Model created in COMSOL Multiphysics 6.4

Minimizing the Charging Time of a Lithium-Ion Battery

Introduction

Optimizing a fast-charging curve for a battery is a multiple-objective problem. At the same time as one strives to minimize the total charging time, the applied high charge rates must not result in excessive aging of the battery. In a typical fast charge cycle for a lithium-ion battery, the initially high charging current is continuously lowered in order not to induce lithium plating or accelerated solid electrolyte interphase (SEI) formation.

This model extends the Lithium-Ion Battery Base Model in 1D with an optimization study, with the objective to minimize the required charging time for charging the battery from 0 to 90% state of charge (SOC). This is achieved by fitting the shape of the charging profile using a control function, subject to a constraint for the maximum allowed degradation during the charge cycle.

Model Definition

CHARGE CURVE DEFINITION AND THE CONTROL FUNCTION

The C rate of a battery is proportional to the battery current, where a C rate of 1 equals the current required to fully charge, or discharge, the battery in 1 h. A total current condition is used as boundary condition for the battery model, with the applied current defined as

$$I_{\mathrm{app}} = \frac{C(\tilde{t})}{1\,\mathrm{h}} Q_{\mathrm{cell}} \tag{1}$$

Here, Q_{cell} is the battery capacity as defined by the Lithium-Ion Battery interface.

The charging function C is defined using a Control Function, based on a five-segment piecewise Bernstein polynomial, resulting in seven control variables (fitting parameters). The argument for the control function, ranging between 0 and 1, represents a dimensionless time $\tilde{t} = t/t_{\mathrm{scale}}$, scaled so that the value 0 represents the time at the beginning of the charge cycle and 1 the final time when the battery has reached the target SOC of 90%. By this definition, the area of the control function equals the average C-rate over the whole charge cycle.

$$C_{\mathrm{avg}} = \int_0^1 C(\tilde{t})\,\mathrm{d}\tilde{t} \tag{2}$$

and the time scale, t_{scale}, can be computed as

$$t_{\text{scale}} = \frac{90\% \cdot 1\text{h}}{C_{\text{avg}}} \tag{3}$$

A stop expression is enabled in optimization study in order to stop the time-dependent solver when the battery has reached 90% SOC (at $t = t_{\text{scale}}$).

The optimization solver is set to maximize the value of the variable C_{avg}.

CONSTRAINING THE PARASITIC REACTIONS

The amount of degradation during the charging cycle is computed using a generalized volumetric Butler–Volmer expression in the negative graphite electrode of the following form.

$$i_{\text{BV}} = 10^4\text{A/m}^3 \cdot \left(\frac{c_l}{1\text{M}}\right)^{0.5}\left(e^{\frac{0.5F\eta}{RT}} - e^{-\frac{0.5F\eta}{RT}}\right) \tag{4}$$

where the overpotential η is defined as

$$\eta = \phi_s - \phi_l - 25\ \text{mV} \tag{5}$$

The volumetric current is defined to be zero for positive (anodic) overpotentials by the expression

$$i_v = \begin{array}{l} 0 \quad \text{if } \eta > 0 \\ i_{\text{BV}} \ \text{if } \eta \le 0 \end{array} \tag{6}$$

The above parasitic aging expression was chosen for tutorial purposes, but could represent, for instance, irreversible SEI formation with an onset potential of 25 mV, or lithium plating (with an added safety margin of 25 mV).

Integrating the volumetric current density in the negative electrode over the course of the whole simulation gives a measure of the total amount of capacity lost due to the parasitic reaction

$$Q_{\text{loss}} = \int_0^T \int_{\text{neg}} i_v \,\mathrm{d}S\,\mathrm{d}t \tag{7}$$

During optimization, charging profiles that result in a degradation larger than 10% over 1000 cycles are prohibited by defining a constraint variable as

$$\text{constr} = \frac{1000}{10\%} \cdot \frac{Q_{\text{loss}}}{Q_{\text{cell}}} \tag{8}$$

The above variable is used as a constraint expression optimization solver, with an upper bound of 1.

Results and Discussion

Figure 1 compares the initial loading cycle with the optimized one.

