

Using the standard

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Battery Parameter eXchange

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1 Introduction

Battery Parameter eXchange (BPX) is an open information-exchange standard expressing the values of parameters defined in commonly used physics-based models describing Li-ion batteries. This standard comprises a specification of a set of equations and a data schema for the encoding of the mathematical coefficients within the specification. The standard additionally supports inclusion of experimental data used to justify the reported parameter values.

Within the standard, parameters are stored in a human-readable, extensible, and easily-shared JSON file format¹. To enable easy adoption, tools to parse and validate² BPX formatted files are provided in the [BPX GitHub repository](#). The repository also includes a [change log](#) detailing all changes to the standard and associated code.

This document outlines the model equations used in the standard and provides a mapping between the parameter symbols used in the equations and the parameter names used in the BPX standard. The BPX standard is based on the Doyle-Fuller-Newman (DFN) model [1; 2; 3; 4]. The specific forms of the DFN model and its simpler variations expressed by the standard follow a recent comprehensive review [5]. A nomenclature table is available in Appendix A. The standard should be read alongside the following critical review of the methods to measure or infer parameters for use within the isothermal DFN framework [6]. A table outlining the experimental techniques often used to extract parameters is given in Appendix B.

2 What is BPX?

This section provides additional context on practical use of the BPX standard.

“Physics-based Li-ion battery models” predict the temperature-dependent voltage–current response and internal state evolution of a Li-ion cell, by solving equations parameterised in terms of physically

¹JSON is an open standard file format and data interchange format that uses human-readable text to store and transmit data objects consisting of attribute-value pairs and arrays (or other serializable values).

²Files are validated against a [JSON schema](#).

identifiable properties. BPX creates a standard for these physical equations, and for identifying the parameters they include. Using BPX, parameter values representing a specific battery can be exchanged between users, who may choose to solve the corresponding model with any of a number of different software implementations. Any software implementation capable of solving a physics-based model can support the BPX format by creating read/write tools compatible with the standard.

Although the characteristic of a physics-based model is the physical identifiability of its parameters, BPX does not enforce a standard for measurement processes used in parameterisation. That is, it creates a standard for a model defined by a set of equations, not for the interpretation of this model in the context of the Li-ion battery as a real-world item. This distinction is intended to align with the needs of practical industrial use of physics-based models. In particular, it allows users to treat parameters in a purely empirical manner if they choose to do so. BPX does support (and encourage) the inclusion of validation data from experiments within the BPX file format.

Diverse phenomena arise in Li-ion cells with various chemistry. BPX does not aim to impose any specified theory for underlying models, nor does it intend to limit creativity in the extension or future substitution of its standard models. Rather, BPX responds to *de facto* commonalities that have arisen naturally in academic research and industrial application, by providing a consistent reporting standard for these common features. User-defined extensions to the standard are supported; users who incorporate such extensions in their BPX files are responsible for communicating the corresponding technical specification of any additions.

The BPX standard requires that a BPX file be complete in order to be considered valid: it must contain sufficient parameter information to compute the stated battery model type. In principle, however, the JSON file format supports a partially complete BPX file. Such files will not be accepted as valid BPX by the BPX tools, but can nonetheless be used for information exchange between users.

BPX is:

- A standardised equation set and parameter-exchange format for physics-based battery modelling.
- A file format supporting inclusion of validation data alongside parameters.
- A data schema and set of tools that can ensure that a parameter set in a BPX file is:
 - correctly formatted
 - internally self-consistent
 - sufficient to compute one of a set of specific battery models (DFN, SPM_e, SPM)

BPX is not:

- A standard for measurement or characterisation methods.
- A standard constraining interpretation or use of parameters reported.

BPX does not require:

- The reported model to be limited to the standard.
 - Miscellaneous, user-defined extensions are supported.

3 Model equations

3.1 Doyle-Fuller-Newman (DFN) model

The BPX standard uses a lumped thermal formulation of the DFN model. Full details of this formulation are given in Sections 2.3 and 5.2 of [5]. Each electrode is assumed to contain a blend of particle types enumerated m . Each particle type comprises equally-sized spherical particles with defined material

properties.

