

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

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# **Acronyms**

**BMS** battery management system

**MEX** Matlab® executable

**OO** object oriented

OOP object oriented programming

# List of Symbols

Symbol	Unit	Description
$C_{dis}$	Ah	discharge capacity
cDoC	%	cycle-depth-of-cycle
DoD	70	depth of discharge
E F	As/mal	•
_	As/mol	_
I	Α	Current
$N_{f}$	-	number of cycles to failure
SoC	%	state of charge
$SoC_{\sf max}$	%	$maximum\ SoC$
$SoC_{max,l}$	%	local maximum in an $SoC$ profile
SoH	%	state of health
R	$J/(mol \cdot K)$	universal gas constant
rmse	various	root mean squared error
T	K or $^{\circ}\text{C}$	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.

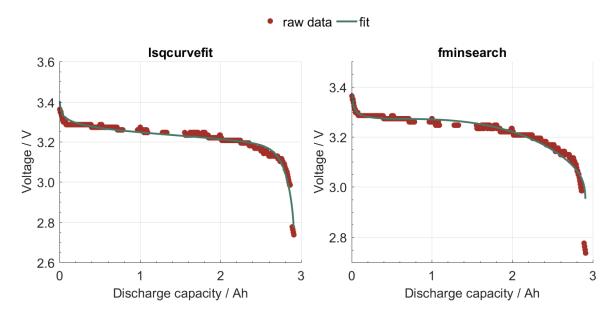


Figure 1: Fit results of the dischargeFit class using the fit methods lsqcurvefit and fminsearch, respectively. The raw data was extracted from [3].





**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.
--	----------	--------------	------------	--------	----------	---------------------	-----

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).

ref section

#### 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 via Matlab's "Events and Listeners<sup>i</sup>" [6]. This way, various age models (predefined or custom) can be dynamically added to a battery model at run time or even left out completely. Ageing can be simulated on the battery pack level (by treating all cells as one entity) or on the cell level (by observing each cell separately). The event oriented age model provided in this package is based solely on cycle counting, for which a mathematical approach developed by [7] is implemented. Descriptions of the counting algorithm and the classes used to implement the age model are provided in the following sections.

#### 2.1 Overview

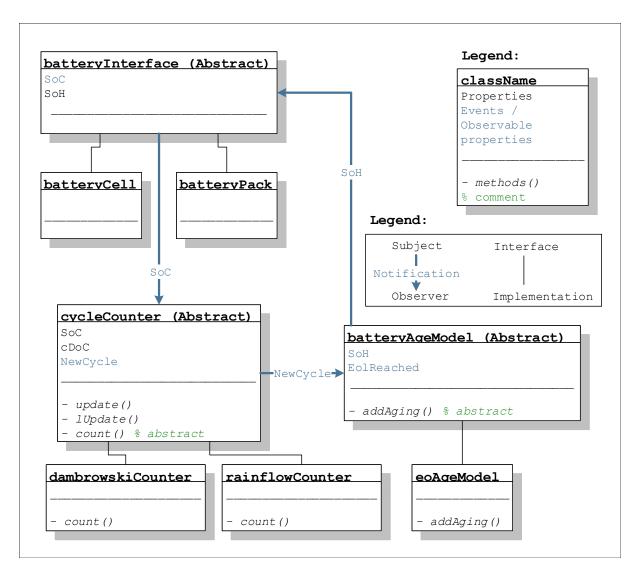
Cycle counting algorithms are designed to count cycles from a set of measured data. A challenge for a running simulation or a battery management system (BMS) that relies on cycle counting is to decide when to count the cycles of an accumulated data set. Counting could be done at fixed time intervals or it could be triggered by a certain event. The latter is the approach implemented by the cycleCounter interface, which acts both as an observer of a battery cell or pack as well as a subject for the eoAgeModel class.

The observation of charge cycles is handled by the abstract cycleCounter interface, in which all methods except for the count () method are predefined. An object that implements the interface is regularly updated with the observed battery's SoC, which is stored within the object's memory. The cycle counting occurs every time the SoC reaches an upper threshold, i.e. the observed battery's maximum SoC. After counting, the NewCycle event is triggered, causing all of the object's observers (i.e. an eoAgeModel object) to be notified that new data is available for simulation. The age model then uses the data to determine the battery's new state of health SoH and passes it on to the battery.

An Observer Pattern class diagram of the age model is depicted in Figure 5. The observation is handled by the respective abstract interfaces, while the actual simulation is handled by the implementations. This makes the model highly flexible. For example, a lightweight implementation could be to observe a batteryPack using a single cycleCounter and a single batteryAgeModel. Another option could be to use multiple cycleCounter and ageModel objects in order to simulate the ageing of each batteryCell within a pack individually. The cycle counting can be implemented by various algorithms (two are provided in this package). And advanced users could even replace the default age model implementation (eoAgeModel) with a custom class that takes other factors into account, e.g. calendar ageing or thermal influences. In large simulations, it may be of interest to neglect the battery ageing in order to save simulation time. This can either be done by simply not linking up the components at runtime or by including a dummyCycleCounter and a dummyAgeModel. These classes

in Matlab $^{\otimes}$ , an observer is often referred to as a "listener". However, "observer" is the more common term in OOP design pattern terminology and will be used throughout this documentation.





