

# Cell Resolved Matlab® OOP Model of a Lithium Iron Phosphate Battery Pack

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# **Abbreviations**

**OO** object oriented

**OOP** object oriented programming

# **List of Symbols**

Symbol	Unit	Description
$C_{\sf dis}$	Ah	discharge capacity
DoD	-	depth of discharge
F	As/mol	Faraday constant
I	Α	Current
SoC	%	state of charge
R	$J/(mol\cdotK)$	universal gas constant
rmse	various	root mean squared error
T	K or $^{\circ}$ C	temperature
V	V	voltage
$z_{Li}$	-	ionic charge number of lithium



## 1 Discharge curves

Many battery data sheets provide measured discharge curves, on which the charging and discharging behaviour of this model is based. Rather than determining the curves according to the internal impedance, a common approach [1], this model determins the curves directly by means of digitizing the images and creating a curve fit. The classes used for fitting and modelling the discharge curves are described in the following subsections.

### 1.1 Single discharge curve

For modelling a single discharge curve, the class dischargeFit is used, which implements the interface curveFitInterface. The curve is fitted according to [2], using a function that is loosely based on the Nernst equation with two exonential functions superimposed as a correction for the voltage drops at the beginning and end of the curve.

$$V(SoC) = x_1 - \frac{R \cdot T}{z_{\text{Li}} \cdot F} \cdot ln\left(\frac{SoC}{1 - SoC}\right) + x_2 \cdot SoC + x_3$$
$$+ (x_4 + (x_5 + x_4 \cdot x_6) \cdot SoC) \cdot exp(-x_6 \cdot SoC)$$
$$+ x_7 \cdot exp(-x_8 \cdot SoC)$$
(1)

where  $x_1, ..., x_8$  are the fit parameters,  $R=8.3144598 \text{ J/(mol} \cdot \text{K)}$  is the universal gas constant,  $z_{\text{Li}}=1$  is the ionic charge number of lithium, F=96485.3328959 As/mol is the Faraday constant, SoC is the state of charge, V is the voltage in V and T is the temperature in K at which the curve was recorded. The curves are fitted using the levenberg-marquardt algorithm and either the <code>lsqcurvefit</code> method, the <code>fminsearch</code> method or a combination of both, depending on the user's preference.

#### 1.1.1 Creation of a dischargeFit object

A dischargeFit object is created with the digitized raw data - the voltage V in V, the discharge capacity  $C_{\text{dis}}$  in Ah, the current I in A at which the curve was recorded and the temperature T in K at which the curve was recorded.

```
1 d = dischargeFit(V, C_dis, I, T);
```

V and C\_dis are vectors containing the digitized raw data from the data sheet. Further options, such as initial values for the fit parameters  $x_1, ..., x_8$  and the fit method can be passed to the constructor using Matlab's name-value pair syntax:

```
1 d = dischargeFit(V, C_dis, I, T, 'OptionName', OptionValue);
```

By default, the initial fit parameters are set to zero and the curve is fit by first using lsqcurvefit, followed by fminsearch. The initial fit parameters are stored in a vector x0

Section describing interface, etc.



of length 8, which can be passed via the option name 'x0', for example using the following syntax:

```
1 x0 = ones(8, 1);
2 d = dischargeFit(V, C_dis, I, T, 'x0', x0);
```

The method used for the curve fitting can be passed to the constructor using the option name 'mode'. The corresponding value must be one of the following three strings:

- 'lsq' for lsqcurvefit
- 'fmin' for fminsearch
- 'both' for lsqcurvefit followed by another fit using fminsearch

e.g.

```
1 d = dischargeFit(V, C_dis, I, T, 'mode', 'fmin');
2 d.plotResults
```

Depending on the curve and on the technology, one of the methods may return a better result.

#### 1.1.2 Visual validation

A visual validation can be performed by calling the class's plotResults method (see above). In Figure 1, the results of two dischargeFit objects using the same raw data are compared.

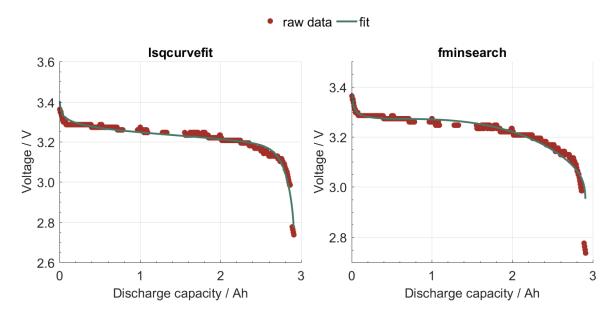


Figure 1: Fit results of the dischargeFit class using the fit methods lsqcurvefit and fminsearch, respectively. The raw data was extracted from [3].





**Figure 2:** Fit results of the dischargeFit class using the fit mode 'both' with the default parameter initialization (left) and with a custom parameter initialization (right). The raw data was extracted from [3].

