

# Diffusion-Induced Stress in a Lithium-Ion Battery

## *Introduction*

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Diffusion-induced stress in lithium-ion battery electrode materials can occur as a result of compositional inhomogeneities during lithium intercalation in the host material particles. These stresses are important since the electrode material can undergo significant volume changes during charging and discharging. The accumulated structural changes can induce electrode failure in the form of particle fracture.

In order to quantify the stress generated in the electrode, the elastic deformation of the material must be related to the intercalation process. Since atomic diffusion in solids is a much slower process than elastic deformation, mechanical equilibrium is established much faster than that of diffusion. Hence, mechanical equilibrium can be treated as a static equilibrium problem ([Ref. 1](#) and [Ref. 2](#)).

This tutorial models diffusion-induced stress caused by concentration changes within the negative host material electrode particles during discharge and relaxation of a lithium-ion battery. The radial and tangential components of stress (considering spherical particles in the negative electrode) and von Mises stress inside a particle in the negative electrode are analyzed. It is seen that, during discharge, the von Mises stress is 0 at the center and reaches a maximum value at the surface of the particle. Similarly, the time evolution of radial and tangential components of the diffusion-induced strain at surface of particles along the length of the negative electrode is analyzed during discharge and relaxation. During de-intercalation of lithium ions from the negative electrode particles (discharge), the diffusion-induced surface strain decreases with time. Finally, the behavior and time evolution of the total elastic strain energy density stored in the negative electrode material particles is analyzed. Note that this quantity provides the driving force for particle fracture.

## *Model Definition*

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The model is set up for a graphite/NMC battery cell, using the Lithium-Ion Battery interface. More background to the base model can be found in [Lithium-Ion Battery Base Model in 1D](#).

The tutorial analyses diffusion-induced stress and strain generated in the negative electrode particles. Assuming the electrode particles to be isotropic linear elastic solids, analytical expressions are calculated at the Particle Intercalation node of the Porous Electrode feature, for several quantities such as stress, hydrostatic stress, von Mises stress, strain, total elastic strain energy density, and so on. These expressions require the relative change in volume of the graphite electrode material, which is typically a function of concentration (that is, state-of-charge) in the particle. For example, graphite material has

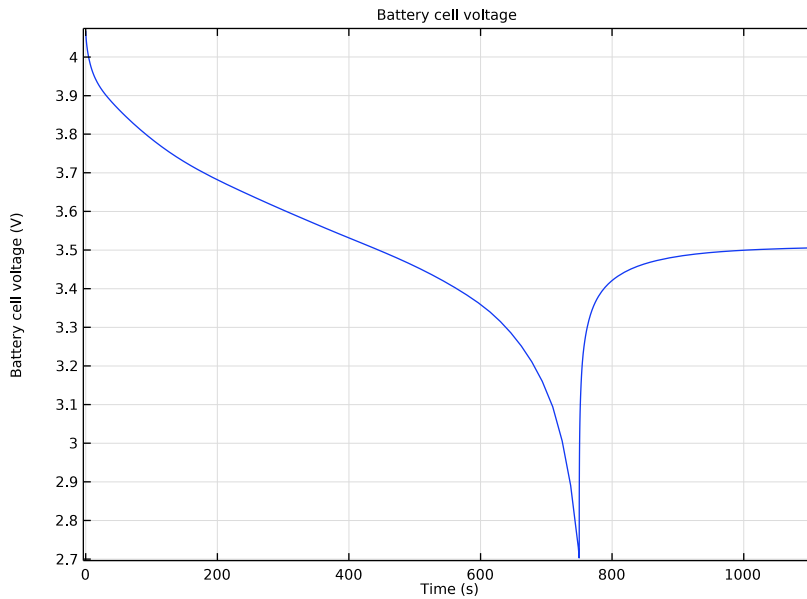
a volumetric expansion of about 10% over state-of-charge values ranging from 0 to 1. Additionally, the stress and strain expressions require elastic properties such as the Young's modulus and Poisson's ratio (note that these elastic properties are assumed to be independent of concentration).

The applied current consists of a discharge current of 4 C that is applied for 750 s, followed by a relaxation period of 350 s.

## Results and Discussion

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The battery cell voltage profile is plotted as a function of time in [Figure 1](#).



*Figure 1: Battery cell voltage profile as a function of time.*

[Figure 2](#) shows the normalized lithium concentration in a particle at a particular position (center) in the negative electrode, at various times during discharge and relaxation. Note in all subsequent plots, the solid and dashed lines refer to the discharge and relaxation periods, respectively. During discharge, which involves de-intercalation of lithium ions from the negative electrode particles, it can be seen that the concentration in the particle

decreases with time. At the end of the relaxation period, the concentration settles at a final value.