Mass conservation in the active material particles gives, for all m :

$$\frac{\partial c_{k,m}}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 N_{k,m}) = 0, \quad N_{k,m} = -D_{k,m}(c_{k,m}, T) \frac{\partial c_{k,m}}{\partial r}, \quad \text{in } 0 \leq r \leq R_{k,m}, \quad (1a)$$

subject to

$$N_{k,m} = 0, \text{ on } r = 0, \quad N_{k,m} = \frac{j_{k,m}(x, t)}{F}, \text{ on } r = R_{k,m}, \quad (1b)$$

and

$$c_{k,m}(r, x, t) = c_{k,m,0}, \quad \text{at } t = 0. \quad (1c)$$

The **initial concentrations in the active material particles** can be calculated from the cell state-of-charge (SOC), z , by solving the following simultaneous equations³ for $k = n$ and $k = p$ respectively, and all m :

$$U_{k,0} = U_{k,m}(\theta_{k,m} = \theta_{k,m,0}, T) \quad (2a)$$

$$z = \sum_m \Theta_{k,m} \frac{\theta_{k,m,0} - \theta_{k,m}^{\min}}{\theta_{k,m}^{\max} - \theta_{k,m}^{\min}}, \quad \text{with } \theta_{k,m} = \frac{c_{k,m}}{c_{k,m}^{\max}}. \quad (2b)$$

where $U_{n,0}$ and $U_{p,0}$ are constants and where the capacity proportion contributed by each particle type i in electrode k is:

$$\Theta_{k,i} = \frac{c_{k,i}^{\max} R_{k,i} b_{k,i}}{\sum_m c_{k,m}^{\max} R_{k,m} b_{k,m}} \quad (2c)$$

If there is only one material in the electrode k , enumerated $m = 1$, these equations simplify to the following statement ($\theta_k \equiv \theta_{k,m=1}$):

$$\theta_{k0} = \theta_k^{\min} + z (\theta_k^{\max} - \theta_k^{\min}) \quad (2d)$$

The assumption of symmetric **Butler-Volmer kinetics** gives

$$j_{k,m} = 2j_{k,m,0} \sinh \left(\frac{F}{2RT} \eta_{k,m} \right), \quad (3a)$$

$$j_{k,m,0} = FK_{k,m}(T) \sqrt{\frac{c_e}{c_{e0}} \frac{c_{k,m}}{c_{k,m}^{\max}} \left(1 - \frac{c_{k,m}}{c_{k,m}^{\max}} \right)} \bigg|_{r=R_{k,m}}, \quad (3b)$$

The **active material electrode thermodynamics** define the reaction overpotential

$$\eta_{k,m} = \phi_k - \phi_e - U_{k,m} \left(c_{k,m}|_{r=R_{k,m}} \right), \quad (4a)$$

with the open circuit potential (OCP) $U_{k,m}$ given by⁴

$$U_{k,m}(\theta_{k,m}, T) = U_{k,\text{ref}}(\theta_{k,m}) + (T - T_{\text{ref}}) \frac{dU_{k,m}}{dT} \bigg|_{T=T_{\text{ref}}}(\theta_{k,m}) \quad (4b)$$

³This calculation assumes that the cell is in equilibrium at the given SOC.

⁴Within BPX the OCP is given as a function of stoichiometry and temperature.

Charge conservation in the electrode matrix, assuming an effective Ohm's law current density in the composite electronic conductor, gives

$$i_{v,k} = \sum_m b_{k,m} j_{k,m} \quad (5a)$$

$$\frac{\partial i_k}{\partial x} = -i_{v,k}, \quad i_k = -\sigma_k \frac{\partial \phi_k}{\partial x}, \quad (5b)$$

subject to

$$\phi_n = 0, \text{ on } x = 0, \quad i_n = 0, \text{ on } x = L_n, \quad i_p = 0, \text{ on } x = L - L_p, \quad (5c)$$

Here $L = L_n + L_s + L_p$.

