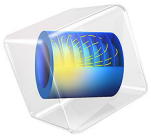


Model created in COMSOL Multiphysics 6.4

Single-Particle Modeling of Lithium-Ion Batteries

Introduction

The single-particle approach (Ref. 1 and Ref. 2) is a way to simplify the intercalating porous electrode formulation in the traditional Doyle–Fuller–Newman (DFN) model (see the 1D Isothermal Lithium-Ion Battery model example). In the single-particle model (SPM), the local potential and concentration gradients in the solution (electrolyte) phase are ignored, and instead the electrolyte potential losses are accounted for using a lumped solution resistance term. At the same time, the potential gradients in the solid phase of the electrodes are also neglected. As for the DFN model, the single-particle formulation accounts for solid diffusion in the electrode particles and the intercalation reaction kinetics. However, all particles are assumed to be identical, and since the reaction current distribution across the porous electrodes is assumed to be uniform, all particles are subjected to the same conditions, with the result that all particles may be treated as one "single" particle.

The assumptions of the single-particle formulation are typically valid for low to medium applied current densities. Additionally, the validity of the assumptions and the applicability of the model also depends on the parameters values and electrode-electrolyte chemistry used in the model. Typically the assumptions are applicable to thin, or highly conductive, electrodes.

The single-particle model formulation is typically used to reduce computational load in, for instance, capacity fade modeling, battery pack simulations, control systems, or parameter estimation applications.

As mentioned above, the traditional SPM model defines the electrolyte as a lumped resistor. However, it is also possible to keep the electrolyte transport model of the DFN model, solving for both the salt concentration and potential in the electrolyte phase, and combine it with the single-particle approach for the electrodes. This extension is often called SPMe in scientific literature.

This tutorial example demonstrates how to use the Thin Porous Electrode nodes in the Lithium-Ion Battery interface for defining SPMe and SPM models, as well as the Two Electrodes option in the Lumped Battery interface for defining a SPM model.

First a DFN model is defined in 1D, and the cell voltage response to a charge–discharge load cycle is computed. The voltage profile is then compared to the different single-particle models.

DOYLE–FULLER–NEWMAN BASE MODEL

The DFN model is based on the Lithium-Ion Battery Base Model in 1D. The model is defined using the **Lithium-Ion Battery** interface, using two **Porous Electrode** and one **Separator** domain node. (Compared with the Lithium-Ion Battery Base Model in 1D, the electrode thicknesses are increased somewhat in order to see larger differences between the DFN and single-particle models.)

SINGLE-PARTICLE MODEL WITH ELECTROLYTE SALT TRANSPORT

The SPMe makes use of a single **Separator** domain node in the **Lithium-Ion Battery** interface, and uses the same **Binary 1:1 liquid electrolyte** charge balance model as the DFN model. The two single-particle electrodes are defined using the **Thin Porous Electrode** boundary nodes.

The length of the single domain L_{el} (m) in the SPMe model is defined as

$$L_{\mathrm{el}} = L_{\mathrm{sep}} + \frac{1}{2}(L_{\mathrm{neg}} + L_{\mathrm{pos}}) \tag{1}$$

where L_{sep} (m), L_{neg} (m), and L_{pos} (m) are the lengths of the separator, negative electrode and positive electrode, respectively.

Apart from the size of the single domain, the SPMe is parameterized in the same way as the DFN model.

SINGLE-PARTICLE MODEL WITH CONSTANT ELECTROLYTE RESISTANCE

The SPM defined in the tutorial uses the same setup as the SPMe, but with the charge balance model set to **Single-ion conductor** using a user-defined effective electrolyte conductivity. This excludes solving for the electrolyte salt concentration in the single separator domain.

The lumped solution resistance R (Ω) of the SPM is defined as

$$R = \frac{E_{\mathrm{IR,\,1C}}}{I_{\mathrm{1C}}} \tag{2}$$

where $E_{\mathrm{IR,1C}}$ (V) is the electrolyte voltage drop when operating the cell at a 1C current, and I_{1C} (A) is the 1C current.

The effective conductivity σ_{eff} (S/m) used in the SPM model is then defined as

$$\sigma_{\text{eff}} = \frac{L_{\text{el}}}{RA_{\text{cell}}} \tag{3}$$

where A_{cell} (m^2) is the cross-sectional area of the cell.

In the tutorial, the computational solution of the SPMe is used to estimate $E_{\text{IR,1C}}$. The resulting effective conductivity of the SPM is slightly lower than for the SPMe due to the impact of concentration polarization effects in the electrolyte.

Due to the simplified equation formulation, a linear discretization may be used in combination with one mesh element only.

SINGLE-PARTICLE MODEL USING THE LUMPED BATTERY INTERFACE

A second SPM (Lumped) model is also defined in the tutorial, using the **Two Electrodes** model option in the **Lumped Battery** interface.

The SPM (Lumped) model is mathematically equivalent to the SPM. There is a difference however with regards to what parameters are used to define the two models. Whereas the Lithium-Ion Battery interface makes use of locally defined parameters in the geometry, the Lumped Battery interface make use of lumped zero-dimensional parameters.

The host capacity Q_{host} (C) of each electrode in the SPM (Lumped) model is defined as

$$Q_{\text{host}} = \varepsilon c_{s,\,\max} F A_{\text{cell}} L \tag{4}$$

where is ε (1) the electrode phase volume fraction, $c_{s,\max}$ (mol/m^3) the maximum concentration of intercalated lithium and L the electrode thickness.