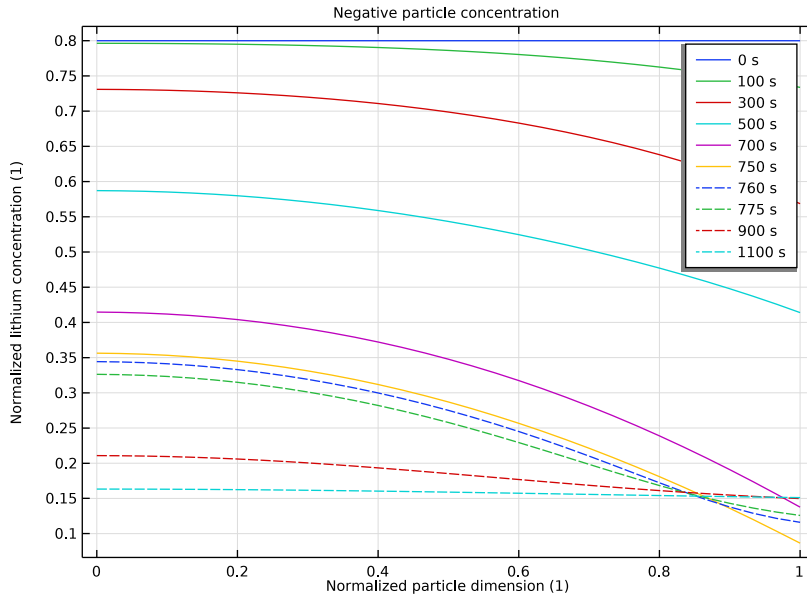


Figure 2: Normalized lithium concentration in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

The radial component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge and relaxation, is shown in Figure 3. During discharge (de-intercalation of lithium ions from the particle), the radial stress is compressive inside the spherical particle. At any given time, the compressive radial stress is

highest at the center and decreases monotonically to 0 at the surface of the particle. During the relaxation period, the compressive radial stress inside the particle relaxes to 0.

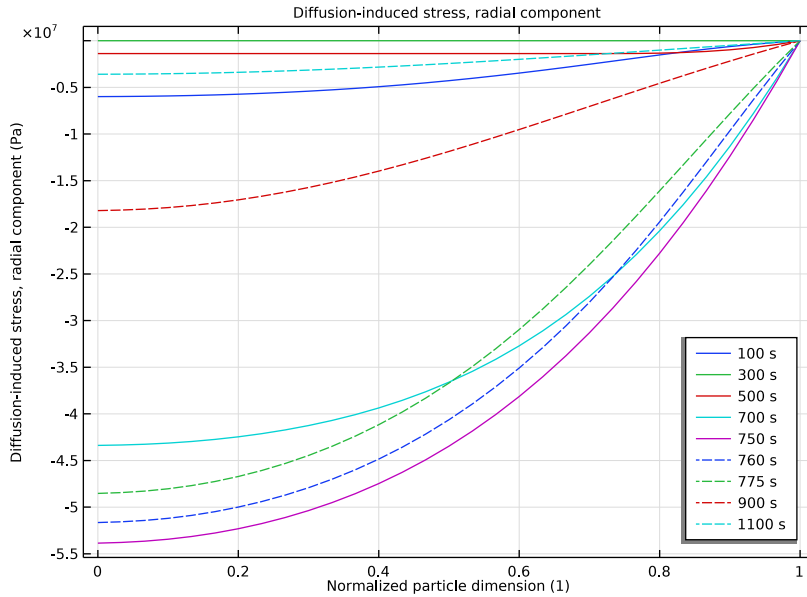


Figure 3: Radial component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

Similarly, Figure 4 shows the tangential component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge and relaxation. During discharge, the tangential stress is compressive at the center and tensile at the surface of the spherical particle. Note that at the center of the particle, the tangential and radial stresses always have the same magnitude so that the stress state at the center of

the particle is purely hydrostatic. The crossover from compressive to tensile occurs at  $r = 1/\sqrt{2}$ , after the stress reaches steady state.