Total cell properties current I (positive for cell charging) and voltage V_{tot} are related to the local macroscopic variables as:

$$\phi_p = V_{\text{tot}}, \quad \text{on } x = L, \quad (6a)$$

$$i_p = -i_{\text{app}}, \quad \text{on } x = L, \quad (6b)$$

where

$$i_{\text{app}}(t) = \frac{I(t)}{AN_p}. \quad (6c)$$

One of equations (6a) or (6b), or a combination of them, must be specified as an independent boundary condition. Assuming a galvanostatic charge/discharge, equation (6b) is set directly, and cell voltage is then computed from (6a), but this boundary condition could be replaced with (for example) one that sets a controlled voltage V_{tot} or power IV_{tot} applied to the cell.

Charge conservation in the electrolyte, assuming a concentrated binary monovalent Li^+ ideal electrolyte, gives

$$\frac{\partial i_e}{\partial x} = i_v(x), \quad i_e = \sigma_e(c_e, T) \mathcal{B}(x) \left(-\frac{\partial \phi_e}{\partial x} + \frac{2RT}{F} (1 - t^+) \frac{1}{c_e} \frac{\partial c_e}{\partial x} \right), \quad (7a)$$

in which

$$i_v(x) = \begin{cases} i_{v,n}, & \text{if } 0 \leq x \leq L_n, \\ 0, & \text{if } L_n < x \leq L - L_p, \\ i_{v,p}, & \text{if } L - L_p < x \leq L, \end{cases} \quad \mathcal{B}(x) = \begin{cases} \mathcal{B}_n, & \text{if } 0 \leq x \leq L_n, \\ \mathcal{B}_s, & \text{if } L_n < x \leq L - L_p, \\ \mathcal{B}_p, & \text{if } L - L_p < x \leq L, \end{cases} \quad (7b)$$

Charge conservation is solved subject to

$$i_e = 0, \quad \text{at } x = 0, L. \quad (7c)$$

Mass conservation in the electrolyte, assuming a concentrated binary monovalent Li^+ ideal electrolyte, gives

$$\varepsilon(x) \frac{\partial c_e}{\partial t} = -\frac{\partial N_e}{\partial x} + \frac{i_v(x)}{F}, \quad N_e = -D_e(c_e, T) \mathcal{B}(x) \frac{\partial c_e}{\partial x} + \frac{t^+}{F} i_e, \quad (8a)$$

with

$$\varepsilon(x) = \begin{cases} \varepsilon_n, & \text{if } 0 \leq x \leq L_n, \\ \varepsilon_s, & \text{if } L_n < x \leq L - L_p, \\ \varepsilon_p, & \text{if } L - L_p < x \leq L, \end{cases} \quad (8b)$$

subject to

$$N_e = 0, \quad \text{at } x = 0, L, \quad (8c)$$

and

$$c_e = c_{e0}, \quad \text{at } t = 0. \quad (8d)$$

Assuming a uniform cell temperature and ignoring reversible heat of mixing, **conservation of energy** leads to a lumped thermal model

$$\rho c_p \frac{dT}{dt} = \frac{AN_p}{V} \int_0^L (\dot{Q}_{\text{irr}} + \dot{Q}_{\text{rev}}) dx - h \frac{A}{V} (T - T_{\text{amb}}), \quad (9a)$$

in which

$$\dot{Q}_{\text{irr}}(x) = \begin{cases} -i_n \frac{\partial \phi_n}{\partial x} - i_e \frac{\partial \phi_e}{\partial x} + \sum_m b_{n,m} j_{n,m} \eta_{n,m}, & \text{if } 0 \leq x \leq L_n, \\ -i_e \frac{\partial \phi_e}{\partial x}, & \text{if } L_n < x \leq L - L_p, \\ -i_p \frac{\partial \phi_p}{\partial x} - i_e \frac{\partial \phi_e}{\partial x} + \sum_m b_{p,m} j_{p,m} \eta_{p,m}, & \text{if } L - L_p < x \leq L, \end{cases} \quad (9b)$$

and

$$\dot{Q}_{\text{rev}}(x) = \begin{cases} T \sum_m b_{n,m} j_{n,m} \frac{\partial U_{n,m}}{\partial T} \Big|_{T=T_{\text{ref}}}, & \text{if } 0 \leq x \leq L_n, \\ 0, & \text{if } L_n < x \leq L - L_p, \\ T \sum_m b_{p,m} j_{p,m} \frac{\partial U_{p,m}}{\partial T} \Big|_{T=T_{\text{ref}}}, & \text{if } L - L_p < x \leq L, \end{cases} \quad (9c)$$