For the solid intercalation, the diffusion time constants τ (s) of the two electrodes are defined as

$$\tau = \frac{r_p^2}{D} \tag{5}$$

where r_p (m) is the electrode particle radius and D (m^2/s) the diffusivity.

An advantage of using the Lumped Battery interface is that the model may be defined in 0D, so that no geometry needs to be defined.

Another difference between the SPM and SPM (Lumped) models is the handling of the Butler–Volmer kinetics-based activation overpotentials. In the SPM (Lumped) model, the activation overpotential is defined using an analytical function of the form

$$\eta = \frac{2RT}{F}\text{asinh}\frac{I}{2I_0} \tag{6}$$

where η is the activation overpotential (V) and I_0 is the exchange current (A). This allows for decoupling of the electrode and electrolyte phase potentials in the equation system and removes the need to solve for the potentials as dependent variables in the model. This lowers the computational complexity of the model. The above equation for the activation overpotential is however only valid for the case of symmetric transfer coefficients and one single electrode reaction.

LOAD CYCLE

A load cycle, starting from 75% SOC, discharging at 1C for 2000 s, resting for 300 s, recharging at 1C for 1000 s, and then resting again for 1700 s, is defined using a step sequence in a **Current** subnode to a **Load Cycle** parent node in each interface.

COMPONENTS AND STUDIES

The DFN, SPMe, SPM, and SPM(Lumped) models are defined in separate components, using separate geometries and meshes.

Each model is solved for in an individual time-dependent study, simulating the same charge–discharge cycle for 5000 s.

Results and Discussion

Figure 1 shows the cell voltage vs time for all four models. The discrepancies between the models are generally relatively small, with the largest deviations seen between the DFN and the other models. These differences are due changes in the current distribution within the

porous electrodes of the DFN models, something the SPMe and SPM models are unable to capture.

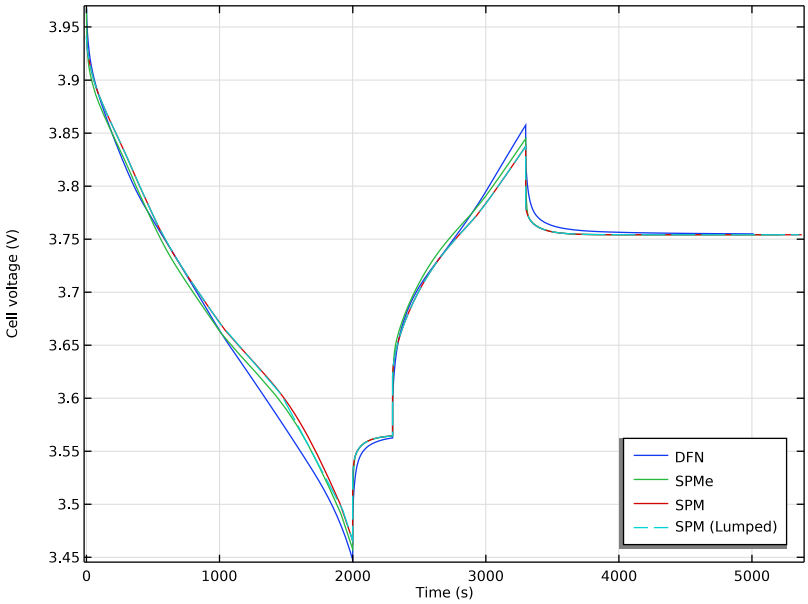


Figure 1: Cell voltage comparison for all four models.

Figure 2 shows a closeup of the cell voltages at the initiation of the charge pulse. The SPMe differs from the SPM models only during the first 20 s after initiation of the charge, during which a steady-state concentration profile in the electrolyte establishes.

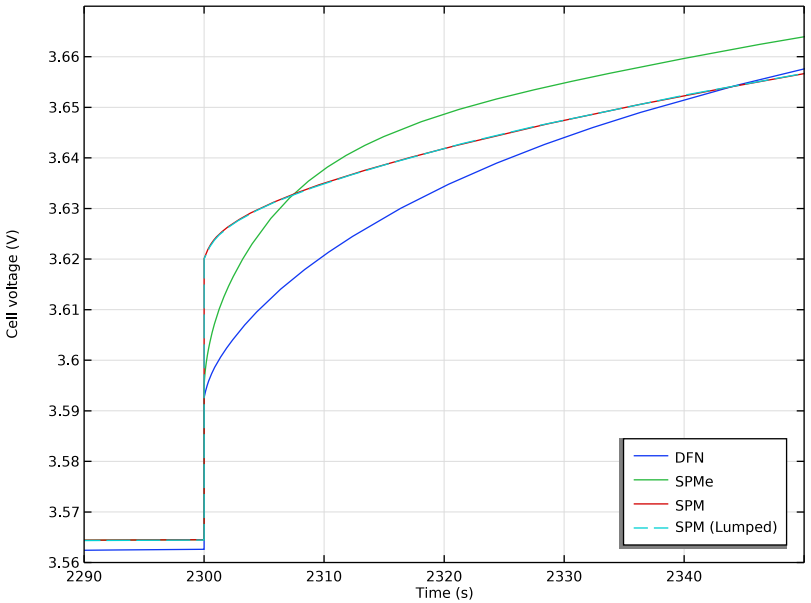


Figure 2: Cell voltage comparison for all four models (closeup).

Table 1 shows the number of degrees of freedoms (DOFs) and solution time as reported in the solver log when solving the four different models (the solution time may vary depending on the used computer). The lower amount of DOFs and shorter solution time for SPM (Lumped) compared to SPM is related to the treatment of the nonlinear activation overpotential, which allows for decoupling of the electrolyte and electrode potentials.

