ANL/CSE-22/1



Battery Performance and Cost Modeling for Electric-Drive Vehicles

A Manual for BatPaC v5.0

Chemical Sciences and Engineering Division Argonne National Laboratory

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A Manual for BatPaC v5.0

prepared by Kevin W. Knehr, Joseph J. Kubal, Paul A. Nelson, and Shabbir Ahmed Chemical Sciences and Engineering Division, Argonne National Laboratory

July, 2022

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ABBREVIATIONS

ASI	area-specific impedance
ASIC	application-specific integrated circuit
BDU	battery disconnect unit
BMS	battery management system
BMU	battery management unit
BOL	beginning of life
DMC	dimethyl carbonate
EC	ethylene carbonate
EG/W	ethylene-glycol/water heat transfer fluid
EMC	ethyl methyl carbonate
EOL	end of life
EV	electric vehicle
Gr	graphite
GSA	General, Sales, and Administration
HEV	hybrid electric vehicle
HEV-HP	high-power assist hybrid electric vehicle
LCO	lithium cobalt oxide
LFP	lithium iron phosphate
Li	lithium
Li-ion	lithium-ion
LMO	lithium manganese spinel
LMR	lithium and manganese rich
LTO	lithium titanate spinel
Mild-HEV	mild power assist hybrid electric vehicle
MW	molecular weight
NCA	lithium nickel cobalt aluminum oxide
NMC	lithium nickel manganese cobalt oxide
NMP	N-Methyl-2-pyrrolidone
OCV	open-circuit voltage
OEM	original equipment manufacturer

PE	polyethylene
PET	polyethylene terephthalate
PHEV	plug-in hybrid electric vehicle
PP	polypropylene
SOC	state of charge

LIST OF SYMBOLS

Section 5

а	ratio of interfacial area to electrode volume, cm ² /cm ³
A	area, cm ²
ASI	area-specific impedance, ohm cm ²
C_j	capacity of <i>j</i> , Ah
C_p	specific heat capacity, J/g K
$E_{a,eff}$	effective activation energy for ASI, J/mol
E_{pack}	total pack energy, Wh
f	factor
F	Faraday constant, 96,485 C/mol
G	mass flowrate, g/s
h	heat transfer coefficient, W/cm ² K
H_{j}	height of component j (see subscripts), cm
<i>i</i> _o	exchange current density related to the interfacial area, A/cm^2
Ι	average current density, A/cm ²
$I_{ionic,lim}$	ionic limiting current density, A/cm ²
I_n	local current density, A/cm ²
I_P	cell current density at rated power, A/cm ²
I total	total current density, A
k	thermal conductivity, W/cm K
ℓ_j	effective length of component j (see subscripts), cm
L_j	length of component j (see subscripts), cm
[L/W]	aspect ratio of pouch cell
m_j	mass of j (see subscripts), g
MW	molecular weight of lithiated compound, g/mol
n	parameter
N_j	number of component <i>j</i> (see subscripts)
[N/P]	negative to positive capacity ratio
Р	power, W
q	heating rate, W
Q	specific capacity of the electrode, mAh/g

C-rate, h ⁻¹
limiting C-rate, h ⁻¹
radius of j (see subscripts), cm
universal gas constant, 8.314 J/mol K
resistance factor
resistance of j (see subscripts), ohm
time, s
temperature, K
open-circuit voltage, V
voltage, V
fraction of the open-circuit voltage
width of component j (see subscripts), cm
compression factor

Greek

δ_j	thickness of j (see subscripts), cm
Е	volume fraction
μ	fluid viscosity, g/cm s
Ø	diameter of j (see subscripts), cm
$ ho_j$	density of j (see subscripts), g/cm ³
σ_j	conductivity of j (see subscripts), S/cm