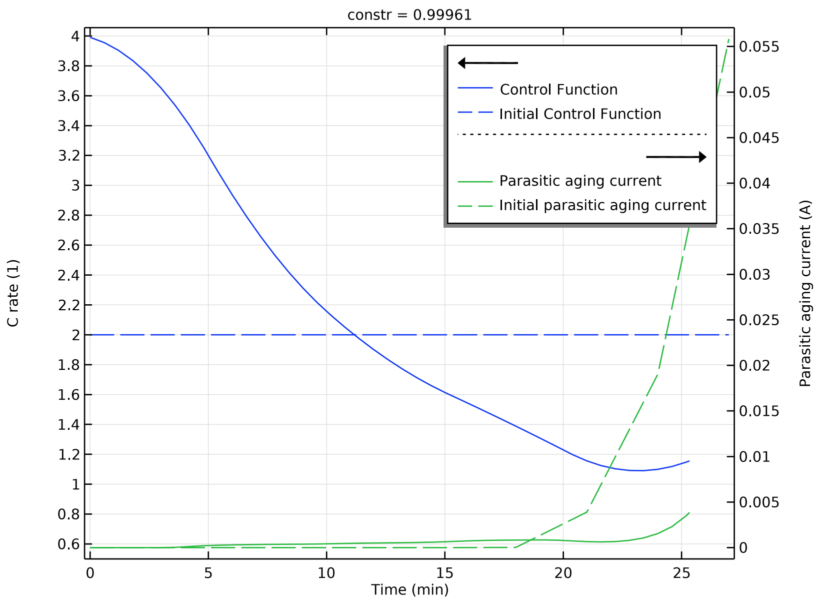


Figure 1: The optimized charge profile is plotted together with the electroplating current.

The optimization reduces the charging time by a factor of 2 relative to the initial charging profile, but this comes at the cost of a nonzero electroplating current. The relationship between these two objectives is plotted in Figure 2, where the charging profile has been optimized for different values of the maximum number of cycles. The figure shows that it is possible to achieve a tenfold improvement in longevity for the battery at the cost of a 20% increase in the charging time.

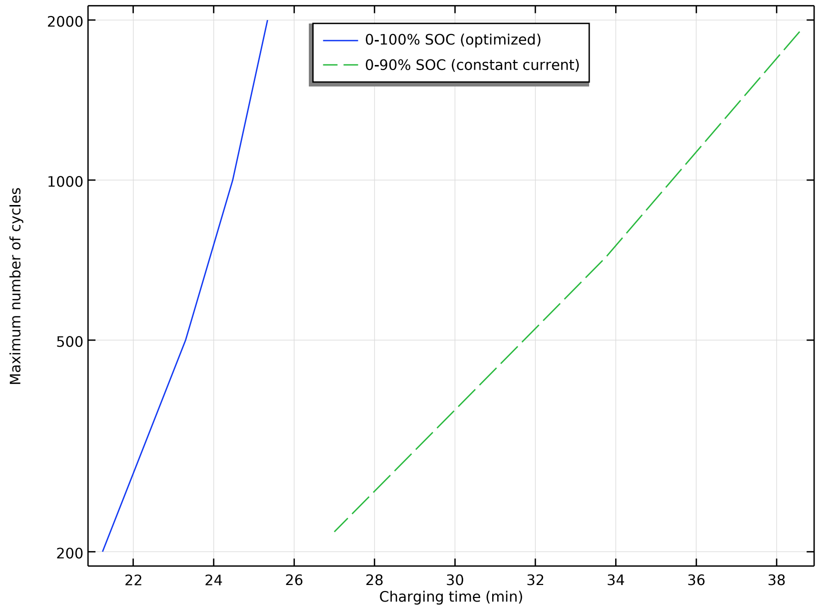


Figure 2: The maximum number of cycles is plotted as a function of the charging time.

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

Modeling Instructions

This example starts from an existing model from the Battery Design Module Application Library.

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_1d** in the tree.

3 Click **Open**.

GLOBAL DEFINITIONS

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
L_pos	70[um]	7E-5 m	Positive electrode thickness

Optimization Parameters

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

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

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

Name	Expression	Value	Description
end_soc	0.9	0.9	State of charge at end of charge
t_1C	end_soc[h]	3240 s	Time required to reach end soc in 1 h
vol_lb	25[mV]	0.025 V	Lower voltage bound
maxCycles	1000[1]	1000	Maximum number of cycles
maxDegradation	10[%]	0.1	Maximum degradation
t	0[s]	0 s	Time
cfunc0	1	1	Initial control function

Use a **Control Function** to optimize the nondimensional charging rate.