TABLE 1: DEGREES OF FREEDOM AND SOLUTION TIMES FOR THE DIFFERENT MODELS.

MODEL	DOFS	SOLVER TIME(S)
DFN	675	5
SPMe	170	4
SPM	26	3
SPM (Lumped)	23	2

References

1. S. Santhanagopalan, Q. Guo, P. Ramadass, and R.E. White, "Review of Models for Predicting the Cycling Performance of Lithium Ion Batteries," *J. Power Sources*, vol. 156, no. 2, pp. 620–628, 2006.

2. M. Guo, G. Sikha, and R.E. White, "Single Particle Model for a Lithium Ion Cell: Thermal Behavior," *J. Electrochem. Soc.*, vol. 158, no. 2, pp. A122–A132, 2011.

Application Library path: `Battery_Design_Module/Lithium-Ion_Batteries,_Performance/lib_single_particle`

Modeling Instructions

APPLICATION LIBRARIES

1 From the **File** menu, choose **Application Libraries**.

2 In the **Application Libraries** window, select **Battery Design Module** > **Lithium-Ion Batteries, Performance** > **lib_base_model_Id** in the tree.

3 Click **Open**.

First define the load cycle for the Doyle-Fuller-Newman (DFN) model. We will compare the probe cell voltage output for the DFN model to the various single-particle models defined later.

COMPONENT 1 - DFN

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

2 In the **Settings** window for **Component**, type `Component 1 - DFN` in the **Label** text field.

LITHIUM-ION BATTERY (LIION)

Load Cycle 1

1 In the **Model Builder** window, expand the **Component 1 - DFN (comp1)** > **Lithium-Ion Battery (liion)** node, then click **Load Cycle 1**.

2 In the **Settings** window for **Load Cycle**, locate the **Continuation Conditions** section.

3 Select the **Use elapsed time only** checkbox.

C Rate 1

1 In the **Model Builder** window, expand the **Load Cycle 1** node, then click **C Rate 1**.

2 In the **Settings** window for **C Rate**, locate the **C-Rate Multiple** section.

3 From the **Input type** list, choose **Step sequence**.

4 In the C_0 text field, type `-1`.

5 Click + **Add**.

6 In the table, enter the following settings:

t_i (s)	C_i (1)
2000[s]	0

7 Click + **Add**.

8 In the table, enter the following settings:

t_i (s)	C_i (1)
2300[s]	1

9 Click + **Add**.

10 In the table, enter the following settings:

t_i (s)	C_i (1)
3300	0

DEFINITIONS (COMP1)

Load Cycle Probe - DFN

1 In the **Model Builder** window, expand the **Component 1 - DFN (comp1)** > **Definitions** node, then click **Load Cycle Probe (liion_lc1_volt)**.

2 In the **Settings** window for **Global Variable Probe**, type `Load Cycle Probe - DFN` in the **Label** text field.

3 Locate the **Expression** section.

4 Select the **Description** checkbox. In the associated text field, type `Cell voltage - DFN`.

GLOBAL DEFINITIONS

DFN Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `DFN Parameters` in the **Label** text field.

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

Name	Expression	Value	Description
L_pos	60[um]	6E-5 m	Positive electrode thickness
soc_init	0.75	0.75	Initial SOC

STUDY 1

Step 2: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then 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 **s**.

4 In the **Output times** text field, type `0 5000`.

5 In the **Model Builder** window, click **Study 1**.

6 In the **Settings** window for **Study**, type `Study 1 - DFN` in the **Label** text field.

7 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

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

RESULTS

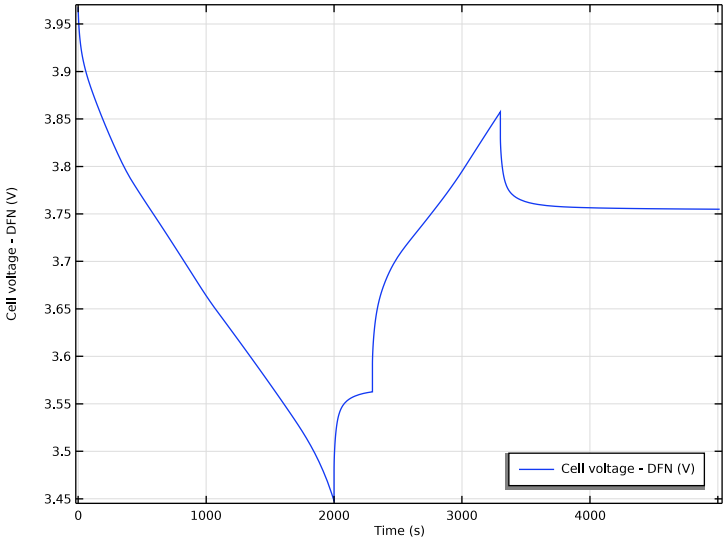
Probe Plot Group 1

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

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

3 From the **Position** list, choose **Lower right**.

4 In the **Probe Plot Group 1** toolbar, click **Plot**.



COMPONENT 1 - DFN (COMP1)

In the **Model Builder** window, collapse the **Component 1 - DFN (comp1)** node.

The next step is to define a model using single particles for the electrodes, but with the same electrolyte transport model as in the DFN model. The new model is referred to as SPMe.

Load some additional lumped parameters from a text file. These parameters will be used to define the simplified single-particle models.