Sub-scripts (j)

act	denotes active material
add	denotes additional amount
Al	denotes aluminum thermal conductor
BB	denotes bus bar
сс	denotes current collector
cell	denotes cell
cell/mod	denotes cells per module
cnct	denotes contact
clnt	denotes coolant
const	denotes constant

cont	denotes container
ct	denotes connection tubes
e	denotes folded edge
Ε	denotes at rated energy
echem	denotes electrochemical processes
excess	denotes excess amounts
ext	denotes external
ft	denotes feedthrough
icnct	denotes interconnect
int	denotes interior
intf	denotes electrochemical interface
I/O	denotes inlet/outlet
jack	denotes pack jacket
layers	denotes layers in cell
max	denotes maximum
mod	denotes module
MRR	denotes module row rack
neg	denotes negative electrode
Р	denotes at rated power
pack	denotes pack
panel	denotes panel
pos	denotes positive electrode
p2t,gap	denotes gap between positive coating and terminal
ref	denotes condition at reference temperature
rstrnt	denotes restraint
sep	denotes separator
SOC	denotes property at rated state of charge
support	denotes support in module row rack
tab	denotes tab
term	denotes terminal
tgt	denotes target value
tol	denotes tolerance for assembly
upper	denotes upper portion of module row rack

wall	denotes wall
0	denotes default condition
//	denotes in parallel
2s,SOC	denotes default two-second ASI at starting SOC for pulse
10s,SOC	denotes default ten-second ASI at started SOC for pulse
10s,SOCe	denotes default ten-second ASI at ending SOC of pulse

Section 6

ASI105,50%	reference area specific resistance at ten seconds and 50% start of charge, $\Omega~\text{cm}^2$
L	length of the cell, cm
Q	specific capacity of active material, mAh/g
t_{chg}	charge time, s
T _{max}	maximum allowable cell temperature, °C
α	slope
β	intercept
δ_{pos}	thickness of positive electrode, cm
hoact/etrode	density of active material in electrode, gactive/cm ³ electrode

Section 7

C_i	applied unit cost of BMS component <i>i</i> , \$/unit
C_o	baseline unit cost of BMS component, \$/unit
$M_{vehicle}$	multiplier for the number of components needed based on vehicle
NASIC	number of ASIC per pack
$N_{cells/ASIC}$	number of cells per ASIC
$N_{cells/mod}$	number of cells per module
$N_{cells,//}$	number of cells in parallel
N_{fixed}	fixed number of components needed
N _{i/ASIC}	number of component <i>i</i> per ASIC
N _{i/pack}	number of component <i>i</i> per pack
$N_{mod/pack}$	number of modules per pack
$N_{mod,//}$	number of modules in parallel
Noffset	offset for the number of components needed

N _{pack/year}	number of packs manufactured per year
Nseries	number of cells in series in the pack
N_0	number of manufactured components in baseline unit cost
p	power factor

Section 8

A	area, cm ²
ASI	area-specific impedance, ohm cm ²
C_P	specific heat capacity, J/g/K
D_H	hydraulic diameter, cm
E	energy, Wh
Ė	energy usage rate, Wh/mile
f	factor, units vary
G	fluid mass flow rate, g/s/cm ²
Gz	Graetz number
h	heat transfer coefficient, W/cm ² /K
Ι	current, A
k_j	thermal conductivity of <i>j</i> , W/cm/K
L	length, cm
m	mass, kg
N_j	number of <i>j</i>
Nu	Nusselt number
Р	power, W
PC	performance coefficient for heat exchanger
Pr	Prandlt number
q	heat generation/transfer, W
$[q/\Delta T]$	denotes heat transfer per temperature difference, $W/^{\circ}C$
Q	volumetric flow rate, cm ³ /s
R	resistance, ohm
Re	Reynolds number
S	vehicle speed, mph
t	denotes time, s
Т	temperature, °C

и	velocity, cm/s
U	pack open circuit voltage for energy, V
V	pack voltage during sustained discharge, V
W	width, cm

Greek

δ_j	thickness of <i>j</i> , cm
ΔT	change in temperature, °C
μ_j	viscosity of <i>j</i> , poise
$\boldsymbol{\rho}_j$	density of j , g/cm ³

