties** section. In the ε_0 text field, type `eps_neg_min`.

7 In the ε_{max} text field, type `eps_neg_max`.

8 In the exm text field, type `exm`.

9 Click to expand the **Equilibrium Potential Handling (Primary Condition)** section. From the **Equilibrium potential based on** list, choose **First reaction**.

Porous Electrode Reaction 1

Now, set up the electrode reactions and the double layer capacitance for the electrodes. Start with the positive electrode discharge reaction.

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Lead-Acid Battery (leadbat)** > **Positive Porous Electrode 1** click **Porous Electrode Reaction 1**.

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

3 From the **Kinetics expression type** list, choose **Lead-acid battery discharge**.

4 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_pos`.

5 In the α_a text field, type `alpha_a_pos`.

6 In the α_c text field, type `alpha_c_pos`.

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

8 In the γ text field, type `gamma_pos`.

9 Locate the **Active Specific Surface Area** section. In the $a_{v,\mathrm{max}}$ text field, type `a_max_pos`.

10 In the ζ text field, type `morph_pos`.

Positive Porous Electrode 1

These steps set up the oxygen evolution reaction, occurring on the positive electrode:

1 In the **Model Builder** window, click **Positive Porous Electrode 1**.

Porous Electrode Reaction 2

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

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `1.23`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Butler–Volmer**.

5 In the i_0 text field, type `i0_O2*(cl/cl_ref)^2`.

6 In the α_a text field, type `alpha_O2`.

7 In the α_c text field, type `alpha_O2`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `a_max_pos*(epsilon-eps_pos_min)/(eps_pos_max-eps_pos_min)`.

9 Locate the **Stoichiometric Coefficients** section. In the ν_{H+} text field, type `-2`.

10 In the ν_{HSO4-} text field, type `0`.

11 In the ν_{H2O} text field, type `1`.

12 In the ν_{PbO2} text field, type `0`.

13 In the ν_{PbSO4} text field, type `0`.

14 Click to expand the **Heat of Reaction** section. From the list, choose **User defined**.

Positive Porous Electrode 1

In the **Model Builder** window, click **Positive Porous Electrode 1**.

Porous Matrix Double Layer Capacitance 1

1 In the **Physics** toolbar, click **Attributes** and choose **Porous Matrix Double Layer Capacitance**.

2 In the **Settings** window for **Porous Matrix Double Layer Capacitance**, locate the **Porous Matrix Double Layer Capacitance** section.

3 In the C_{dl} text field, type `C_dl_pos`.

4 In the $a_{v,dl}$ text field, type `a_max_pos`.

Porous Electrode Reaction 1

Set up the negative electrode discharge reaction in the following way:

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Lead-Acid Battery (leadbat)** > **Negative Porous Electrode 1** click **Porous Electrode Reaction 1**.

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

3 From the **Kinetics expression type** list, choose **Lead-acid battery discharge**.

4 In the $i_{0,ref}(T)$ text field, type `i0_ref_neg`.

5 In the α_a text field, type `alpha_a_neg`.

6 In the α_c text field, type `alpha_c_neg`.

7 In the $c_{l,ref}$ text field, type `cl_ref`.

8 In the γ text field, type `gamma_neg`.

9 Locate the **Active Specific Surface Area** section. In the $a_{v,max}$ text field, type `a_max_neg`.

10 In the ζ text field, type `morph_neg`.

Negative Porous Electrode 1

Set up the hydrogen evolution reaction on the negative electrode in the following way:

1 In the **Model Builder** window, click **Negative Porous Electrode 1**.

Porous Electrode Reaction 2

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

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. In the associated text field, type `0`.

4 Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Butler–Volmer**.

5 In the i_0 text field, type `i0_H2*cl/cl_ref`.

6 In the α_a text field, type `alpha_H2`.

7 In the α_c text field, type `alpha_H2`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `a_max_neg*(epsilon-eps_neg_min)/(eps_neg_max-eps_neg_min)`.

9 Locate the **Stoichiometric Coefficients** section. In the ν_{H+} text field, type `-2`.

10 In the ν_{HSO4-} text field, type `0`.

11 In the ν_{Pb} text field, type `0`.

12 In the ν_{PbSO4} text field, type `0`.

13 Click to expand the **Heat of Reaction** section. From the list, choose **User defined**.

Negative Porous Electrode 1

In the **Model Builder** window, click **Negative Porous Electrode 1**.

Porous Matrix Double Layer Capacitance 1

1 In the **Physics** toolbar, click **Attributes** and choose **Porous Matrix Double Layer Capacitance**.

2 In the **Settings** window for **Porous Matrix Double Layer Capacitance**, locate the **Porous Matrix Double Layer Capacitance** section.

3 In the C_{dl} text field, type `C_dl_neg`.

4 In the $a_{v,dl}$ text field, type `a_max_neg`.

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`.