**Figure 5:** Overview of the Observer implementation of the age model with communication flows and inheritance links.

implement the cycleCounter and batteryAgeModel interfaces, respectively. However, calling their methods does nothing. The former option is faster, due to reduced method overhead, but the latter may be more robust in some cases.

## 2.2 Cycle counting

In this pack, two classes have been created to implement the cycleCounter's count() method. A cycleCounter subclass can be constructed in one of the following ways:



where cycleCounter must be replaced with the name of the respective class that is being constructed (e.g. dambrowskiCounter or rainflowCounter). To register the object as an observer of a battery object bat<sup>i</sup>, the initAgeModel() method can be used.

ref section

```
1 % Extract intitial SoC and max. SoC from battery
2 init_soc = bat.SoC;
3 soc_max = bat.socMax;
4 % Replace "cycleCounter" with the respective subclass
5 c = cycleCounter(init_soc, soc_max);
6 % Intitialize event oriented age model with cycle counter c
7 bat.initAgeModel('ageModel', 'EO', 'cycleCounter', c)
```

Note that the 'ageModel' option must be specified, otherwise bat will internally replace c with a dummyCycleCounter object to prevent runtime errors. If this happens, a warning message is printed to the command window.

#### 2.2.1 The rainflowCounter class

The state of the art algorithm for cycle counting, "rainflow", was originally developed for mechanical stress modelling [8] and has recently become popular in the field of battery charge cycle counting [9]. The rainflowCounter class was added to this package for the purpose of demonstrating the flexibility of the age model implementation. It acts as an adapter for the popular FileExchange contribution, "Rainflow Counting Algorithm" by Adam Nieslony [10]. In order for the class to work, the MEX functions must be downloaded from [10] and placed within Matlab's search path. They are not included in this package and attempting to construct a rainflowCounter object will fail if they are not found. To register a rainflowCounter with a battery bat, the above syntax must be used, whereby cycleCounter (init\_soc, ... soc\_max) is replaced by rainflowCounter (init\_soc, soc\_max).

#### 2.2.2 The dambrowskiCounter class

In 2012, J. Dambrowski, S. Pichlmaier and A. Jossen developed a mathematical definition of a battery's charge cycles along with an algorithm for counting them [7]. Since the counting algorithm was not named, the dambrowskiCounter class that implements it in this package was named after one of the authors. In their approach, so-called pre-cycles are counted and compared with each other. This is visualized in Figure 6. The twice depicted SoC curve (grey) has two local maxima  $SoC_{\max,l,i}$ , since the last value is counted as a local maximum. Starting from an  $SoC_{\max,l,i}$ , a pre-cycle of "prior equality" is defined as the SoC within an interval between the respective  $SoC_{\max,l}$  and the last point at which the SoC was equal to  $SoC_{\max,l}$ . Two such pre-cycles are depicted in Figure 6 (left) and coloured in red and blue, respectively. A pre-cycle of "subsequent equality" (Figure 6, right, coloured in blue) is defined as the SoC

bat can be an object of any class that implements the batteryInterface.





**Figure 6:** Qualitative visualization of pre-cycle counting according to [7]: Two pre-cycles of prior equality (left) and a pre-cycle of subsequent equality (right).

within an interval between the respective  $SoC_{\max,l}$  and the subsequent point at which the SoC is equal to  $SoC_{\max,l}$ . Finally, a pre-cycle is counted as a cycle if there is no larger pre-cycle that encompasses the same interval and shares the same local minimum. This is not the case for the small cycle (coloured red) in Figure 6 (left); so the depicted curve contains two cycles.

In this package, dambrowskiCounter is the default cycle counter if an age model is specified. Thus, it does not have to be passed as an argument in a battery's initAgeMode() method.

```
1 bat.initAgeModel('ageModel', 'EO')
```

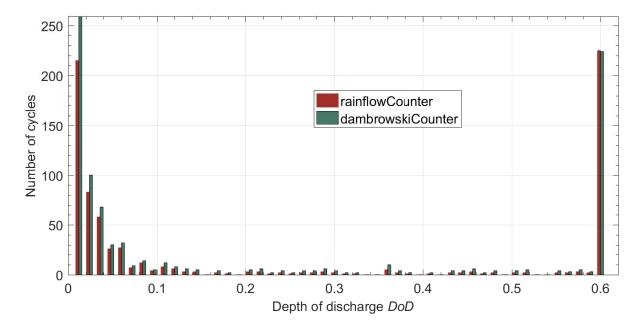
- 2 % Automatically initializes a dabrowskiCounter object with init\_soc
- 3 % and soc\_max set according to the battery's properties and links.