DEFINITIONS (COMP1)

Control Function 1 (cfunc1)

1 In the **Definitions** toolbar, click **Control Variables** and choose **Control Function**.

2 In the **Settings** window for **Control Function**, locate the **Output** section.

3 In the f_{max} text field, type 4.

4 In the c_0 text field, type 1.

5 Locate the **Control Variable Discretization** section. From the **Control type** list, choose **Piecewise Bernstein polynomial**.

6 Locate the **Output** section. In the c_0 text field, type `cfunc0`.

7 Locate the **Units** section. Click **Select Input Quantity**.

8 In the **Physical Quantity** dialog, select **General** > **Dimensionless (1)** in the tree.

9 Click **OK**.

Variables 2 - Negative Electrode

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

2 In the **Settings** window for **Variables**, type `Variables 2 - Negative Electrode` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

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

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Unit	Description
eta_aging	phis-phil-vol_lb	V	Overpotential of plating reaction (with added 25 mV margin offset)
i_aging	if(eta_aging<0, 1e4[A/m^3]*(cl[1/M])^0.5*(exp(0.5*eta_aging*F_const/(R_const*T))-exp(-0.5*eta_aging*F_const/(R_const*T))),0)	A/m^3	Parasitic aging current density to use in constraint variable

Domain Probe 1 (dom1)

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

2 In the **Settings** window for **Domain Probe**, type `total_aging_current` in the **Variable name** text field.

3 Locate the **Probe Type** section. From the **Type** list, choose **Integral**.

4 Locate the **Source Selection** section. From the **Selection** list, choose **Negative Electrode**.

5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **i_aging - Parasitic aging current density to use in constraint variable - A/m^3**.

6 Locate the **Expression** section. In the **Expression** text field, type `-i_aging*A_cell`.

LITHIUM-ION BATTERY (LIION)

Electrode Current 1

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

2 Right-click **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** and choose **Electrode Phase** > **Electrode Current**.

3 Select Boundary 4 only.

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

5 From the list, choose **C-rate multiple**.

6 In the C_{rate} text field, type `cfunc1(t*avg_C_rate/t_1C)`.

Using `cfunc1(t*avg_C_rate/t_1C)` instead of `cfunc1(t)` ensures that the entire range of the **Control Function** is utilized.

Load Cycle 1

In the **Model Builder** window, right-click **Load Cycle 1** and choose **Delete**.

Particle Intercalation 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** > **Porous Electrode - Negative** node, then click **Particle Intercalation 1**.

2 In the **Settings** window for **Particle Intercalation**, click to expand the **Particle Discretization** section.

3 Select the **Fast assembly in particle dimension** checkbox to reduce the computational time.

Particle Intercalation 1

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Lithium-Ion Battery (liion)** > **Porous Electrode - Positive** node, then click **Particle Intercalation 1**.

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

3 Select the **Fast assembly in particle dimension** checkbox.

COMPONENT 1 (COMP1)

Add an ODE to compute the parasitic aging charge as the integral of the parasitic aging current.

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 **Mathematics** > **ODE and DAE Interfaces** > **Global ODEs and DAEs (ge)**.

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

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

GLOBAL ODES AND DAES (GE)

Global Equations 1 (ODE1)

1 In the **Settings** window for **Global Equations**, locate the **Global Equations** section.

2 In the table, enter the following settings:

Name	f(u,ut,utt,t) (1)	Initial value (u_0) (1)	Initial value (ut_0) (1/s)	Description
Q_aged	Q_agedt-total_aging_current	0	0	Integrated charge of aging reactions

3 Locate the **Units** section. Click **Define Dependent Variable Unit**.

4 In the **Dependent variable quantity** table, enter the following settings:

Dependent variable quantity	Unit
Custom unit	C

5 Click **Select Source Term Quantity**.

6 In the **Physical Quantity** dialog, select **General** > **Current (A)** in the tree.

7 Click **OK**.

DEFINITIONS (COMP1)

Variables 1 - Global

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Definitions** click **Variables 1**.

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

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

Name	Expression	Unit	Description
constr	Q_aged*maxCycles/maxDegradation/liion.Q_cell		Constraint
avg_C_rate	cfunc1.avg		Average C rate (to be maximized)

This corresponds to allowing a degradation of 10% after 1000 cycles.

STUDY 1

Step 1: Current Distribution Initialization

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Current Distribution Initialization**.