GLOBAL DEFINITIONS

Lumped Parameters

1 In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.

2 In the **Settings** window for **Parameters**, type `Lumped Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `lib_single_particle_parameters.txt`.

ROOT

Define the SMPe model in a separate component, using a different geometry and mesh than the DFN model.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component** > **1D**.

COMPONENT 2 - SPME

1 In the **Model Builder** window, click **Component 2 (comp2)**.

2 In the **Settings** window for **Component**, type `Component 2 - SPMe` in the **Label** text field.

GEOMETRY 2

Interval 1 (i1)

1 In the **Model Builder** window, under **Component 2 - SPMe (comp2)** right-click **Geometry 2** and choose **Interval**.

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

3 In the table, enter the following settings:

Coordinates (m)
0
L_el

The length **L_el** of the domain, defined in the parameter file you imported before, is longer than the separator domain length in the DFN model.

ADD PHYSICS

1 In the **Home** toolbar, click **Windows** and choose **Add Physics**.

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

3 In the tree, select **Electrochemistry** > **Batteries** > **Lithium-Ion Battery (liion)**.

4 Click the **Add to Component 2 - SPMe** button in the window toolbar.

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

LITHIUM-ION BATTERY 2 (LIION2)

1 In the **Settings** window for **Lithium-Ion Battery**, locate the **Cross-Sectional Area** section.

2 In the A_c text field, type `A_cell`.

Separator 1

The settings for the **Separator** node are identical to the DFN model.

1. In the **Model Builder** window, under **Component 2 - SPMe (comp2)** > **Lithium-Ion Battery 2 (liion2)** click **Separator 1**.
2. In the **Settings** window for **Separator**, locate the **Electrolyte Properties** section.
3. From the **Electrolyte material** list, choose **LiPF6 in 3:7 EC:EMC (Liquid, Li-ion Battery) (mat1)**.
4. Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsl_sep`.

Thin Porous Electrode 1

1. In the **Physics** toolbar, click **Boundaries** and choose **Thin Porous Electrode**.
2. Select Boundary 1 only.
3. In the **Settings** window for **Thin Porous Electrode**, locate the **Porous Matrix Properties** section.
4. In the d_{pe} text field, type `L_neg`.
5. In the ε_s text field, type `epss_neg`.

Particle Intercalation 1

The settings for the **Particle Intercalation** and **Porous Electrode Reaction** child nodes are identical to the corresponding settings in the DFN model.

1. In the **Model Builder** window, click **Particle Intercalation 1**.
2. In the **Settings** window for **Particle Intercalation**, locate the **Material** section.
3. From the **Particle material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
4. Locate the **Particle Transport Properties** section. In the r_p text field, type `rp_neg`.

Porous Electrode Reaction 1

1. In the **Model Builder** window, click **Porous Electrode Reaction 1**.
2. In the **Settings** window for **Porous Electrode Reaction**, locate the **Material** section.
3. From the **Material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.
4. Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_ref_neg`.

Thin Porous Electrode 2

1. In the **Physics** toolbar, click **Boundaries** and choose **Thin Porous Electrode**.
2. Select Boundary 2 only.

3 In the **Settings** window for **Thin Porous Electrode**, locate the **Porous Matrix Properties** section.

4 In the d_{pe} text field, type `L_pos`.

5 In the ε_{s} text field, type `epss_pos`.

Particle Intercalation 1

1 In the **Model Builder** window, click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, locate the **Material** section.

3 From the **Particle material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

4 Locate the **Particle Transport Properties** section. In the r_{p} text field, type `rp_pos`.

Porous Electrode Reaction 1

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

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

3 From the **Material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

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

5 In the **Model Builder** window, click **Lithium-Ion Battery 2 (liion2)**.

6 In the **Settings** window for **Lithium-Ion Battery**, locate the **Cell Settings** section.

7 Select the **Define cell state of charge (SOC) and initial charge inventory** checkbox.

SOC and Initial Charge Distribution 1

1 In the **Model Builder** window, under **Component 2 - SPMe (comp2)** > **Lithium-Ion Battery 2 (liion2)** click **SOC and Initial Charge Distribution 1**.

2 In the **Settings** window for **SOC and Initial Charge Distribution**, locate the **Electrode Selection Type** section.

3 From the **Negative electrode** list, choose **Boundary**.

4 From the **Positive electrode** list, choose **Boundary**.

5 Locate the **Initial Cell Charge Distribution** section. In the SOC_0 text field, type `soc_init`.

Negative Electrode Boundary Selection 1

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

2 Select Boundary 1 only.

Positive Electrode Boundary Selection 1

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

2 Select Boundary 2 only.

Thin Porous Electrode 2

1 In the **Model Builder** window, under **Component 2 - SPMe (comp2)** > **Lithium-Ion Battery 2 (liion2)** click **Thin Porous Electrode 2**.

2 In the **Settings** window for **Thin Porous Electrode**, locate the **Electrode Phase Potential Condition** section.

3 From the **Electrode phase potential condition** list, choose **Load cycle**.

LITHIUM-ION BATTERY (LIION)

C Rate 1

1 In the **Model Builder** window, expand the **Component 1 - DFN (comp1)** > **Lithium-Ion Battery (liion)** node.

2 Right-click **Component 1 - DFN (comp1)** > **Lithium-Ion Battery (liion)** > **Load Cycle 1** > **C Rate 1** and choose **Copy**.

3 In the **Model Builder** window, collapse the **Lithium-Ion Battery (liion)** node.

LITHIUM-ION BATTERY 2 (LIION2)

Load Cycle 1

1 In the **Model Builder** window, under **Component 2 - SPMe (comp2)** > **Lithium-Ion Battery 2 (liion2)** > **Thin Porous Electrode 2** click **Load Cycle 1**.