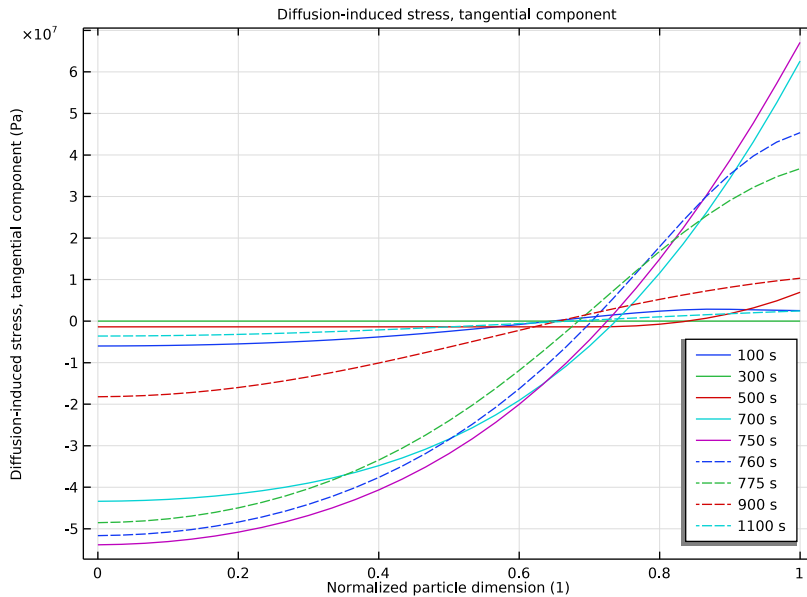


Figure 4: Tangential component of the diffusion-induced stress in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

Figure 5 shows the von Mises stress in a particle at the center of the negative electrode, at various times during discharge and relaxation. During discharge, the von Mises stress is 0

at the center of the particle and reaches a maximum value at the surface of the spherical particle. During the relaxation period, the stress inside the particle relaxes to 0.

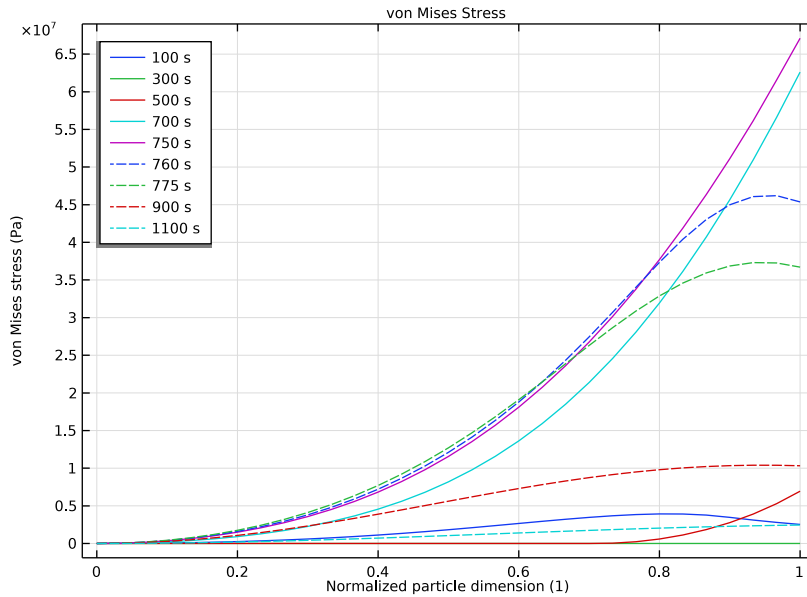


Figure 5: von Mises stress in a particle at the center of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

Figure 6 and Figure 7 show the radial and tangential components, respectively, of the diffusion-induced strain at surface of particles along the length of the negative electrode, at various times during discharge and relaxation. During de-intercalation of lithium ions from the particle, the surface strain decreases with time in the negative electrode. Also, the surface value of strain is not uniform across the electrode because of variation in particle concentration across the electrode. The maximum value of surface strain is observed at the

current collector end. At the end of the relaxation period, the strain eventually reaches a value corresponding to the final particle concentration.

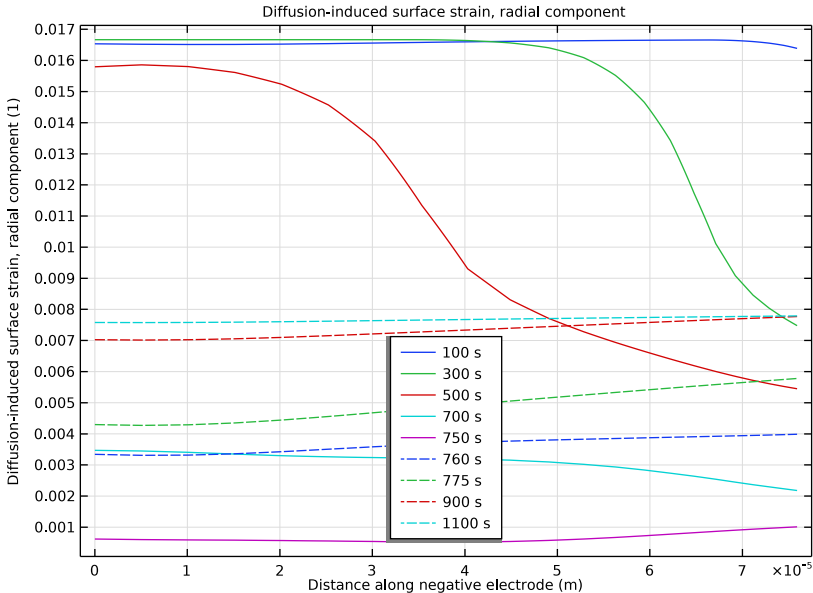


Figure 6: Radial component of diffusion-induced surface strain along the length of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).