2 In the **Settings** window for **Current Distribution Initialization**, locate the **Physics and Variables Selection** section.

3 In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Global ODEs and DAEs (ge)**.

Step 2: Time Dependent

1 In the **Model Builder** window, 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(0,0.1/cfunc0,0.9/cfunc0)`.

4 Click to expand the **Results While Solving** section. From the **Probes** list, choose **None**.

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

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

7 In the **Study** toolbar, click **= Compute**.

RESULTS

1D Plot Group 7

1 In the **Model Builder** window, expand the **Results** > **1D Plot Group 7** node.

2 Right-click **1D Plot Group 7** and choose **Delete**.

STUDY 1: INITIAL

1 In the **Model Builder** window, click **Study 1: Initial**.

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

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

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

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

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
cfunc0 (Initial control function)	`range(1.4,0.2,2)`	

5 Locate the **Output While Solving** section. From the **Probes** list, choose **None**.

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

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 **Empty Study**.

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 1: INITIAL

Step 1: Current Distribution Initialization, Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 1: Initial**, Ctrl-click to select **Step 1: Current Distribution Initialization** and **Step 2: Time Dependent**.

2 Right-click and choose **Copy**.

STUDY 2

In the **Model Builder** window, right-click **Study 2** and choose **Paste Multiple Items**.

General Optimization

1 In the **Study** toolbar, click **Optimization** and choose **General Optimization**.

2 In the **Settings** window for **General Optimization**, locate the **Optimization Solver** section.

3 From the **Method** list, choose **GCMMA**.

4 From the **Study step** list, choose **Time Dependent**.

5 Click **Add Expression** in the upper-right corner of the **Objective Function** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **comp1.avg_C_rate - Average C rate (to be maximized) - 1**.

6 Locate the **Objective Function** section. From the **Type** list, choose **Maximization**.

7 Select the **Condition-based final time** checkbox.

8 In the **Stop expression** text field, type `t_1C-t*comp1.avg_C_rate`, so that the total charge becomes fixed.

9 Click **Add Expression** in the upper-right corner of the **Constraints** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **comp1.constr - Constraint - 1**.

10 Locate the **Constraints** section. In the table, enter the following settings:

Expression	Lower bound	Upper bound	Evaluate for
comp1.constr		1	Time Dependent

11 Click to expand the **Output** section. From the **Probes** list, choose **None**.

Step 2: Time Dependent

1 In the **Model Builder** window, 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(0,0.01[h],3*t_1C)`.

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

5 In the **Settings** window for **Study**, type `Study 2: Optimization` in the **Label** text field.

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

7 In the **Study** toolbar, click **Get Initial Value**, so that a plot can be setup to be shown while solving.

RESULTS

Control Function

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

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

3 From the **Dataset** list, choose **Study 2: Optimization/Solution 8 (sol8)**.

4 In the **Label** text field, type `Control Function`.

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

6 In the **Title** text area, type `constr = eval(constr)`.

Global 1

1 Right-click **Control Function** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
cfunc1(t*avg_C_rate/t_1C)	1	Control Function

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

5 In the **Expression** text field, type t.

6 From the **Unit** list, choose **min**.

Global 2

1 Right-click **Global 1** and choose **Duplicate**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **total_aging_current - Domain Probe 1 - A**.

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
total_aging_current	A	Parasitic aging current

Global 3

1 In the **Model Builder** window, under **Results** > **Control Function** right-click **Global 1** and choose **Duplicate**.

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

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

4 In the **Control Function** toolbar, click **Plot**.

5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
cfunc1(t*avg_C_rate/t_1C)	1	Initial Control Function

6 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Cycle (reset)**.

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

Global 4

1 In the **Model Builder** window, under **Results** > **Control Function** right-click **Global 2** and choose **Duplicate**.

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

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

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`total_aging_current`	`A`	`Initial parasitic aging current`

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

Control Function

1 In the **Model Builder** window, click **Control Function**.

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

3 Select the **Two y-axes** checkbox.

4 In the table, select the **Plot on secondary y-axis** checkboxes for **Global 2** and **Global 4**.

5 Select the **y-axis label** checkbox. In the associated text field, type `C rate (1)`.

6 Select the **Secondary y-axis label** checkbox. In the associated text field, type `Parasitic aging current (A)`.

STUDY 2: OPTIMIZATION

General Optimization

1 In the **Model Builder** window, under **Study 2: Optimization** click **General Optimization**.

2 In the **Settings** window for **General Optimization**, locate the **Output** section.

3 Select the **Plot** checkbox.

4 In the table, enter the following settings:

Plot group	Plot window
Control Function	Graphics

Solver Configurations

In the **Model Builder** window, expand the **Study 2: Optimization** > **Solver Configurations** node.