Energy conservation is solved subject to

$$T(0) = T_0. \quad (9d)$$

Within the BPX standard, $D_{k,m}$, D_e , σ_e and $K_{k,m}$ are assumed to have an Arrhenius temperature relationship, i.e.

$$f(c, T) = f_{\text{ref}}(c) \exp \left(\frac{E_f}{R} \left(\frac{1}{T_{\text{ref}}} - \frac{1}{T} \right) \right), \quad (10)$$

where f is the parameter of interest, f_{ref} is the parameter's value at the reference temperature.

3.2 Single Particle Model with electrolyte (SPMe)

A single particle model with electrolyte (SPMe) is a simplification of the DFN model in which each active material particle type in each electrode is represented by a single particle, without spatial variation. The following particle-specific variables therefore become independent of x in the SPMe: $i_{v,k}(t)$, $\eta_{k,m}(t)$, $U_{k,m}(t)$, $\phi_{k,m}(t)$, $c_{k,m}(r, t)$.

A variety of different mathematical simplifications reductions of the DFN model are described by the term “SPMe”. Some of the most prominent have been reviewed in Section 3.1 of the review paper [5], including the asymptotic ‘canonical’ SPMe [7]. Note that there is an error in [5] in equations (28c) and (28e): the b_k parameter (surface area per unit volume) needs to be included in (28e) and removed from (28c) for everything to be consistent.

Common variations of the SPMe require the same set of parameters as the DFN model (see Table 1). For this reason, BPX does not enforce a specific mathematical specification of SPMe as being uniquely compatible. This decision is under review and may be changed in future.

3.3 Single Particle Model (SPM)

The SPM represents a further simplification of the SPMe, neglecting concentration variation in the electrolyte, and potential variation in the electrolyte and electrodes across the cell. Compared to the DFN model or SPMe, the following variables therefore also become independent of x : $c_e(t)$, $\phi_e(t)$, $\phi_k(t)$, $j_{k,m,0}(t)$.

The SPM therefore consists of the two diffusion equations given by equations (1a)-(1c), solved with spatially independent equivalents of equations (3a)-(3b), (4a)-(4b). Total cell properties relate to microscopic properties according to (6a)-(6c), combined with a statement of uniform current density for each electrode:

$$i_{v,n} = -\frac{i_{app}(t)}{b_n L_n}, \quad i_{v,p} = \frac{i_{app}(t)}{b_p L_p}, \quad (11)$$

Applying the following substitutions to the DFN model, over all x , allows the heat sources in equations (9a)-(9d) to be used for the SPM.

$$\phi_n = 0, \quad (12a)$$

$$\phi_p = V_{tot}, \quad (12b)$$

$$\frac{\partial \phi_e}{\partial x} = 0, \quad (12c)$$

$$c_e = c_{e0}. \quad (12d)$$

The SPM requires a smaller set of parameters than the SPMe or DFN. The specific parameters required for each model supported by the standard are outlined in Table 1.

4 BPX Schema

The BPX schema is organised into three main sections:

- "Header", containing general information such as the BPX version or a description of the cell
- "Parameterisation", containing the parameter values associated with the cell
- "Validation", optionally containing additional test data that can be used to validate the model (e.g. time, current, voltage data)

Header information optionally includes a title, description, BPX version number, and compatible model. Allowed entries in the "Model" field are "DFN" (section 3.1), "SPMe" (section 3.2), or "SPM" (section 3.3). Parameters required for each model are given in Table 1.

Within the "Parameterisation" section, parameters are stored by their domain:

- "Cell"
- "Electrolyte"
- "Separator"
- "Negative electrode"
- "Positive electrode"
- "User-defined"

Table 1 details the allowed string names given to each of the parameters, along with allowed type and any functional dependence. So, for example, the negative particle radius R_n is stored in the JSON file at the following node:

- ["Parameterisation"]["Negative electrode"]["Particle radius [m]"]

The special type "FloatFunctionTable" allows parameters to be provided as a float, a function of a single variable⁵, or a table of data⁶. A complete example BPX-compliant JSON file is given in Appendix C.