2 In the **Settings** window for **Load Cycle**, locate the **Continuation Conditions** section.

3 Select the **Use elapsed time only** checkbox.

C Rate 1

Right-click **Load Cycle 1** and choose **Paste C Rate**.

DEFINITIONS (COMP2)

Global Variable Probe - SPMe

1 In the **Definitions** toolbar, click  **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - SPMe` in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 - SPMe (comp2)** > **Lithium-Ion Battery 2** > **liion2.phis_tpce2 - Electric potential - V**.

4 Locate the **Expression** section.

5 Select the **Description** checkbox. In the associated text field, type `Cell Voltage - SPMe`.

6 Click to expand the **Table and Window Settings** section. Click **Add Table**.

7 From the **Plot window** list, choose **Probe Plot 1**.

Also add an integration operator. This operator will be used later when computing the total electrolyte potential drop.

Integration 1 (intop1)

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

2 In the **Settings** window for **Integration**, type `intop_neg` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Geometric entity level** list, choose **Boundary**.

4 Select Boundary 1 only.

ADD STUDY

1 In the **Home** toolbar, click **Windows** and choose **Add Study**.

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 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Lithium-Ion Battery (liion)**.

5 Find the **Studies** subsection. Right-click and choose **Add Study**.

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

STUDY 2

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 2** 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 `0 5000`.

4 Click to expand the **Results While Solving** section. From the **Probes** list, choose **Manual**.

5 In the **Probes** list box, select **Load Cycle Probe - DFN (liion_lc1_volt)**.

6 Under **Probes**, click **Delete**.

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

8 In the **Settings** window for **Study**, type `Study 2 - SPMe` in the **Label** text field.

9 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

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

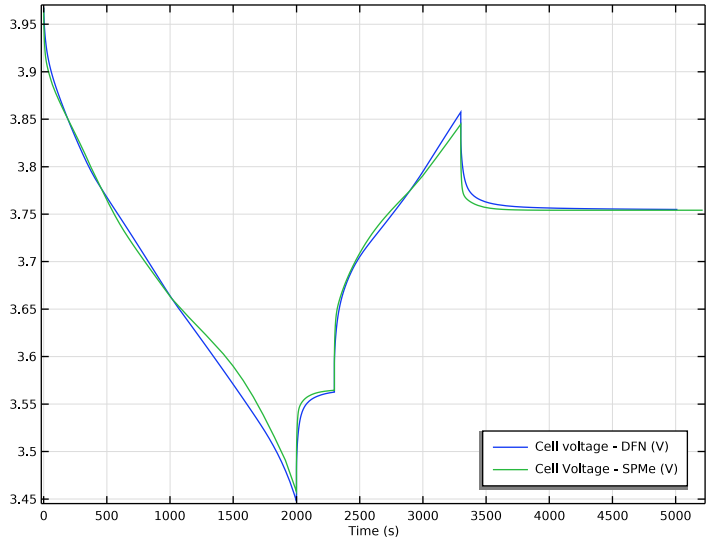
RESULTS

Probe Plot Group 1

The probe plot should now show a comparison between the DFN and SPMe cell voltage outputs.

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

2 In the **Probe Plot Group 1** toolbar, click **Plot**.



Electrolyte domain potential drop in SPMe model

The next step is to create a single particle model where we treat the electrolyte transport as a constant resistor, which will be called SPM. In order to compute the corresponding resistivity, we evaluate the total electrolyte potential drop of the SPMe model as follows:

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

2 In the **Settings** window for **1D Plot Group**, type `Electrolyte domain potential drop in SPMe model` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 - SPMe/ Solution 3 (5) (sol3)**.

Point Graph 1

1 Right-click **Electrolyte domain potential drop in SPMe model** and choose **Point Graph**.

2 Select Boundary 2 only.

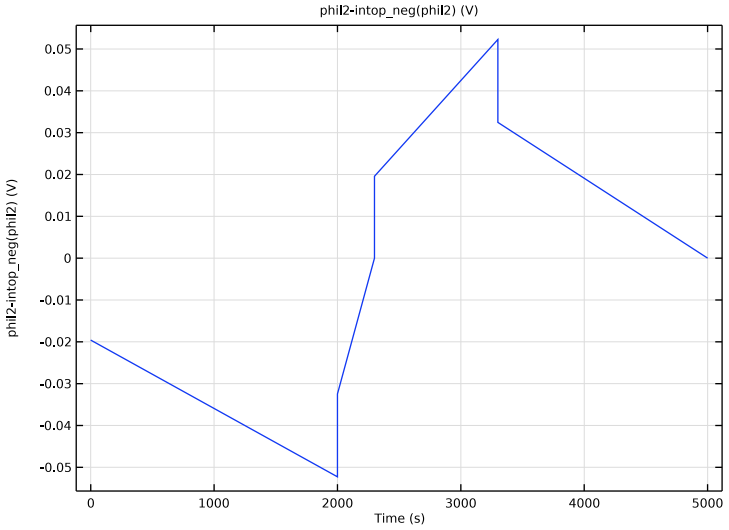
3 In the **Settings** window for **Point Graph**, locate the **y-Axis Data** section.

4 In the **Expression** text field, type `phil2-intop_neg(phil2)`.

Electrolyte domain potential drop in SPMe model

1 In the **Model Builder** window, click **Electrolyte domain potential drop in SPMe model**.

2 In the **Electrolyte domain potential drop in SPMe model** toolbar, click **Plot**.



Note that the voltage drop at the end of the 1C current loads is about 45 mV.