Sub-scripts

a	denotes accessory power
ad,dch	denotes adiabatic discharge
ad,pulse	denotes adiabatic power pulse
amb	denotes from ambient conditions
Al	denotes aluminum thermal conductor
c2w	denotes cell center to coolant wall
cells	denotes cells
cell,e	denotes heat rejection through pouch cell edge
cell,s	denotes heat rejection through pouch cell side
cells,//	denotes cells in parallel
clnt	denotes coolant
clnt,in	denotes coolant inlet
C,amb	denotes cold ambient conditions
d	denotes aerodynamic drag power
е	denotes efficiency from battery to wheels and accessories
Ε	denotes pack energy
e,dch	denotes discharge efficiency
exchg	denotes heat exchanger
f	denotes rolling friction power
heat	denotes heating
H,amb	denotes hot ambient conditions

insulation	denotes insulation in pack jacket
metal	denotes metal components between cell and coolant
<i>mod</i> ,//	denotes modules in parallel
pack	denotes pack
pos	denotes positive electrode
pulse	denote power pulse
ритр	denotes pump
p,add	denotes additional pressure drop
Р	denotes pack power
S	denotes sustained discharge
SS	denotes power to sustain speed S
start	denotes at start
w2f	denotes coolant wall to bulk fluid
x	denotes parallel to layers in cell
у	denotes across layers in cell

Section 9

С	capital cost of installed equipment for the designed battery, \$
C_o	capital cost of installed equipment for the baseline plant battery, \$
р	power factor
R	designed battery processing rate for specific process step
R_o	baseline plant processing rate for specific process step

ACKNOWLEDGEMENTS

The authors wish to thank Brian Cunningham, David Howell, Stephen Boyd, Peter Faguy, Tien Duong, Samuel Gillard, and Haiyan Croft of the U.S. Department of Energy's (DOE), Energy Efficiency and Renewable Energy (EERE), Vehicle Technologies Office (VTO) for supporting the development of the BatPaC model. The authors wish to thank David Robertson, Kevin Gallagher, Dennis Dees, Juhyun Song, Zhe Liu, Abhas Deva, and Gary Henriksen of Argonne National Laboratory. The authors also wish to thank Top Material Co., Ltd for their contributions to the manufacturing plant design. The authors express their gratitude to the many industrial partners that privately reviewed our work resulting in an improved final product. Default data was collected from cells produced and tested at the DOE Cell Analysis, Modeling, and Prototyping (CAMP) Facility at Argonne National Laboratory. The CAMP Facility is fully supported by the DOE, EERE, VTO.

EXECUTIVE SUMMARY

This manual details the fifth version of the Battery Performance and Cost (BatPaC v5.0) model developed at Argonne National Laboratory for lithium-ion battery packs used in transportation (file "BatPaC 5.0 2022-07-22.xlsm"). BatPaC is a publicly available model that performs a bottom-up lithium-ion battery design and cost calculation. The model designs the battery for a specified power, energy, and vehicle type (*i.e.*, hybrid, plug-in hybrid, or full-electric). The cost of the designed battery is calculated by accounting for every step in the lithium-ion battery manufacturing process. The original model and manual were publicly peer-reviewed by battery experts assembled by the U.S. Environmental Protection Agency. This revised model and manual include changes made in response to comments received from users and the observed trajectory of the industry.

BatPaC determines the size, weight, and cost of near-future electric vehicle packs assuming they are comprised of modules containing prismatic, stiff, pouch cells (Section 2). The design is calculated to meet performance, configuration, and manufacturing requirements set by the user. The inputs into BatPaC contain sufficient detail to facilitate the study of a range of topics that influence battery size and cost. This includes, but is not limited to, pack configuration, material properties, energy/power requirements, manufacturing steps, and production scale (Section 3). Default input values are provided for commercially relevant cell chemistries and vehicle types. The user can modify all relevant inputs and add new sets of default conditions (Section 4).