LEAD-ACID BATTERY (LEADBAT)

Now, provide the boundary conditions. Ground the negative electrode and set a current density at the positive electrode.

Electric Ground 1

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

2 Select Boundary 5 only.

Electrode Current Density 1

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

2 Select Boundary 1 only.

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

4 In the $i_{n,s}$ text field, type `I_disch*step1(t/1[s])`.

Initial Values 2

Finally, provide initial conditions for the battery at the start of the discharge.

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

2 Select Domains 1 and 2 only.

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

4 In the *cl* text field, type `cl_init`.

5 In the *epsilon* text field, type `eps_pos_init`.

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 *cl* text field, type `cl_init`.

4 In the *epsilon* text field, type `eps_neg_init`.

STUDY 1

Start by setting up a 21 h study using the C/20 current setting from the parameter file.

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 In the **Output times** text field, type `range(0,1800,21*3600)`.

Solution 1 (sol1)

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

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

Store the actual steps taken by the solver to make sure to capture any sudden steep voltage changes.

3 In the **Model Builder** window, under **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** click **Time-Dependent Solver 1**.

4 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

5 From the **Times to store** list, choose **Steps taken by solver**.

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

RESULTS

Cell Voltage C/20

1 In the **Settings** window for **1D Plot Group**, type `Cell Voltage C/20` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

3 In the **Title** text area, type `Cell voltage during a C/20 discharge + 1 h relaxation`.

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Time (h)`.

6 Select the **y-axis label** checkbox. In the associated text field, type `Cell Voltage (V)`.

Point Graph 1

1 In the **Model Builder** window, expand the **Cell Voltage C/20** node, then click **Point Graph 1**.

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

3 From the **Parameter** list, choose **Expression**.

4 In the **Expression** text field, type `t/3600`.

5 In the **Cell Voltage C/20** toolbar, click **Plot**.

Electrolyte Salt Concentration C/20

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

2 In the **Settings** window for **1D Plot Group**, type `Electrolyte Salt Concentration C/20` in the **Label** text field.

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

4 In the **Title** text area, type `Electrolyte concentration profile during a C/20 discharge + 1 h relaxation period`.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `Distance across the lead-acid cell [m]`.

7 Select the **y-axis label** checkbox. In the associated text field, type `c<sub>l</sub> [mol/m<sup>3</sup>]`.

8 Locate the **Data** section. From the **Time selection** list, choose **Interpolated**.

9 In the **Times (s)** text field, type `3600 10*3600 20*3600 21*3600`.

Line Graph 1

1 Right-click **Electrolyte Salt Concentration C/20** and choose **Line Graph**.

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

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

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lead-Acid Battery** > **cl - Electrolyte salt concentration - mol/m³**.

5 Click to expand the **Legends** section. Select the **Show legends** checkbox.

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

7 In the table, enter the following settings:

Legends
`1 h (After 1 h of discharge)`
`10 h (After 10 h of discharge)`
`20 h (At end of discharge)`
`21 h (After 1 h relaxation)`

8 In the **Electrolyte Salt Concentration C/20** toolbar, click **Plot**.

Electrode SOC During a C/20 Discharge

1 In the **Model Builder** window, right-click **Electrolyte Salt Concentration C/20** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Electrode SOC During a C/20 Discharge` in the **Label** text field.

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

4 Locate the **Data** section. In the **Times (s)** text field, type `3600 10*3600 20*3600`.

5 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Electrode state of charge (1)`.

Line Graph 1

1 In the **Model Builder** window, expand the **Electrode SOC During a C/20 Discharge** 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)** > **Lead-Acid Battery** > **leadbat.soc - Electrode state of charge - 1**.

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

Legends
1 h
10 h
20 h

4 In the **Electrode SOC During a C/20 Discharge** toolbar, click **Plot**.

GLOBAL DEFINITIONS

Now set up the 20C study by changing the current. Also add a nonlocal coupling for use in a stop condition to stop the simulation when the cell voltage drops below 1.5 V.

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 In the table, enter the following settings:

Name	Expression	Value	Description
C_factor	20	20	Current multiplicative factor

DEFINITIONS

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, locate the **Source Selection** section.

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

4 Select Boundary 1 only.

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Time Dependent with Initialization**.

4 Click the **Add Study** button in the window toolbar.

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

STUDY 2

Step 2: Time Dependent

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

2 In the **Output times** text field, type `range(0,1,60)`.

Solution 3 (sol3)

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

2 In the **Model Builder** window, expand the **Solution 3 (sol3)** node.

3 Right-click **Study 2** > **Solver Configurations** > **Solution 3 (sol3)** > **Time-Dependent Solver 1** and choose **Stop Condition**.

4 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

5 Click **Add**.

6 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.intop1(comp1.phis)<1.5`	True (>=1)	√	`Stop expression 1`

Specify that the solution is to be stored both before and after the stop condition is reached.