In this example, 'lsq' appears to return better results for the voltage drop at the end of the curve, while 'fmin' results in a more precise fit for the voltage drop at the beginning of the curve. Further differences can be seen in the fits' curvatures. The 'lsq' option results in a slightly flatter curve than the 'fmin' mode. The results of a dischargeFit object using the 'both' option are presented in Figure 2. Using the default fit parameter initialization of zeros (left) appears to improve the curvature and voltage drops slightly, compared to the other modes. Further improvements can be made by passing custom initial fit parameters to the constructor via the option 'x0' (see Figure 2, right).

#### 1.1.3 Object properties

Further fit quality analysis can be performed via the mean difference in voltage between the raw data and the curve fit at the respective positions of the raw data  $\overline{\Delta V}$  in V and the maximum difference between the raw data and the curve fit at the respective positions  $\Delta V_{\rm max}$  in V. Additionally, every curve fit class (i.e. dischargeCurves, woehlerFit, etc.) in this package implements the curveFitInterface, which contains the root mean square error rmse as a property. The rmse for a curve fit with the raw data  $y_{\rm raw}$  and the fitted data  $y_{\rm fit}$  at the same respective x coordinates is defined as

$$rmse = \sqrt{\frac{\sum_{i=1}^{n} (|y_{\mathsf{raw},i} - y_{\mathsf{fit},i}|)^2}{n}} \tag{2}$$

where i is the index of the measurement and n is the number of measurements. In the case of a dischargeFit object,  $y_{\text{raw},i}$  is the measured voltage at the discharge capacity  $C_{\text{dis},i}$  and  $y_{\text{fit},i}$  is the fitted voltage at  $C_{\text{dis},i}$ . Often used for forecasting models, the rmse provides



	Table 1:	: Accessible	properties	of the	discharc	geFit. <b>cla</b> :	SS.
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Name	Description	Unit	Set access
Х	8x1 vector of fit parameters	-	public
dV_mean	Mean voltage difference between raw data and fit	V	read only
dV_max	Max voltage difference between raw data and fit	V	read only
T	Temperature at which the curve was recorded	K	immutable
Z	Current of the curve	Α	immutable
mode	Method used for fitting ('fmin', 'lsq' or 'both')	-	public
rmse	Root mean square error	V	read only

a good measure of accuracy when comparing two models of the same data set [4]. In the previous examples, the curve fit using the 'lsq' method (Figure 1, left) has an rmse of 0.0244 V. Using the 'fmin' mode (Figure 1, right) improves the rmse to a value of 0.0162 V and using the fit mode 'both' (Figure 2, left) further improves it to 0.0157 V. The lowest rmse (0.0106 V) is achieved with the custom fit parameter initialization (Figure 2, right). A list of the class's accessible properties is provided in Table 1. The z property is inherited from the curveFitInterface. Setting the x or mode properties will cause the object to re-run the fitting algorithm, thus likely resulting in different values for x than were set by the user.

#### 1.1.4 Usage of a dischargeFit object

In order to calculate a voltage for a given discharge capacity, the object can be treated like a function handle, by using subsref indexing.

```
1 d = dischargeFit(V, C_dis, I, T, 'mode', 'fmin');
2 Cd = 1.5; % Discharge capacity in Ah
3 V = d(Cd); % Voltage in V
4 Cd_vect = linspace(0, 3, 1000); % Vector of discharge capacities in Ah
5 V_vect = d(Cd_vect); % Corresponding vector of voltages in V
```

A dischargeFit object is not accessed directly by the battery model, but rather stored in a dischargeCurves object. After creating a dischargeFit, it can be added to a dischargeCurves collection by using the add() method (see section 1.2). Alternatively, it can be added directly to a subclass of the batteryInterface (see section) using it's addcurves() method.

section ref



#### 1.2 Collection of discharge curves

A single discharge curve can be used to model the behaviour of a battery for a given current. However, in reality, a battery will often be charged or discharged with different currents. In many cases, the current may change from one simulation time step to another. In order to be able to determine the voltage as a function of  $C_{\rm dis}$  and I, multiple dischargeFit objects are wrapped by a dischargeCurves object, which is described in the following sections.

#### 1.2.1 Creation of a dischargeCurves object

There are two ways to initialize a dischargeCurves object. The first option is to create an empty object and using the class's dischargeFit() method to add curve fits. The dischargeFit() method has the same syntax as the dischargeFit class's constructor.

```
1 dC = dischargeCurves;
2 I = [0.6; 1; 3; 5; 10; 20]; % Vector of currents in A
3 T = 293; % Temperature in K
4 for i = 1:6
5     dC.dischargeFit(raw(i).V, raw(i).Cd, I(i), T)
6 end
7 % raw is a struct array containing the measured curve data
8 % from the data sheet.
```

This option has the advantage of reducing clutter in the workspace. However, changing the parameters and analysing the accuracy of the individual curve fits is more complicated. Alternatively, the dischargeFit objects can be created, modified and then passed to the dischargeCurves constructor.