BatPaC uses an iterative process to generate a cell design that satisfies all user inputs. The resulting cell design is used to calculate the dimensions and performance of the modules and pack (Section 5). A major outcome of the design calculation is the thicknesses of the electrodes, which are determined to meet the power requirements of the cell. For all-electric vehicles, the thicknesses may also depend on charging requirements of the pack (Section 6). The cell, module, and pack designs are used to determine the battery management (Section 7) and thermal management (Section 8) systems for the pack. Liquid cooled systems are assumed for all packs in BatPaC v5.0. The results of the battery management and thermal designs are used to determine the final structure of the battery pack. The final pack design is used to inform the manufacturing cost model (Section 9) and recyclable quantities (Section 10). The manufacturing cost is calculated assuming a highly automated plant operating in the near-future. The costs of raw materials and purchased items assume near-future costs based on economies of scale.

1. INTRODUCTION

1.1 Motivation and History

The penetration of lithium-ion (Li-ion) batteries into the vehicle market has prompted interest in projecting and understanding the costs of Li-ion battery packs used to electrify the automotive powertrain. The model described here-in was developed at Argonne National Laboratory (ANL) for estimating performance metrics and manufacturing cost of Li-ion batteries for electric-drive vehicles. The model was developed to meet the following requirements:

- 1. Open and available to the entire community
- 2. Transparent in the assumptions made and method of calculation
- 3. Capable of designing a battery specifically for the requirements of an application
- 4. Accounts for the physical limitations that govern battery performance
- 5. Based on a bottom-up calculation approach to account for every cost factor

The Battery Performance and Cost (BatPaC) model is the product of long-term research and development at ANL. The BatPaC model and report (ANL-11/32) were first openly distributed to the public, free of charge, in November 2011 from the website <u>www.cse.anl.gov/batpac</u> [1]. This model was based on previously developed methods for designing Li-ion batteries for electric-drive vehicles using Microsoft[®] Office Excel spreadsheets [2–10]. It also included modeling of the manufacturing costs of the batteries. This original version of BatPaC was subjected to a public peer-review by battery experts assembled by the U.S. Environmental Protection Agency.

Since its original release, several versions of BatPaC have been developed to improve functionality, address comments received from users, and revise the model to match the trajectory of the industry. In late 2012, the model was updated to BatPaC v2.1 and a second edition of the manual (ANL-12/55) was made available [11]. In late 2017, BatPaC v3.1 was released, and the third edition of the manual (ANL/CSE-19/2) followed in early 2019 [12]. BatPaC v4.0 was released in early 2020 along with an addendum listing major changes. In addition to the major version releases, the model has been frequently updated, and the new versions have been made available on the same website with brief descriptions of the improvements. Over all versions, there have been 3000+ downloads from government agencies, leading universities, laboratories, and companies around the world.

1.2 Additions from Previous Versions

This is the fourth edition of the manual, which is being released in conjunction with BatPaC v5.0. The major updates from BatPaC v3.1 (third edition of the manual) to BatPaC v4.0 were as follows:

- Added the 'Dashboard,' 'Summary of Results,' 'BMU,' 'Recycle,' and 'Lists' worksheets
- Added VBA Macros for resetting the calculation and selecting default pack designs
- Included an NMC811-Graphite default chemistry couple
- Remodeled the 'Chem' worksheet and updated the default chemistry couple parameters

The major updates from BatPaC v4.0 to BatPaC v5.0 are as follows:

- Redesigned the cell, module, and pack to align with observed best-practices in industry
- Improved the calculation used to limit the electrode thickness based on fast-charge requirements of an all-electric vehicle
- Included the ability to design packs based on exceptional power requirements not encompassed by the default vehicles (*i.e.*, new pulse lengths and states of charge)
- Created energy- and power-type cells for all default chemistry couples
- Developed a tool contained in a new worksheet for generating new chemistry couples with self-consistent open circuit voltages and specific capacities (mAh/g) that depend on inputs for the desired negative-to-positive capacity ratio and losses during formation
- Added the ability to include additives in the cells
- Removed cabin-air as a cooling option
- Updated the battery management system (BMS, formerly BMU) calculation
- Added the operating temperature as an input, which modifies the area-specific impedance
- Included two new worksheets ("Vehicle Considerations" and "Default Vehicle Configurations") for modifying/adding default vehicles
- Redesigned the manufacturing plant, including changes to the processing steps, capital equipment costs, labor, plant size, plant utilities, scaling factors, and default size
- Provided the ability to adjust the percent utilization of the manufacturing plant
- Provided options for pack manufacturing method (*i.e.*, all manufacturing done in-house, purchase cells from third party, or purchase modules from third party) and pack cost (*i.e.*, with and with-out profits and warranty)
- Expanded the 'Recycle' worksheet to track recoverable scrap from the manufacturing floor
- Provided an "Errors and Warnings" section in the 'Dashboard' worksheet to guide the user away from common pitfalls in battery design
- Re-formatted and re-organized all worksheets
- Updated costs of raw materials and purchased items

This version of the manual contains constants and default inputs for the cost, materials, and vehicles. The constants in the manual correspond to those in "BatPaC 5.0 2022-07-22.xlsm," which is the latest version of BatPaC released with the manual. BatPaC may undergo slight modifications after this release to improve the accuracy and useability of the tool. As such, some of the constants in future versions of BatPaC v5.0 may deviate from those listed herein. The current version of BatPaC is listed on the following website: <u>https://www.anl.gov/cse/batpac-model-software</u>.

1.3 Overview of BatPaC Model

BatPaC takes user-defined performance requirements of a battery pack and designs a battery from cell to pack to meet the requirements, with a minimal demand of experimental data. The design information is then coupled with a manufacturing cost model to determine the total cost of the battery pack. A broad overview of this process is shown in Figure 1.1. In general, BatPaC starts by calculating a cell, module, and pack design based on user inputs (*e.g.*, pack power, pack energy,

fast charging requirements, physical constraints, etc.). Next, information and constraints from the designs are used to determine the battery management and thermal management systems for the pack. The results of the battery management and thermal designs are used to determine the final structure of the battery pack. Finally, BatPaC determines the manufacturing cost, recyclable quantities, and the total cost of the pack. Note that, although the schematic indicates the pack power, pack energy, design inputs, and constraints feed into the battery design, many of these parameters propagate throughout the BatPaC model.

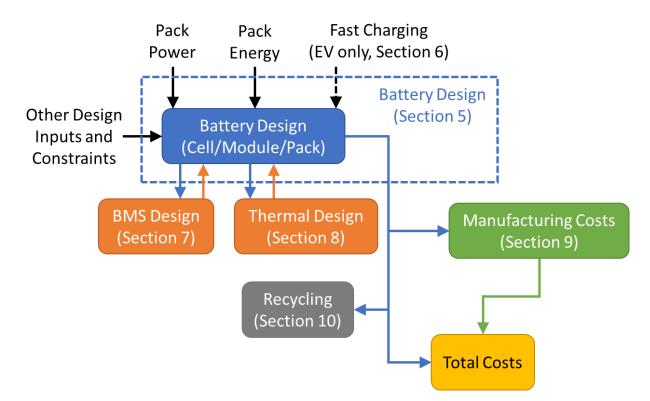


Figure 1.1. Overview of the process used by BatPaC to determine pack design and total cost.

This manual provides the information, assumptions, and equations necessary to use, modify, and understand the underlying calculations in the BatPaC tool. The manual starts with a description of the cell, module, and pack design assumed by the model (Section 2). Next, Section 3 provides an overview of the spreadsheet model, including instructions for using and modifying the tool. Section 4 describes how to add/modify the default vehicle options in the model. The remaining sections provide detailed information on the calculations in BatPaC. Section 5 discusses the battery design and performance modeling. Section 6 describes how BatPaC adjusts the design to account for electric vehicle charging. Section 7 details the battery management system calculations. Section 8 provides information on the thermal management system. Section 9 discusses the manufacturing cost calculations. Finally, section 10 describes an accounting system used to keep track of the recoverable materials at the end of life and during manufacturing of the pack.