Within the "Negative electrode" or "Positive electrode" domain, certain parameters may be specified either once, or several times, to indicate several types of contributing active materials in a blended electrode (enumerated m). For those parameters listed in Table 1 as "according to "Particle" rules", one of the following options is allowed:

1. To specify all particles in the electrode as a common material, include each parameter and its value exactly once, directly within "Negative electrode" or "Positive electrode" as appropriate.
2. To specify a blended electrode comprising different types of particle, include a "Particle" node within "Negative electrode" or "Positive electrode" as appropriate. Within the "Particle", specify one or many nodes as required for the number of particle types used. Each node can have any user-defined name describing the specific particle type (for example, "Particle Type 1"). Within the node for each particle type, include each parameter and its value for that particle type. A partial example BPX JSON file showing a "Positive electrode" field with two particle types is given in Appendix D.

Outside the "User-defined" domain of the "Parameterisation" section, the allowed parameter names are strictly constrained to those specified by the standard as allowed in the corresponding domain (Table 1). Within the dedicated "User-defined" domain, however, users may include any other parameters that they wish to report, even when these fall outside the equations and parameters specified by this document. The BPX standard requires that all entries under "User-defined" are of type "FloatFunctionTable"; with the exception of the specification of interpolants, no JSON hierarchy is permitted in this node. Where users report user-defined parameters with this method, it is their responsibility to communicate the corresponding extension to Section 3 and Table 1, in order that the mathematical specification of user-defined parameters is clear.

⁵The schema currently supports the following operations: *, /, -, +, **, exp, tanh. Here, ** denotes exponentiation, as in Python.

⁶One-dimensional data can be provided as, e.g., "x": [0, 0.1, 1], "y": [1.72, 1.2, 0.06]. When the file is parsed, a linear interpolant is created using the data.

Symbol	BPX name	Type	Function of	SPM	SPMe	DFN
"Cell"						
A	"Electrode area [m2]"	float	-	✓	✓	✓
\mathcal{A}	"External surface area [m2]"	float	-	✓	✓	✓
\mathcal{V}	"Volume [m3]"	float	-	✓	✓	✓
N_p	"Number of electrode pairs connected in parallel to make a cell"	int	-	✓	✓	✓
V_{\min}	"Lower voltage cut-off [V]"	float	-	✓	✓	✓
V_{\max}	"Upper voltage cut-off [V]"	float	-	✓	✓	✓
Q_{nom}	"Nominal cell capacity [A.h]"	float	-	✓	✓	✓
T_{amb}	"Ambient temperature [K]"	float	-	✓	✓	✓
T_0	"Initial temperature [K]"	float	-	✓	✓	✓
T_{ref}	"Reference temperature [K]"	float	-	✓	✓	✓
ρ	"Density [kg.m-3]"	float	-	✓	✓	✓
c_p	"Specific heat capacity [J.K-1.kg-1]"	float	-	✓	✓	✓
\mathcal{K}	"Thermal conductivity [W.m-1.K-1]"	float	-	✓	✓	✓
"Electrolyte"						
c_{e0}	"Initial concentration [mol.m-3]"	float	-		✓	✓
t^+	"Cation transference number"	float	-		✓	✓
$D_{e,\text{ref}}$	"Diffusivity [m2.s-1]"	FloatFunctionTable	c_e		✓	✓
E_{D_e}	"Diffusivity activation energy [J.mol-1]"	float	-		✓	✓
$\sigma_{e,\text{ref}}$	"Conductivity [S.m-1]"	FloatFunctionTable	c_e		✓	✓
E_{σ_e}	"Conductivity activation energy [J.mol-1]"	float	-		✓	✓
"Negative electrode"/"Separator"/"Positive electrode"						
L_k	"Thickness [m]"	float	-	*	✓	✓
ε_k	"Porosity"	float	-		✓	✓
\mathcal{B}_k	"Transport efficiency"	float	-		✓	✓
"Negative electrode"/"Positive electrode"						
σ_k	"Conductivity [S.m-1]"	float	-		✓	✓
"Negative electrode"/"Positive electrode" according to "Particle" rules, see above						
$\theta_{k,m}^{\min}$	"Minimum stoichiometry"	float	-	✓	✓	✓
$\theta_{k,m}^{\max}$	"Maximum stoichiometry"	float	-	✓	✓	✓
$c_{k,m}^{\max}$	"Maximum concentration [mol.m-3]"	float	-	✓	✓	✓
$R_{k,m}$	"Particle radius [m]"	float	-	✓	✓	✓
$b_{k,m}$	"Surface area per unit volume [m-1]"	float	-	✓	✓	✓
$D_{k,m,\text{ref}}$	"Diffusivity [m2.s-1]"	FloatFunctionTable	θ_k	✓	✓	✓
$E_{D_{k,m}}$	"Diffusivity activation energy [J.mol-1]"	float	-	✓	✓	✓
$U_{k,m,\text{ref}}$	"OCP [V]"	FloatFunctionTable	θ_k	✓	✓	✓
$\frac{dU_{k,m}}{dT}\bigg _{T=T_{\text{ref}}}$	"Entropic change coefficient [V.K-1]"	FloatFunctionTable	θ_k	✓	✓	✓
$K_{k,m,\text{ref}}$	"Reaction rate constant [mol.m-2.s-1]"	float	-	✓	✓	✓
$E_{K_{k,m}}$	"Reaction rate constant activation energy [J.mol-1]"	float	-	✓	✓	✓