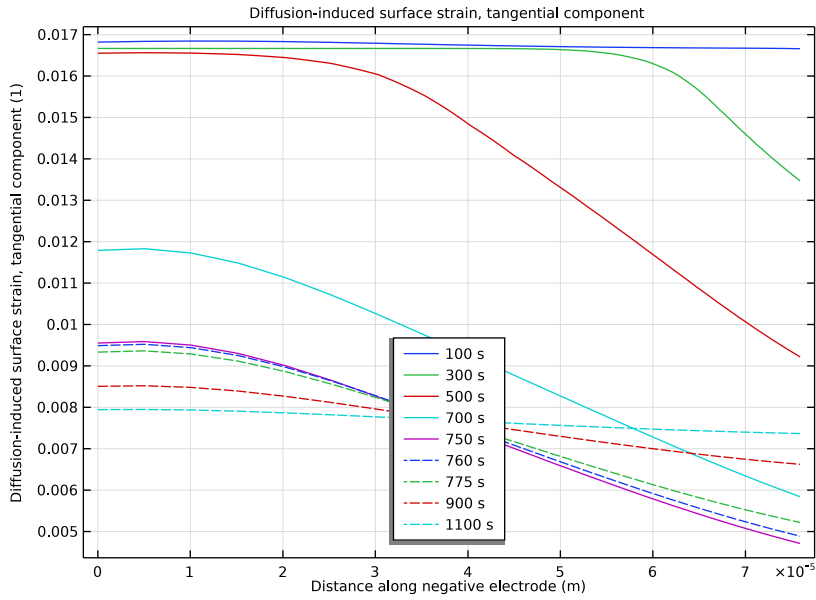
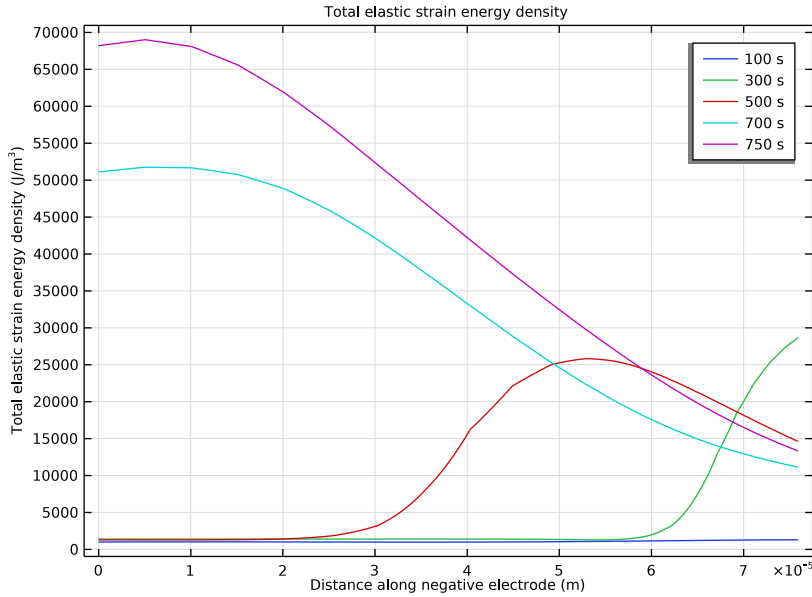


Figure 7: Tangential component of diffusion-induced surface strain along the length of the negative electrode, at various times during discharge (solid lines) and relaxation (dashed lines).

The total elastic strain energy density that is stored in the negative electrode material particles provides the driving force for particle fracture. This quantity is plotted along the