COMPONENT 2 - SPME (COMP2)

Make a copy of the whole SPMe model and paste it into a new component. We will use the new component to create the SPM model.

1 In the **Model Builder** window, right-click **Component 2 - SPMe (comp2)** and choose **Copy**.

COMPONENT 2 - SPME 1 (COMP3)

In the **Model Builder** window, right-click the root node and choose **Paste Multiple Items**.

COMPONENT 2 - SPME 1 (COMP3), DEFINITIONS (COMP3), GEOMETRY 2, LITHIUM-ION BATTERY 2 (LIION3), MESH 2

1 In the **Messages from Paste** dialog, click **OK**.

In the copy operation the name of the `liion2` interface was pasted as `liion3`. As a result of this, you will have to update various variable names in order to get the SPM model to work properly.

COMPONENT 2 - SPME (COMP2)

In the **Model Builder** window, collapse the **Component 2 - SPMe (comp2)** node.

COMPONENT 3 - SPM

1 In the **Model Builder** window, click **Component 2 - SPMe 1 (comp3)**.

2 In the **Settings** window for **Component**, type `Component 3 - SPM` in the **Label** text field.

DEFINITIONS (COMP3)

Global Variable Probe - SPM

1 In the **Model Builder** window, under **Component 3 - SPM (comp3)** > **Definitions** click **Global Variable Probe - SPMe (var2)**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - SPM` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `liion3.phis_tpce2`.

4 In the **Description** text field, type `Cell Voltage - SPM`.

5 Locate the **Table and Window Settings** section. Click + **Add Table**.

Variables 2

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

As conductivity value we will use a constant effective conductivity value based on the average electrolyte potential drop value we estimated in the SPMe model. Define this as a variable here for later use when defining the **Separator** domain.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
sigmal_eff	liion3.I_1C_cell*L_el/(E_IR_1C*A_cell)	S/m	

E_IR_1C equals 45 mV in the parameter list.

LITHIUM-ION BATTERY 3

The difference between the SPMe and the SPM model lies in the electrolyte transport formulation. The SPM model models the electrolyte as a resistor. This can be accomplished by using the **Single-Ion Conductor** model in the **Lithium-Ion Battery** interface.

1 In the **Model Builder** window, under **Component 3 - SPM (comp3)** click **Lithium-Ion Battery 2 (liion3)**.

2 In the **Settings** window for **Lithium-Ion Battery**, type Lithium-Ion Battery 3 in the **Label** text field.

3 Locate the **Charge Balance Model** section. From the list, choose **Single-ion conductor**.

Since there are no source terms present in the single separator domain in the SPM model, it suffices to use a linear discretization of the electrolyte potential. This saves computational resources.

4 Click to expand the **Discretization** section. From the **Electrolyte potential** list, choose **Linear**.

Separator 1

1 In the **Model Builder** window, expand the **Component 3 - SPM (comp3)** > **Lithium-Ion Battery 3 (liion3)** node, then click **Separator 1**.

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

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

4 Locate the **Effective Transport Parameter Correction** section. From the **Electrolyte conductivity** list, choose **No correction**.

MESH 2

Edge 1

In the **Mesh** toolbar, click  **Edge**.

Distribution 1

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

Since there are no source terms present in the single domain in the SPM model, it suffices to use a single mesh element. This also saves computational resources.

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

3 In the **Number of elements** text field, type `1`.

ADD STUDY

1 In the **Home** toolbar, click **Windows** and choose **Add Study**.

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 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Lithium-Ion Battery (liion)** and **Lithium-Ion Battery 2 (liion2)**.

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

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

STUDY 3

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 3** 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 `0 5000`.

4 Locate the **Results While Solving** section. From the **Probes** list, choose **Manual**.

5 In the **Probes** list, choose **Load Cycle Probe - DFN (liion_lc1_volt)** and **Global Variable Probe - SPMe (var1)**.

6 Under **Probes**, click **Delete**.

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

8 In the **Settings** window for **Study**, type `Study 3 - SPM` in the **Label** text field.

9 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

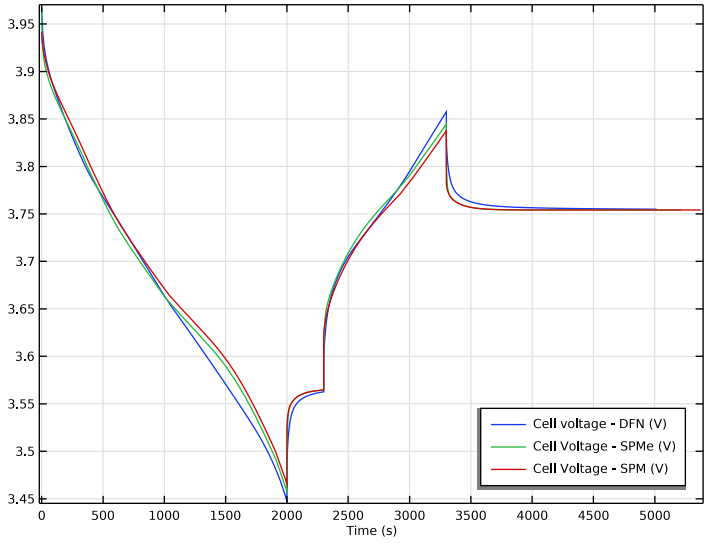
10 In the **Study** toolbar, click **Compute**.