Table 1: Parameter symbols, corresponding BPX names, types, functional dependencies, and the models. Symbol ✓ means that the parameter is needed for the model; symbol * means that the parameter is needed only for the negative and positive electrodes and not for the separator. The parameters within the table are grouped by component. A slash between component names indicates the parameter has a value in each domain (e.g. "Thickness [m]" is defined for both the negative and positive electrodes, and the separator).

Appendices

A Nomenclature

The symbols and corresponding units used within this standard are detailed below.

Variables (with units)		
$c_{k,m}$	inserted lithium concentration	mol m^{-3}
c_e	lithium electrolyte concentration	mol m^{-3}
i_k	macroscopic effective current density, electron-conducting phase	A m^{-2}
i_{app}	applied geometric current density	A m^{-2}
i_e	macroscopic effective electrolyte current density	A m^{-2}
$i_{v,k}$	volumetric Li insertion reaction current density	A m^{-3}
I	cell current	A
$j_{k,m}$	microscopic Li insertion reaction current density	A m^{-2}
$j_{k,m,0}$	exchange current density	A m^{-2}
$N_{k,m}$	molar flux of inserted lithium	$\text{mol m}^{-2} \text{s}^{-1}$
N_e	effective molar flux of Li^+ in the electrolyte	$\text{mol m}^{-2} \text{s}^{-1}$
\dot{Q}_{irr}	irreversible volumetric heat source	W m^{-3}
\dot{Q}_{rev}	reversible volumetric heat source	W m^{-3}
Q_{irr}	total cell irreversible heat source	W
Q_{rev}	total cell reversible heat source	W
r	microscopic radial coordinate	m
t	time	s
T	temperature	K
V_{OCV}	open-circuit voltage	V
V_{tot}	cell voltage	V
x	macroscopic (through-cell) coordinate	m
z	cell state-of-charge (SOC)	-
$\eta_{k,m}$	overpotential at the electrode–electrolyte interface	V
θ_{k0}	initial electrode stoichiometry	-
$\theta_{k,m}$	inserted Li stoichiometry (by particle type)	-
$\Theta_{k,m}$	capacity contribution (by particle type)	-
ϕ_k	electric potential	V