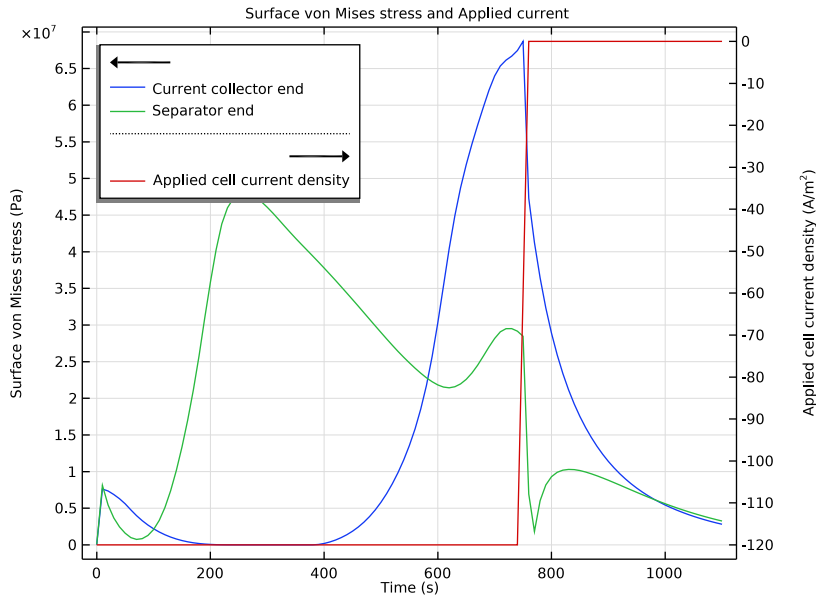
length of the negative electrode in [Figure 8](#), at various times during discharge. The maximum value is observed near the current collector end at the end of discharge.



*Figure 8: Total elastic strain energy density stored in the negative electrode material particles, plotted along the length of the negative electrode, at various times during discharge.*

All the above plots show a quantity plotted either across the particle dimension or along the length of the negative electrode, at various times during discharge. Alternatively, it is useful to plot the time evolution of any quantity at different positions in the negative electrode. The von Mises stress at the surface of particles at two positions in the negative electrode (current collector end and separator end) is plotted versus time in [Figure 9](#). The plot also includes the applied current for reference. The von Mises stress contains contribution from both the radial and tangential components of the diffusion-induced stress. As seen from [Figure 3](#) and [Figure 4](#), the surface value of the radial component of the diffusion-induced stress is 0. So, the surface von Mises stress essentially mimics the behavior of the tangential component of the diffusion-induced surface stress. In [Figure 9](#), it can be seen that the von Mises stress initially increases at the separator end and subsequently at the current collector end. The stress induced in the electrode particles varies at different positions along the negative electrode due to concentration gradients in the porous electrode. Similarly, it can be expected that the total elastic strain density, that provides the driving force for fracture, also varies at different positions along the negative

electrode. It can be seen in [Figure 9](#) that the surface von Mises stress is higher at the current collector end as compared to the separator end, toward the end of the discharge period. Finally, the stress in the particles relaxes to 0 during the relaxation period.



*Figure 9: Time evolution of the von Mises stress at the surface of the particles at two positions in the negative electrode. The applied current is also plotted for reference.*

## References

1. Y-T. Cheng, and M.W. Verbrugge, "Evolution of stress within a spherical insertion electrode particle under potentiostatic and galvanostatic operation," *Journal of Power Sources*, vol. 190, pp. 453–460, 2009.
2. V. Malave, J.R. Berger, and P.A. Martin, "Concentration-dependent chemical expansion in lithium-ion battery cathode particles," *Journal of Applied Mechanics*, vol. 81, pp. 091005 1–9, 2014.

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**Application Library path:** Battery\_Design\_Module/Batteries,\_Lithium-Ion/  
diffusion\_induced\_stress

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### ROOT

Start this tutorial by opening a template file that contains a 1D battery model. Alternatively, you may build the template model yourself by following the instructions found in the template model.

### APPLICATION LIBRARIES

- 1 From the **File** menu, choose **Application Libraries**.
- 2 In the **Application Libraries** window, select **Battery Design Module>Batteries, Lithium-Ion>lib\_base\_model\_Id** 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
soc_init	100[%]	I	Initial SOC
E	10[GPa]	IE10 Pa	Young's modulus

#### Step 1 (step1)

Define a step function that will be used later to set up the applied current.

- 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 **From** text field, type 1.
- 4 In the **To** text field, type 0.

### COMPONENT 1 (COMP1)

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

## DEFINITIONS (COMPI)

### Variables I

- 1 In the **Model Builder** window, expand the **Component I (comp1)>Definitions** node, then click **Variables I**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 In the table, enter the following settings:

Name	Expression	Unit	Description
I_app	$(-I_{1C} \cdot 4) \cdot \text{step1}((t - 750)[1/s])$	A/m <sup>2</sup>	Applied cell current density

## LITHIUM-ION BATTERY (LIION)


### Electrode Current Density I

- 1 In the **Model Builder** window, expand the **Component I (comp1)>Lithium-Ion Battery (liion)** node, then click **Electrode Current Density I**.
- 2 In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.
- 3 In the  $i_{n,s}$  text field, type I\_app.

## GLOBAL DEFINITIONS

### Relative volume change as function of soc

Define an interpolation function that defines the relative expansion of graphite material as a function of state-of-charge.