RESULTS

Probe Plot Group 1

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

2 In the **Probe Plot Group 1** toolbar, click **Plot**.



COMPONENT 3 - SPM (COMP3)

In the **Model Builder** window, collapse the **Component 3 - SPM (comp3)** node.

It is also possible to create a SPM model by using the **Lumped Battery** interface, we will now proceed to make such a model, which we will call SPM (Lumped). By the use of the **Lumped Battery** interface, no geometry needs to be defined, and the model may hence be created in 0D.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component** > **0D**.

COMPONENT 4 - SPM (LUMPED)

In the **Settings** window for **Component**, type `Component 4 - SPM (Lumped)` in the **Label** text field.

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** > **Batteries** > **Lumped Battery, Two Electrodes (lb)**.

4 Click the **Add to Component 4 - SPM (Lumped)** button in the window toolbar.

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

LUMPED BATTERY (LB)

1 In the **Settings** window for **Lumped Battery**, locate the **Operation Mode** section.

2 From the **Operation mode** list, choose **Load cycle**.

The SPM (Lumped) model makes use of a number of lumped parameters, defined in the parameters file you imported earlier.

3 Locate the **Initial Capacity** section. In the $Q_{\mathrm{host,neg},0}$ text field, type `Q_host_neg`.

4 In the $Q_{\mathrm{host,pos},0}$ text field, type `Q_host_pos`.

5 Locate the **Initial Cell Charge Distribution** section. In the $\mathrm{SOC}_{\mathrm{cell},0}$ text field, type `soc_init`.

LITHIUM-ION BATTERY (LIION)

C Rate 1

1 In the **Model Builder** window, expand the **Component 1 - DFN (comp1)** > **Lithium-Ion Battery (liion)** node.

2 Right-click **Component 1 - DFN (comp1)** > **Lithium-Ion Battery (liion)** > **Load Cycle 1** > **C Rate 1** and choose **Copy**.

LITHIUM-ION BATTERY (LIION)

In the **Model Builder** window, collapse the **Component 1 - DFN (comp1)** > **Lithium-Ion Battery (liion)** node.

LUMPED BATTERY (LB)

Load Cycle 1

1 In the **Model Builder** window, under **Component 4 - SPM (Lumped) (comp4)** > **Lumped Battery (lb)** click **Load Cycle 1**.

2 In the **Settings** window for **Load Cycle**, locate the **Continuation Conditions** section.

3 Select the **Use elapsed time only** checkbox.

C Rate 1

Right-click **Load Cycle 1** and choose **Paste C Rate**.

Negative Equilibrium Potential 1

1 In the **Model Builder** window, under **Component 4 - SPM (Lumped) (comp4)** > **Lumped Battery (lb)** click **Negative Equilibrium Potential 1**.

2 In the **Settings** window for **Negative Equilibrium Potential**, locate the **Material** section.

3 From the **Electrode material** list, choose **Graphite, LixC6 MCMB (Negative, Li-ion Battery) (mat2)**.

4 Locate the **Model Input** section. In the *T* text field, type `T`.

Positive Equilibrium Potential 1

1 In the **Model Builder** window, click **Positive Equilibrium Potential 1**.

2 In the **Settings** window for **Positive Equilibrium Potential**, locate the **Material** section.

3 From the **Electrode material** list, choose **NMC 111, LiNi0.33Mn0.33Co0.33O2 (Positive, Li-ion Battery) (mat3)**.

4 Locate the **Model Input** section. In the *T* text field, type `T`.

DEFINITIONS (COMP4)

Also add some variable expressions for the lumped exchange current densities as follows:

Variables 3

1 In the **Model Builder** window, under **Component 4 - SPM (Lumped) (comp4)** right-click **Definitions** and choose **Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`J0_neg`	`(lb.DOC_neg_surface*(1-lb.DOC_neg_surface))^0.5*2*i0_ref_neg*(3/rp_neg)/(cs_max_neg*F_const/1[h])`		`Dimensionless exchange current density, negative electrode`
`J0_pos`	`(lb.DOC_pos_surface*(1-lb.DOC_pos_surface))^0.5*2*i0_ref_pos*(3/rp_pos)/(cs_max_pos*F_const/1[h])`		`Dimensionless exchange current density, positive electrode`

LUMPED BATTERY (LB)

Voltage Losses 1

1 In the **Model Builder** window, under **Component 4 - SPM (Lumped) (comp4)** > **Lumped Battery (lb)** click **Voltage Losses 1**.

2 In the **Settings** window for **Voltage Losses**, locate the **Ohmic Overpotential** section.

3 In the $\eta_{IR,1C}$ text field, type `E_IR_1C`.

4 Locate the **Model Input** section. In the T text field, type `T`.

5 Locate the **Activation Overpotential, Negative** section. In the $J_{0,neg}$ text field, type `J0_neg`.

6 Locate the **Activation Overpotential, Positive** section. In the $J_{0,pos}$ text field, type `J0_pos`.

7 Locate the **Concentration Overpotential, Negative** section. Select the **Include concentration overpotential, negative** checkbox.

8 In the τ_{neg} text field, type `tau_neg`.

9 Locate the **Concentration Overpotential, Positive** section. Select the **Include concentration overpotential, positive** checkbox.

10 In the τ_{pos} text field, type `tau_pos`.

DEFINITIONS (COMP4)

Global Variable Probe - SPM (Lumped)

1 In the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe - SPM (Lumped)` in the **Label** text field.

3 Locate the **Expression** section.

4 Select the **Description** checkbox. In the associated text field, type `Cell potential, SPM (Lumped)`.

5 Locate the **Table and Window Settings** section. Click **Add Table**.

6 From the **Plot window** list, choose **Probe Plot 1**.

ADD STUDY

1 In the **Home** toolbar, click **Windows** and choose **Add Study**.

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Time Dependent**.