ϕ_e	electrolyte potential	V
Parameters and functions (with units)		
A	electrode cross-sectional (geometric) area	m^2
$b_{k,m}$	particle surface area per unit of volume	m^{-1}
$c_{k,m}^{\max}$	maximum particle concentration	mol m^{-3}
c_{e0}	initial/rest lithium ion concentration in the electrolyte	mol m^{-3}
c_p	specific heat capacity	$\text{J K}^{-1} \text{kg}^{-1}$
$D_{k,m}$	lithium diffusivity in particle	$\text{m}^2 \text{s}^{-1}$
$D_{k,m,\text{ref}}$	reference lithium diffusivity in particle	$\text{m}^2 \text{s}^{-1}$
D_e	lithium ion diffusivity in electrolyte	$\text{m}^2 \text{s}^{-1}$
$D_{e,\text{ref}}$	reference lithium ion diffusivity in electrolyte	$\text{m}^2 \text{s}^{-1}$
$E_{D_{k,m}}$	activation energy of lithium diffusivity in particle	J mol^{-1}
E_{D_e}	activation energy of lithium-ion diffusivity in electrolyte	J mol^{-1}
E_{σ_e}	activation energy of conductivity (electrolyte)	J mol^{-1}
$E_{K_{k,m}}$	activation energy of normalised reaction rate constant	J mol^{-1}
h	heat transfer coefficient	$\text{W m}^{-2} \text{K}^{-1}$
I	applied current	A
$K_{k,m}$	normalised reaction rate constant	$\text{mol m}^{-2} \text{s}^{-1}$
$K_{k,m,\text{ref}}$	reference normalised reaction rate constant	$\text{mol m}^{-2} \text{s}^{-1}$
L_k	electrode and separator thicknesses	m
N_p	number of electrode pairs connected in parallel to make a cell	-
Q_{nom}	nominal cell capacity	A h
$R_{k,m}$	particle radius	m
t^+	cation transference number	-
T_0	initial temperature	K
T_{amb}	ambient temperature	K
T_{ref}	reference temperature	K
$U_{k,0}$	initial open-circuit potential (OCP) of electrode	V
$U_{k,m}$	open-circuit potential (OCP)	V
$U_{k,m,\text{ref}}$	open-circuit potential (OCP) at reference temperature	V
$\left. \frac{dU_{k,m}}{dT} \right _{T=T_{\text{ref}}}$	entropic change coefficient	V K^{-1}
V_{\min}	lower voltage cut-off	V

V_{\max}	upper voltage cut-off	V
\mathcal{A}	cell external surface area	m ²
\mathcal{B}_k	transport efficiency / inverse MacMullin number	-
\mathcal{K}	thermal conductivity	W m ⁻¹ K ⁻¹
\mathcal{V}	cell volume	m ³
ε_k	electrolyte volume fraction (porosity)	-
$\theta_{k,m}^{\max}$	maximum particle stoichiometry	-
$\theta_{k,m}^{\min}$	minimum particle stoichiometry	-
ρ	density	kg m ⁻³
σ_k	conductivity (electrode)	S m ⁻¹
σ_e	conductivity (electrolyte)	S m ⁻¹
$\sigma_{e,\text{ref}}$	reference conductivity (electrolyte)	S m ⁻¹
Constants (with units)		
F	Faraday constant	C mol ⁻¹
R	gas constant	J K ⁻¹ mol ⁻¹
Subscripts		
e	in electrolyte	
n	in negative electrode/particle ("Negative electrode")	
p	in positive electrode/particle ("Positive electrode")	
s	in separator	
solid	in electron-conducting solids	
k	in domain $k \in \{\text{n, s, p}\}$	
m	for particle type m	
0	initial value	

B Parameter extraction techniques

Technique	Parameter(s) extracted
Microscopy	$L_k, R_k, \varepsilon_k, \mathcal{B}_k$
Electrochemical Impedance Spectroscopy (EIS) †	$\mathcal{B}_k, K_k, D_k, D_e, \sigma_e, t^+$
X-ray powder Diffraction (XRD)	R_k
Hg porosimetry	ε_k, b_k
Brunauer–Emmett–Teller (BET) adsorption	b_k
Electronic conductivity probe	σ_k
pseudo-OCV †	U_k
Galvanostatic Intermittent Titration Technique (GITT) †	U_k, D_k
Staircase Galvanostatic Intermittent Titration Technique (SC GITT) †	K_k
Cyclic Voltammetry (CV) †	K_k, D_k
Potentiostatic Intermittent Titration Technique (PITT) †	K_k, D_k
Polarisation-relaxation cells	D_e, t^+

Table 2: Experimental techniques and parameters that they measure. Techniques marked with a dagger (†) can be applied to full-cells, but in order to isolate the components of a single electrode, cells are often torn down and reassembled as half-cells. Techniques that are not marked with a dagger necessarily require teardown. Reproduced from [6].