- 1 In the **Home** toolbar, click  **Functions** and choose **Global>Interpolation**.
- 2 In the **Settings** window for **Interpolation**, type Relative volume change as function of soc in the **Label** text field.
- 3 Locate the **Definition** section. In the table, enter the following settings:

t	f(t)
0	0
0.5	0.05
0.75	0.05
1	0.1

- 4 In the **Function name** text field, type fvol.

5 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Piecewise cubic**.

6 Locate the **Units** section. In the **Argument** table, enter the following settings:

Argument	Unit
t	1

7 In the **Function** table, enter the following settings:

Function	Unit
fvol	1

## LITHIUM-ION BATTERY (LIION)

### *Porous Electrode - Negative*

The physics has already been set up in the template model. Next, set up the inputs required for stress and strain calculations in the **Particle Intercalation** node of the porous electrode domain corresponding to the negative electrode (graphite material). Also, specify the reference exchange current density for the electrode kinetics in the **Porous Electrode Reaction** nodes of the negative and positive electrodes. Finally, specify the applied current (that corresponds to a discharge current of 4C for 850 s followed by a relaxation period for the next 250 s) in the **Electrode Current** node.

### *Particle Intercalation I*

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

2 In the **Settings** window for **Particle Intercalation**, click to expand the **Stress and Strain** section.

3 Select the **Calculate stress and strain** check box.

The negative electrode material (graphite) has built-in properties for Young's modulus and Poisson's ratio, that are functions of the solid phase concentration. However, the stress-strain expressions in the **Particle Intercalation** node assumes that these elastic properties are independent of concentration. Hence, concentration-independent values are set for these elastic properties.

4 In the  $E$  text field, type E.


5 In the  $\Delta V/V_0$  text field, type `fvol(liion.cs_pce1/liion.csmax)`.

It is essential to have a finer resolution along the graphite particle dimension and this can be done by setting a linear distribution with 30 elements.

- 6 Click to expand the **Particle Discretization** section. From the **Distribution** list, choose **Linear**.
- 7 In the  $N_{el}$  text field, type 30.

## STUDY I


### *Step 1: Time Dependent*

- 1 In the **Model Builder** window, expand the **Study I** node, then click **Step 1: 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 range(0,10,1100).
- 5 In the **Model Builder** window, click **Study I**.
- 6 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 7 Clear the **Generate default plots** check box.
- 8 In the **Home** toolbar, click  **Compute**.

## RESULTS

### *Battery cell voltage*

The probe plot show the battery cell voltage (Figure 1).

- 1 In the **Model Builder** window, under **Results** click **Probe Plot Group 1**.
- 2 In the **Settings** window for **ID Plot Group**, type Battery cell voltage in the **Label** text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **Label**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **y-axis label** check box. In the associated text field, type Battery cell voltage (V).
- 6 Locate the **Legend** section. Clear the **Show legends** check box.
- 7 In the **Battery cell voltage** toolbar, click  **Plot**.

### *Study 1/Solution 1 (sol1)*


To plot along the graphite particle dimension, you need to create a Solution dataset that refers to the extra dimension that is set up by the Porous Electrode node corresponding to the negative electrode.

### *Study 1/Solution 1 (3) (sol1)*

- 1 In the **Model Builder** window, expand the **Results>Datasets** node.
- 2 Right-click **Results>Datasets>Study 1/Solution 1 (sol1)** and choose **Duplicate**.
- 3 In the **Settings** window for **Solution**, locate the **Solution** section.
- 4 From the **Component** list, choose  
**Extra Dimension from Particle Intercalation 1 (liion\_pce1\_pin1\_xdim)**.

### *Negative particle concentration*

Next, follow the steps below to plot the normalized lithium concentration in a particle at a particular position (say center) in the negative electrode, at various times during discharge and relaxation. Note in all the subsequent plots in the model, the solid and dashed lines refer to the discharge period and the relaxation period, respectively. (Figure 2).

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type **Negative particle concentration** in the **Label** text field.

### *Line Graph 1*


- 1 Right-click **Negative particle concentration** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Solution 1 (3) (sol1)**.
- 4 From the **Time selection** list, choose **Interpolated**.
- 5 In the **Times (s)** text field, type 0, 100, 300, 500, 700, 750.
- 6 Locate the **Selection** section. From the **Selection** list, choose **All domains**.
- 7 Locate the **y-Axis Data** section. In the **Expression** text field, type `comp1.atxd1 (15e-6, liion.cs_pce1/liion.csmax)`.
- 8 Click to expand the **Legends** section. Select the **Show legends** check box.

### *Line Graph 2*

- 1 Right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 In the **Times (s)** text field, type 760, 775, 900, 1100.
- 4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 5 From the **Color** list, choose **Cycle (reset)**.