2. BATTERY DESIGN FOR BATPAC

This section presents the key aspects to the battery pack design along with key terminology for using BatPaC effectively. It is suggested that one read this section before proceeding to the next sections.

2.1 Overview of Battery Design

A battery pack for an electrified vehicle consists of numerous cells linked together in combinations of series and parallel configurations to reach the desired pack voltage, energy, and power requirements. BatPaC calculates the mass, size, and cost of a battery pack assuming the pack is composed of modules containing stiff pouch cells. An overview of the elements in the battery pack is provided in Figure 2.1. Details on the components are provided in the next subsections.

The cell is the basic building block of the pack. It contains all the active materials. BatPaC assumes a stiff pouch cell, which indicates the type of enclosure and form-factor of the cell. The next level is the module, which contains multiple cells. The cells may be connected in combinations of series or parallel. The module also contains aluminum heat conductors wrapped around each cell for thermal management, a module management control system, terminals, and an enclosure. The module in Figure 2.1 is open on one side to show the cells stacked inside. The module is fully enclosed around the cells in the BatPaC design.

Next, BatPaC assumes that multiple modules are placed within a row rack. The row rack provides structural support to maintain compression on the modules. It also includes cooling panels to manage the heat generated by the cells in the modules. Finally, BatPaC assumes all row racks are connected to form the entire pack. The full pack includes the full battery management system and additional features for the thermal management system. Bus bars and terminals are also included for drawing power to and from the pack. Rows of modules and modules within rows can be connected in combinations of series and parallel to achieve the desired pack voltage. Note that unique design decisions will result in modifications to the generic pack structure described herein - *i.e.*, packs containing only one module or one row of modules. Details on how BatPaC accommodates these unique designs are provided in Section 5.

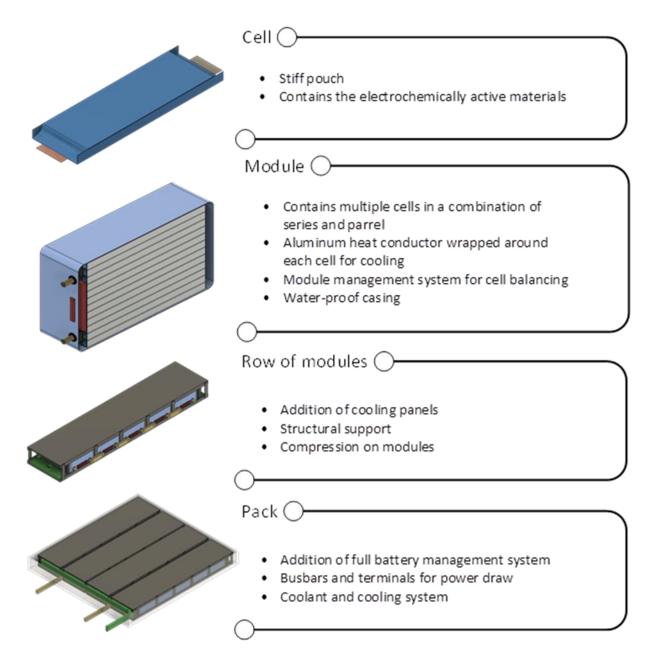


Figure 2.1. Overview of the pack design assumed by BatPaC v5.0. Packs are composed of rows of modules, which contain stiff pouch-cell batteries.

BatPaC contains four default vehicle types – mild hybrid-electric (mildHEV), high-power hybrid electric (HEV-HP), plug-in hybrid-electric (PHEV), and all-electric (EV) vehicles. BatPaC applies the same general pack format presented in Figure 2.1 for all vehicle types. That is, all vehicle packs are composed of modules containing stiff pouch cells. BatPaC modifies the cell and pack designs to account for different features required by the batteries in these vehicles. An overview of the important features for each vehicle type is provided in Table 2.1. Details on how the BatPaC calculation is modified to account for these features can be found in Sections 4.2 (overview), 4.3 (pack configuration), 5.7 (design inputs), and 9.2.3 (cost).