If a dischargeFit is passed to a dischargeCurves object that already holds a reference to a dischargeFit with the same current, the stored reference is replaced by the new one. Similarly, if two or more dischargeFit objects with the same current are passed to a dischargeCurves constructor, the first one is ignored.



#### 1.2.2 Interpolation between curves

The calculation of the voltage for any given current and discharge capacity is done via Matlab's built-in griddedInterpolant class, which is called from within the interp() method. The syntax for a dischargeCurves object dC is as follows:

```
1 V = dC.interp(I, Cd);
2 V = interp(dC, I, Cd); % equivalent
```

Where V is the voltage in V, I is the charging or discharging current in A and Cd is the discharge capacity after charging or discharging in Ah. If I is equal to one of the stored dischargeFit objects' currents, Cd is simply passed on to the respective object, which returns the voltage. If I does not match any of the stored objects and either of the input arguments is not found in the object's cache, Cd is passed on to each of the stored dischargeFit references, creating a vector of voltages for the different currents. Finally, a griddedInterpolant is created using the sample points, I is passed to it and the interpolated voltage is returned and cached. The interpolation method (the default is 'spline') can be changed by setting the property interpMethod.

A visual validation of the interpolation using the 'linear' and 'spline' methods, respectively, is depicted in Figure 3. A collection of dischargeFit objects for six currents was created and the fit results were plotted. Then, all fits except for the one at 10 A were added to a dischargeCurves object. Finally, the interp() method was called for a current of 10 A and a range of discharge capacities, in an attempt to replicate the dischargeFit results using interpolation. The linearly interpolated curve (Figure 3, left) is almost identical to the fit until the beginning of the voltage drop at the end. However, the spline interpolation results



**Figure 3:** Comparison of the dischargeCurves results using linear interpolation and spline interpolation, respectively. The raw data was extracted from [3].





**Figure 4:** Result of the interp() method for a current below the lowest measured current without output limitation (left) and with output limitation (right). The raw data was extracted from [3].

in an overall more precise replication of the fit if the entire curve is regarded. This indicates that the most suitable interpolation method may depend on the maximum depth of discharge DoD of the modelled battery. As can be seen in Figure 3, the interpolation bends slightly at the end of the curve (close to a discharge capacity of 3 Ah). This is due to the fact that the voltage returned by a dischargeFit object is limited to the minimum and maximum of the raw data, respectively. If it were not limited, it could return -Inf or Inf, causing the interpolation to fail. Since most lithium ion batteries' DoD are limited to 0.8 or 0.9, this bend should rarely cause any issues.

As demonstrated Figure 4 (left), the interp method using spline interpolation does not provide a good extrapolation of currents. In order to correct this, the voltage output is limited by the curve fit with the lowest current  $I_{\min}$  and by the curve fit with the highest current  $I_{\max}$ , respectively. As a result, the dischargeFit recorded at  $I_{\min}$  is called for any current below  $I_{\min}$  (see Figure 4, left) and the dischargeFit recorded at  $I_{\max}$  is called for any current above  $I_{\max}$ . In this model, the battery's maximum discharging current is limited by the dischargeCurves object's  $I_{\max}$  (see section).

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#### 1.2.3 Usage of a dischargeCurves object

Similarly to a dischargeFit, the results of a dischargeCurves object can be visually validated using the plotResults() method. Individual curve fit references removed using the remove() method and the respective currents.



```
1 % d = dischargeFit object
2 % I = current
3 dC.add(d) % add d to dischargeCurves dC
4 dC.remove(I) % remove the dischargeFit object with current I from dC
```

In order to access the dischargeFit references stored within a dischargeCurves object, the createIterator() method can be used. This creates an iterator object, a Matlab<sup>®</sup> implementation of the java.util.iterator interface [5]. The object can be used to iterate through the wrapped dischargeFit objects using a similar syntax to that of a JAVA<sup>™</sup> iterator.

```
1 it = dC.createIterator; % returns an scIterator object
2 while it.hasNext % returns true if there is another object to
3 % iterate through
4 d = it.next; % returns a dischargeFit object
5 % more code here
6 end
7 it.reset % resets the scIterator
```

For usage in a battery model, a dischargeCurves object is passed to an implementation of the batteryInterface (see section) using it's addCurves() method.

section



## 2 Age model

The age model is implemented using the Observer design pattern. This way, various age models (predefined or custom) can be dynamically added to a battery model at run time or even left out completely. The event oriented age model provided in this package is based solely on cycle counting, for which A mathematical approach developed by [6] is implemented. A description of the counting algorithm and the classes used to implement the age model is provided in the following sections.

## 2.1 Cycle counter



## References

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