#### 2.2.3 Comparison of the cycle counters

Each cycleCounter object's count () method converts the saved SoC profile into a cycle-Depth-of-Cycle cDoC curve - a vector containing the depths of discharge DoD of all the counted cycles. The simulation results of two batteries using a dambrowskiCounter and a rainflowCounter, respectively, are compared in Figure 7. The cycles' DoDs are each sorted into 50 BINs and compared in a histogram. Overall, the histograms appear very similar, thus proving that both classes produce good results. However, more cycles are counted using the dambrowskiCounter class, possibly causing the simulated battery to age slightly faster. While both classes use different methods for determining the extrema<sup>i</sup>, the amount local maxima found is the same. Thus, the determination of extrema can be ruled out as a cause

idambrowskiCounter uses cycleCounter's iMaxima() method and rainflowCounter uses the sig2ext() function [10].





**Figure 7:** Comparison of the counted cycles and their DoD between two simulations using the rainflowCounter and the dambrowskiCounter using the same SoC profile.

and the root of the discrepancy must lie within the different counting approaches.

## 2.3 Event oriented ageing model

The event oriented ageing model - a very simple and lightweight model - is implemented by the eoAgeModel class, which subclasses the abstract batteryAgeModel interface. Cycle ageing is calculated based on a curve fit of the battery's number of cycles to failure  $N_{\rm f}$  vs DoD curve.

#### 2.3.1 Cycle life curve fits

Due to the fact that the cycle ageing can vary strongly between technologies, it can be difficult to find a good fit for the  $N_{\rm f}$  vs DoD curve. In order to provide some flexibility, three different classes, each implementing the curveFitInterface, are provided for fitting such curves in this package: woehlerFit, nrelcFit and deFit. They only differ in their class names, the number of fit parameters and in the functions used for fitting. The function used in woehlerFit is based on a metal fatigue curve (also known as a "Wöhler curve") [11]

$$N_{\mathsf{f}}(DoD) = x_1 \cdot DoD^{-x_2} \tag{3}$$

with the fit parameters  $x_1$  and  $x_2$ . The nrelcFit class bases it's fit method on an older model [12].

$$N_{f}(DoD) = x_{1} \cdot \frac{1}{DoD} \cdot exp\left(x_{2} \cdot \left(1 - \frac{1}{DoD}\right)\right) \tag{4}$$

Finally, the deFit class uses a double exponential function that was originally developed for lead-acid batteries [13]. However, it also seems to provide decent results for lithium-ion



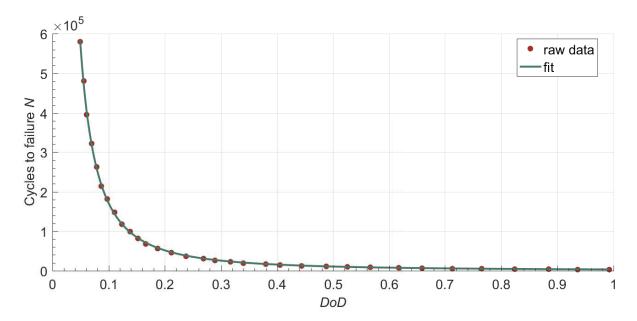


Figure 8: Example for a lithium ion battery's  $N_f$  vs DoD cycle life curve fitted using the woehlerFit class.

batteries in some cases.

$$N_{\mathsf{f}}(DoD) = x_1 + x_2 \cdot exp(-x_3 \cdot DoD) + x_4 \cdot exp(-x_5 \cdot DoD) \tag{5}$$

An example for the fit results of a woehlerFit object is depicted in Figure 8. Due to a lithium-ion battery's extremely large amount of cycles to failure at low DoDs, large relative errors can occur - especially at DoDs close to 1. In order to reduce the rmse, as many raw data points as possible should be provided for fitting.

# 2.4 Creating a user-defined age model

```
1 classdef myCalendarAgeModel < lfpBattery.eoAgeModel</pre>
  %MYCUSTOMAGEMODEL: An example for a user-defined age model.
  %Combines the event oriented age model with a linear calendar age model.
      properties
           L_cal; % calendar life in s
      end
7
      methods
           function obj = myCalendarAgeModel(1, varargin)
10
               % l = calendar life in years
11
               % varargin = input args of eoAgeModel constructor
12
               %% call superclass constructor
13
               obj = obj@lfpBattery.eoAgeModel(varargin{:});
14
               obj.L_cal = 1 * 525600 / obj.eolAc; % set L_cal in
15
```





# References

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