Battery related features for selected vehicles	mildHEV	HEV-HP	PHEV	EV
Start/stop system	✓	✓	✓	✓
Regenerative braking	×	\checkmark	\checkmark	\checkmark
Pulse power for short acceleration	×	✓	✓	✓
Charge depleting	×	×	\checkmark	\checkmark
Rechargeable	×	×	✓	✓
Pure electric	×	×	×	\checkmark
Power requirements (kW)	10 - 40	50 - 250	75 - 300	100 - 800
Energy requirements (kWh)	~1	1 – 10	10 - 20	50 - 200

Table 2.1. Overview of battery features accounted for by BatPaC

2.2 Cell Design

BatPaC uses a stiff pouch for the cell format. A full explanation of the cell sizing is provided in Section 5.2. A schematic showing the main features of the cell is shown in Figure 2.2. The cell is comprised of positive and negative electrodes coated on current collectors with separators placed between the layers. Figure 2.2a shows a schematic of a single bi-cell layer within the pouch and a detailed view is shown in Figure 2.3. The bi-cell layer contains enough material to make two unit-cells – *i.e.*, one positive foil coated on both sides with positive electrodes, one negative foil coated on both sides with negative electrodes, and two separators. The positive and negative electrodes are composite materials containing quantities of active materials, carbon conductors, and binders. The active materials are signified as the large spheres in Figure 2.3.

The schematic in Figure 2.2a is not to scale since the thickness of the electrodes (μ m length-scale) is much smaller than the length of the cell (cm length-scale) in a real cell. The schematic demonstrates how the separator overlaps the electrodes to prevent shorting. The exact dimensions of this overlap (and dimensions for the electrodes) are discussed in more detail in Section 5.2.5. The schematic also accentuates how the positive and negative foils extend past the coated electrode regions to provide current collectors.

In the cell, tens to hundreds of bi-cell layers are stacked on top of each other and welded to positive and negative tabs through the current collectors (see Figure 2.2b). The entire, welded stack is then inserted into a stiff pouch composed of polymer-coated aluminum, filled with electrolyte, and sealed. The positive and negative tabs extend out of the sealed pouch for electrical connection (see Figure 2.2c).

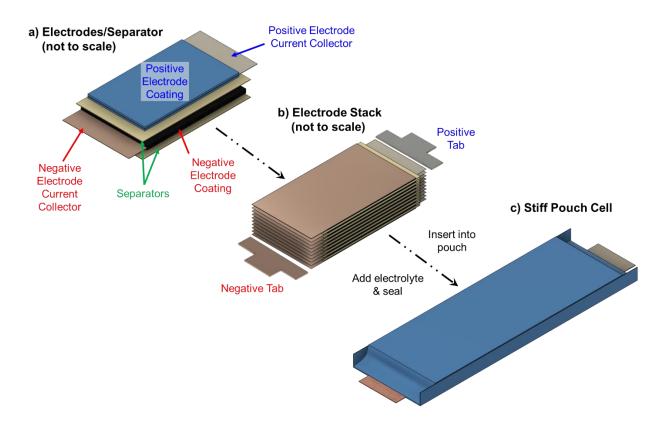


Figure 2.2. Schematic of the stiff pouch cell design showing a) a single bi-cell layer of electrodes and separators, b) a full electrode stack and tabs that will be welded to the current collectors, and c) the final stiff pouch cell containing the electrode stack and filled with electrolyte. Images are drawn to accentuate features. Thicknesses in a) and b) are not to scale.

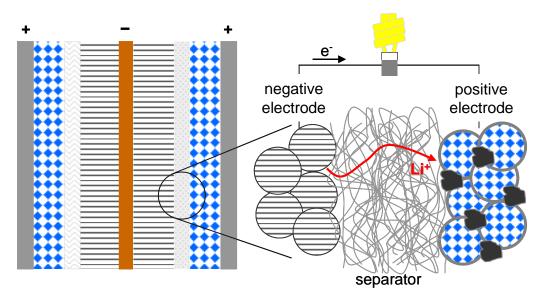


Figure 2.3. Detailed schematic of a bi-cell layer within the pouch cell.