### *Negative particle concentration*

- 1 In the **Model Builder** window, click **Negative particle concentration**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **Label**.
- 4 Locate the **Plot Settings** section.
- 5 Select the **x-axis label** check box. In the associated text field, type Normalized particle dimension (1).
- 6 Select the **y-axis label** check box. In the associated text field, type Normalized lithium concentration (1).
- 7 In the **Negative particle concentration** toolbar, click  **Plot**.

Now, create a plot of the radial component of the diffusion-induced stress in a particle (Figure 3) at the center of the negative electrode, at various times during discharge and relaxation. This can be done by duplicating the previous plot.

### *Diffusion-induced stress, radial component*

- 1 Right-click **Negative particle concentration** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Diffusion-induced stress, radial component in the **Label** text field.
- 3 Locate the **Plot Settings** section. In the **y-axis label** text field, type Diffusion-induced stress, radial component (Pa).


### *Line Graph 1*

- 1 In the **Model Builder** window, expand the **Diffusion-induced stress, radial component** node, then click **Line Graph 1**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 In the **Times (s)** text field, type 100, 300, 500, 700, 750.
- 4 Locate the **y-Axis Data** section. In the **Expression** text field, type `comp1.atxd1(15e-6, liion.sr_pce1)`.
- 5 Click to expand the **Quality** section. From the **Resolution** list, choose **No refinement**.

### *Line Graph 2*

- 1 In the **Model Builder** window, click **Line Graph 2**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `comp1.atxd1(15e-6, liion.sr_pce1)`.
- 4 Locate the **Quality** section. From the **Resolution** list, choose **No refinement**.

#### *Diffusion-induced stress, radial component*

- 1 In the **Model Builder** window, click **Diffusion-induced stress, radial component**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Lower right**.
- 4 In the **Diffusion-induced stress, radial component** toolbar, click  **Plot**.

Now, create a plot of the tangential component of the diffusion-induced stress in a particle (Figure 4) at the center of the negative electrode, at various times during discharge and relaxation. This can be done by duplicating the previous plot.

#### *Diffusion-induced stress, tangential component*

- 1 Right-click **Diffusion-induced stress, radial component** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Diffusion-induced stress, tangential component in the **Label** text field.
- 3 Locate the **Plot Settings** section. In the **y-axis label** text field, type Diffusion-induced stress, tangential component (Pa).


#### *Line Graph 1*

- 1 In the **Model Builder** window, expand the **Diffusion-induced stress, tangential component** node, then click **Line Graph 1**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `comp1.atxd1(15e-6,liion.stheta_pce1)`.

#### *Line Graph 2*

- 1 In the **Model Builder** window, click **Line Graph 2**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `comp1.atxd1(15e-6,liion.stheta_pce1)`.

#### *Diffusion-induced stress, tangential component*

- 1 In the **Model Builder** window, click **Diffusion-induced stress, tangential component**.
- 2 In the **Diffusion-induced stress, tangential component** toolbar, click  **Plot**.

Now, create a plot of the von Mises stress in a particle (Figure 5) at the center of the negative electrode, at various times during discharge and relaxation. This can be done by duplicating the previous plot.

#### *von Mises Stress*

- 1 Right-click **Diffusion-induced stress, tangential component** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type von Mises Stress in the **Label** text field.

- 3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `von Mises stress (Pa)`.


#### *Line Graph 1*

- 1 In the **Model Builder** window, expand the **von Mises Stress** node, then click **Line Graph 1**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `comp1.atxd1(15e-6,liion.mises_pce1)`.

#### *Line Graph 2*


- 1 In the **Model Builder** window, click **Line Graph 2**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 In the **Expression** text field, type `comp1.atxd1(15e-6,liion.mises_pce1)`.

#### *von Mises Stress*

- 1 In the **Model Builder** window, click **von Mises Stress**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Upper left**.
- 4 In the **von Mises Stress** toolbar, click  **Plot**.

Next, create a plot of the radial component of the diffusion-induced surface strain (Figure 6) along the length of the negative electrode.

#### *Diffusion-induced surface strain, radial component*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type `Diffusion-induced surface strain, radial component` in the **Label** text field.


#### *Line Graph 1*

- 1 Right-click **Diffusion-induced surface strain, radial component** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Solution 1 (1) (sol1)**.
- 4 From the **Time selection** list, choose **Interpolated**.
- 5 In the **Times (s)** text field, type `100,300,500,700,750`.
- 6 Select Domain 1 only.
- 7 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Lithium-Ion Battery>Stress and strain>liion.er\_surface\_pce1 - Diffusion-induced surface strain, radial component**.
- 8 Locate the **Legends** section. Select the **Show legends** check box.