Solution 8 (sol8)

1 In the **Model Builder** window, expand the **Study 2: Optimization** > **Solver Configurations** > **Solution 8 (sol8)** > **Optimization Solver 1** > **Time-Dependent Solver 1** node, then click **Advanced**.

2 In the **Settings** window for **Advanced**, click to expand the **Assembly Settings** section.

3 Clear the **Reuse sparsity pattern** checkbox to avoid messages in the log for every reassembly of the sparsity pattern.

Use a **Parametric Sweep** to investigate the relative cost of degradation versus charging rate for optimal charging profiles.

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

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

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
maxCycles (Maximum number of cycles)	200 500 1000 2000	1

5 Locate the **Output While Solving** section. From the **Probes** list, choose **None**.

6 Click to expand the **Advanced Settings** section. Select the **Reuse solution from previous step** checkbox to reduce the computational time.

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

RESULTS

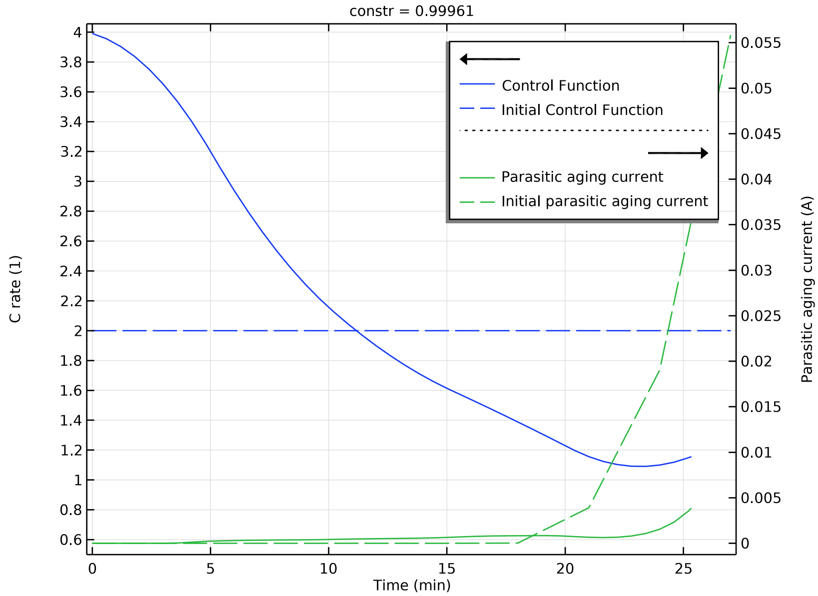
Control Function

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

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

3 In the **y minimum** text field, type `0.5`.

4 In the **Control Function** toolbar, click **Plot**.



Pareto-Optimal Front

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

2 In the **Settings** window for **1D Plot Group**, type `Pareto-Optimal Front` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Optimization/ Parametric Solutions 2 (sol10)**.

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

5 Locate the **Title** section. From the **Title type** list, choose **None**.

6 Locate the **Plot Settings** section.

7 Select the **y-axis label** checkbox. In the associated text field, type `Maximum number of cycles`.

8 Locate the **Axis** section. Select the **y-axis log scale** checkbox.

9 Locate the **Legend** section. From the **Position** list, choose **Upper middle**.

Global 1

1 Right-click **Pareto-Optimal Front** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
maxCycles	1	0-100% SOC (optimized)

4 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **Outer solutions**.

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

6 In the **Expression** text field, type `t_1C/cfunc1.avg`.

7 From the **Unit** list, choose **min**.

8 Select the **Description** checkbox. In the associated text field, type `Charging time`.

9 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Solution** checkbox.

Global 2

1 Right-click **Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 1: Initial/Parametric Solutions 1 (sol3)**.

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

5 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
maxCycles/constr	1	0-90% SOC (constant current)

6 Locate the **x-Axis Data** section. From the **Axis source data** list, choose **All solutions**.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

8 Locate the **x-Axis Data** section. In the **Expression** text field, type `t`.

9 In the **Pareto-Optimal Front** toolbar, click **Plot**.