C BPX JSON example

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1 {
2   "Header": {
3     "BPX": 0.1,
4     "Title": "Parameterisation example of an NMC111|graphite 12.5 Ah pouch cell",
5     "Description": "NMC111|graphite 12.5 Ah pouch cell. Parameterisation by About:Energy Limited (
      aboutenergy.io), December 2022, based on cell cycling data, and electrode data gathered
      after cell teardown. Electrolyte properties from Nyman et al. 2008 (doi:10.1016/j.electacta
      .2008.04.023). Negative electrode entropic coefficient data are from O'Regan et al. 2022 (
      doi:10.1016/j.electacta.2022.140700). Positive electrode entropic coefficient data are from
      Viswanathan et al. 2010 (doi:10.1016/j.jpowsour.2009.11.103). Other thermal properties are
      estimated.",
6     "Model": "DFN"
7   },
8   "Parameterisation": {
9     "Cell": {
10       "Ambient temperature [K]": 298.15,
11       "Initial temperature [K]": 298.15,
12       "Reference temperature [K]": 298.15,
13       "Lower voltage cut-off [V]": 2.7,
14       "Upper voltage cut-off [V]": 4.2,
15       "Nominal cell capacity [A.h]": 12.5,
16       "Specific heat capacity [J.K-1.kg-1]": 913,
17       "Thermal conductivity [W.m-1.K-1]": 2.04,
18       "Density [kg.m-3]": 1847,
19       "Electrode area [m2]": 0.016808,
20       "Number of electrode pairs connected in parallel to make a cell": 34,
21       "External surface area [m2]": 0.0379,
22       "Volume [m3]": 0.000128
23     },
24     "Electrolyte": {
25       "Initial concentration [mol.m-3]": 1000,
26       "Cation transference number": 0.2594,
27       "Conductivity [S.m-1]": "0.1297 * (x / 1000) ** 3 - 2.51 * (x / 1000) ** 1.5 + 3.329 * (x /
        1000)",
28       "Diffusivity [m2.s-1]": "8.794e-11 * (x / 1000) ** 2 - 3.972e-10 * (x / 1000) + 4.862e-10",
29       "Conductivity activation energy [J.mol-1]": 17100,
30       "Diffusivity activation energy [J.mol-1]": 17100
31     },
32     "Negative electrode": {
33       "Particle radius [m]": 4.12e-06,
34       "Thickness [m]": 5.62e-05,
35       "Diffusivity [m2.s-1]": 2.728e-14,
36       "OCP [V]": "9.47057878e-01 * exp(-1.59418743e+02 * x) - 3.50928033e+04 + 1.64230269e-01 *
        tanh(-4.55509094e+01 * (x - 3.24116012e-02)) + 3.69968491e-02 * tanh(-1.96718868e+01
        * (x - 1.68334476e-01)) + 1.91517003e+04 * tanh(3.19648312e+00 * (x - 1.85139824e+00))
        + 5.42448511e+04 * tanh(-3.19009848e+00 * (x - 2.01660395e+00))",
37       "Entropic change coefficient [V.K-1]": "-0.1112 * x + 0.02914 + 0.3561 * exp(-(x -
        0.08309) ** 2) / 0.004616) + 0 * (tanh(63.9 * (x - (0.4955 - 0.1122))) - tanh(63.9 * (
        x - (0.4955 + 0.1122))))",
38       "Conductivity [S.m-1]": 0.39,
39       "Surface area per unit volume [m-1]": 499522,
40       "Porosity": 0.253991,
41       "Transport efficiency": 0.128,
42       "Reaction rate constant [mol.m-2.s-1]": 5.199e-06,
43       "Minimum stoichiometry": 0.005504,
44       "Maximum stoichiometry": 0.75668,
45       "Maximum concentration [mol.m-3]": 29730,
46       "Diffusivity activation energy [J.mol-1]": 30000,
47       "Reaction rate constant activation energy [J.mol-1]": 55000
48     },
49     "Positive electrode": {
50       "Particle radius [m]": 4.6e-06,
```


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