### *Line Graph 2*

- 1 Right-click **Line Graph 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 In the **Times (s)** text field, type 760, 775, 900, 1100.
- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 5 From the **Color** list, choose **Cycle (reset)**.

### *Diffusion-induced surface strain, radial component*

- 1 In the **Model Builder** window, click **Diffusion-induced surface strain, radial component**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **Manual**.
- 4 In the **Title** text area, type Diffusion-induced surface strain, radial component.
- 5 Locate the **Plot Settings** section.
- 6 Select the **x-axis label** check box. In the associated text field, type Distance along negative electrode (m).
- 7 Locate the **Legend** section. From the **Position** list, choose **Lower middle**.
- 8 In the **Diffusion-induced surface strain, radial component** toolbar, click  **Plot**.

Next, create a plot of the tangential component of the diffusion-induced surface strain (Figure 7) along the length of the negative electrode. This can be done by duplicating the previous plot.

### *Diffusion-induced surface strain, tangential component*

- 1 Right-click **Diffusion-induced surface strain, radial component** and choose **Duplicate**.
- 2 In the **Settings** window for **ID Plot Group**, type Diffusion-induced surface strain, tangential component in the **Label** text field.
- 3 Locate the **Title** section. In the **Title** text area, type Diffusion-induced surface strain, tangential component.

### *Line Graph 1*


- 1 In the **Model Builder** window, expand the **Diffusion-induced surface strain, tangential component** 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)>Lithium-**

**Ion Battery>Stress and strain>liion.etheta\_surface\_pce I - Diffusion-induced surface strain, tangential component.**

#### *Line Graph 2*


- 1 In the **Model Builder** window, click **Line Graph 2**.
- 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 (comp 1)>Lithium-Ion Battery>Stress and strain>liion.etheta\_surface\_pce I - Diffusion-induced surface strain, tangential component**.

#### *Diffusion-induced surface strain, tangential component*

- 1 In the **Model Builder** window, click **Diffusion-induced surface strain, tangential component**.
- 2 In the **Diffusion-induced surface strain, tangential component** toolbar, click  **Plot**.

#### *Total elastic strain energy density*

Next, create a plot of the total elastic strain energy density stored in the negative electrode material particles (Figure 8) along the length of the negative electrode.


- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Total elastic strain energy density in the **Label** text field.

#### *Line Graph 1*

- 1 Right-click **Total elastic strain energy density** and choose **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Study 1/Solution 1 (I) (sol1)**.
- 4 From the **Time selection** list, choose **Interpolated**.
- 5 In the **Times (s)** text field, type 100, 300, 500, 700, 750.
- 6 Select Domain 1 only.
- 7 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp 1)>Lithium-Ion Battery>Stress and strain>liion.Ws\_tot\_pce I - Total elastic strain energy density - J/m<sup>3</sup>**.
- 8 Locate the **Legends** section. Select the **Show legends** check box.


#### *Total elastic strain energy density*

- 1 In the **Model Builder** window, click **Total elastic strain energy density**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **Label**.

- 4 Locate the **Plot Settings** section.
- 5 Select the **x-axis label** check box. In the associated text field, type **Distance along negative electrode (m)**.
- 6 In the **Total elastic strain energy density** toolbar, click  **Plot**.

#### *Surface von Mises stress versus time*

Finally, create a plot that shows the time evolution of the von Mises stress at the surface of the particles (Figure 9) at two positions in the negative electrode (current collector end and separator end). Also include the applied current on the same plot for reference.

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type **Surface von Mises stress versus time** in the **Label** text field.

#### *Point Graph 1*

- 1 Right-click **Surface von Mises stress versus time** and choose **Point Graph**.
- 2 Select **Boundaries 1** and **2** only.
- 3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Lithium-Ion Battery>Stress and strain>liion.mises\_surface\_pcel - Surface von Mises stress - Pa**.
- 4 Click to expand the **Legends** section. Select the **Show legends** check box.
- 5 From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:


<b>Legends</b>
Current collector end
Separator end

#### *Global 1*

- 1 In the **Model Builder** window, right-click **Surface von Mises stress versus time** and choose **Global**.
- 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> Variables>I\_app - Applied cell current density - A/m<sup>2</sup>**.

#### *Surface von Mises stress versus time*

- 1 In the **Model Builder** window, click **Surface von Mises stress versus time**.

- 2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.
- 3 Select the **Two y-axes** check box.
- 4 In the table, select the **Plot on secondary y-axis** check box for **Global I**.
- 5 Locate the **Title** section. From the **Title type** list, choose **Manual**.
- 6 In the **Title** text area, type **Surface von Mises stress and Applied current**.
- 7 Locate the **Legend** section. From the **Position** list, choose **Upper left**.
- 8 In the **Surface von Mises stress versus time** toolbar, click  **Plot**.