7 Locate the **Output at Stop** section. From the **Add solution** list, choose **Steps before and after stop**.

8 Clear the **Add information** checkbox.

9 In the **Model Builder** window, click **Study 2**.

10 In the **Settings** window for **Study**, locate the **Study Settings** section.

11 Clear the **Generate default plots** checkbox.

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

RESULTS

Electrolyte Salt Concentration at 20 C

1 In the **Model Builder** window, right-click **Electrolyte Salt Concentration C/20** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Electrolyte Salt Concentration at 20 C` in the **Label** text field.

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

4 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 3 (sol3)**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electrolyte Salt Concentration at 20 C** node, then click **Line Graph 1**.

2 In the **Settings** window for **Line Graph**, click to expand the **Legends** section.

3 Clear the **Show legends** checkbox.

Color Expression 1

1 Right-click **Line Graph 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

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

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Viridis**.

Electrolyte Salt Concentration at 20 C

1 In the **Model Builder** window, under **Results** click **Electrolyte Salt Concentration at 20 C**.

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

3 Select the **Show units** checkbox.

4 In the **Electrolyte Salt Concentration at 20 C** toolbar, click **Plot**.

Electrode SOC During a 20 C Discharge

1 In the **Model Builder** window, right-click **Electrode SOC During a C/20 Discharge** and choose **Duplicate**.

2 In the **Settings** window for **1D Plot Group**, type `Electrode SOC During a 20 C Discharge` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 3 (sol3)**.

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

Line Graph 1

1 In the **Model Builder** window, expand the **Electrode SOC During a 20 C Discharge** node, then click **Line Graph 1**.

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

3 Clear the **Show legends** checkbox.

Color Expression 1

1 Right-click **Line Graph 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

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

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Viridis**.

Electrode SOC During a 20 C Discharge

1 In the **Model Builder** window, under **Results** click **Electrode SOC During a 20 C Discharge**.

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

3 Select the **Show units** checkbox.

4 In the **Electrode SOC During a 20 C Discharge** toolbar, click **Plot**.

GLOBAL DEFINITIONS

For the self-discharge study, set the current to 0 and add a new study node.

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 In the table, enter the following settings:

Name	Expression	Value	Description
`C_factor`	`0`	`0`	`Current multiplicative factor`

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Time Dependent with Initialization**.

4 Click the **Add Study** button in the window toolbar.

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

STUDY 3

Step 2: Time Dependent

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

2 In the **Output times** text field, type `0 range(1,7*24*3600,365*24*3600)`.

3 In the **Model Builder** window, click **Study 3**.

4 In the **Settings** window for **Study**, locate the **Study Settings** section.

5 Clear the **Generate default plots** checkbox.

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

RESULTS

Cell Voltage Comparison

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

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

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Time (s)`.

6 Select the **y-axis label** checkbox. In the associated text field, type `Cell Voltage (V)`.

7 Locate the **Axis** section. Select the **x-axis log scale** checkbox.

8 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Point Graph 1

1 Right-click **Cell Voltage Comparison** and choose **Point Graph**.

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

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

4 Select Boundary 1 only.

5 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lead-Acid Battery** > **phis - Electric potential - V**.

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

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

8 In the table, enter the following settings:

Legends
`C/20 + 1 h relaxation`

Point Graph 2

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

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

3 From the **Dataset** list, choose **Study 2/Solution 3 (sol3)**.

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

Legends
`20C`

Point Graph 3

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

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

3 From the **Dataset** list, choose **Study 3/Solution 5 (sol5)**.

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

Legends
`Self discharge (One year)`

5 In the **Cell Voltage Comparison** toolbar, click **Plot**.

SOC During a One-Year Self Discharge

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

2 In the **Settings** window for **1D Plot Group**, type `SOC During a One-Year Self Discharge` in the **Label** text field.

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** checkbox. In the associated text field, type `Distance across the lead-acid cell (m)`.

6 Select the **y-axis label** checkbox. In the associated text field, type `Electrode state of charge (1)`.

Line Graph 1

1 Right-click **SOC During a One-Year Self Discharge** and choose **Line Graph**.

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

3 From the **Dataset** list, choose **Study 3/Solution 5 (sol5)**.

4 Locate the **Selection** section. From the **Selection** list, choose **All domains**.

5 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Lead-Acid Battery** > **leadbat.soc - Electrode state of charge - 1**.

Color Expression 1

1 Right-click **Line Graph 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Expression** section.

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

4 From the **Unit** list, choose **d**.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Viridis**.

SOC During a One-Year Self Discharge

1 In the **Model Builder** window, under **Results** click **SOC During a One-Year Self Discharge**.

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

3 Select the **Show units** checkbox.

4 In the **SOC During a One-Year Self Discharge** toolbar, click **Plot**.