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Lithium-Ion Battery (liion)**, **Lithium-Ion Battery 2 (liion2)**, and **Lithium-Ion Battery 3 (liion3)**.

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

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

STUDY 4

Step 1: Time Dependent

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

2 In the **Output times** text field, type `0 5000`.

3 Locate the **Results While Solving** section. From the **Probes** list, choose **Manual**.

4 In the **Probes** list, choose **Load Cycle Probe - DFN (liion_lc1_volt)**, **Global Variable Probe - SPMe (var1)**, and **Global Variable Probe - SPM (var2)**.

5 Under **Probes**, click **Delete**.

6 In the **Model Builder** window, click **Study 4**.

7 In the **Settings** window for **Study**, type `Study 4 - SPM (Lumped)` in the **Label** text field.

8 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

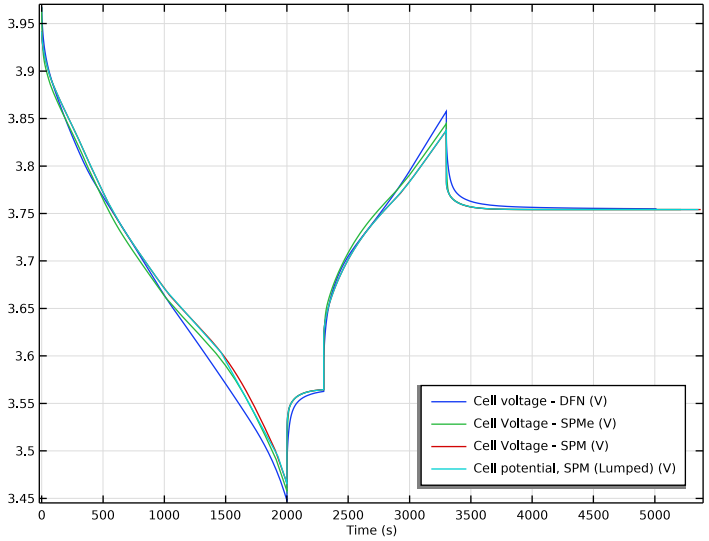
9 In the **Study** toolbar, click **Compute**.

RESULTS

Cell Voltage Comparison

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

2 In the **Probe Plot Group 1** toolbar, click **Plot**.



Finally, polish the cell voltage comparison plot as follows:

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

4 Locate the **Plot Settings** section.

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

Probe Table Graph 1

1 In the **Model Builder** window, expand the **Cell Voltage Comparison** node, then click **Probe Table Graph 1**.

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

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

4 In the table, enter the following settings:

Legends
DFN

Probe Table Graph 2

1 In the **Model Builder** window, click **Probe Table Graph 2**.

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

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

4 In the table, enter the following settings:

Legends
SPMe

Probe Table Graph 3

1 In the **Model Builder** window, click **Probe Table Graph 3**.

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

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

4 In the table, enter the following settings:

Legends
SPM

Probe Table Graph 4

1 In the **Model Builder** window, click **Probe Table Graph 4**.

2 In the **Settings** window for **Table Graph**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

4 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

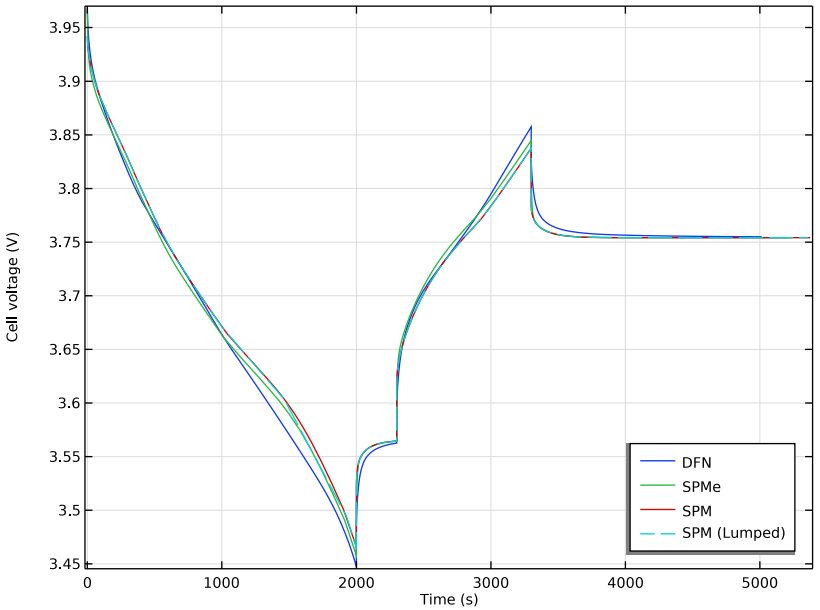
5 In the table, enter the following settings:

Legends
SPM (Lumped)

Cell Voltage Comparison

1 In the **Model Builder** window, click **Cell Voltage Comparison**.

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



3 In the **Settings** window for **1D Plot Group**, locate the **Axis** section.

4 Select the **Manual axis limits** checkbox.

5 In the **x minimum** text field, type 2290.

6 In the **x maximum** text field, type 2350.

7 In the **y minimum** text field, type 3.56.

8 In the **y maximum** text field, type 3.67.

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