2.3 Module Design

BatPaC v5.0 assumes all cells in the pack are contained within modules. There are several advantages to containing the cells in modules, as opposed to free standing cells within the pack. These advantages include easier manufacturing, easier scaling of the pack, increased safety, and improved monitoring. Figure 2.4 provides an overview of all components in the module. The cells in the modules are stacked on-top of each other with an aluminum thermal conductor placed in between each cell. Front and back interconnect panels are used to connect the positive and negative tabs from each cell. Both panels contain cell interconnects. The interconnects are welded to the cell tabs and can be configured to connect cells in series or parallel (see Figure 2.5). The front interconnect panel also includes tabs to connect to the module terminals.

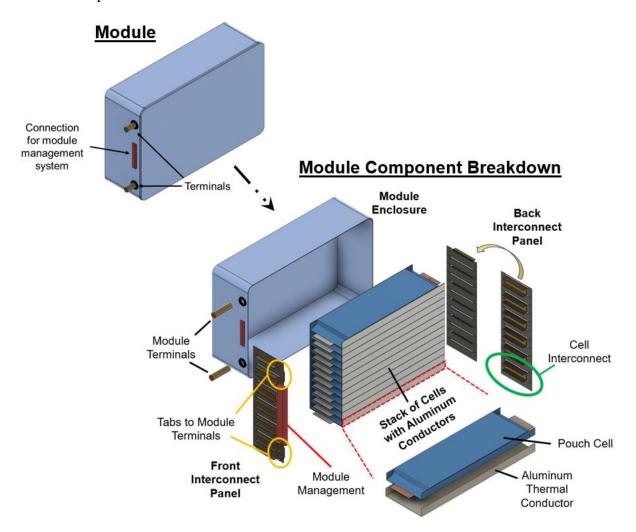


Figure 2.4 Breakdown of key components in the battery module.

The module terminals are used to connect between modules. A space is left near the front interconnect panel for the module management unit, which is tied into the larger battery management system (see Section 7). The entire set of components (cells, aluminum conductors,

interconnects, and module management) are contained within an enclosure. BatPaC assumes the enclosure is made of steel. The components fit tightly within the enclosure, whereby there is direct contact between the aluminum thermal conductors around the cells and the wall of the enclosure. This is necessary for the cooling system to work effectively (see Section 8Error! Reference source not found.). The enclosure also includes a provision for gas release (not shown) to protect the system in the event of a cell failure.

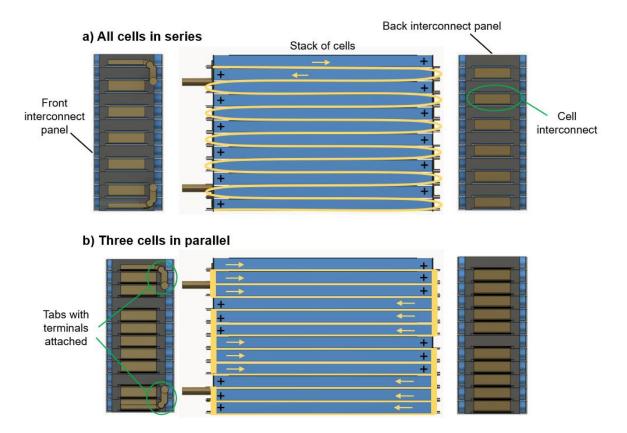


Figure 2.5. Two example cell configurations in the module, which demonstrate the ability of the cell interconnect system to accommodate a variety of cell configurations: a) all cells in series and b) three cells in parallel. Positive sign denotes the polarity of the cell in the stack. Yellow lines and arrows show the electron path through the cell stack.

2.4 Row-of-Modules Design

BatPaC v5.0 assumes all modules are placed within rows before constructing the pack. Figure 2.6 provides a breakdown of all the components which go into the row, which is also referred to as a row rack. Multiple modules are connected using module interconnects, and polymer pads are placed in between the modules for support. The module interconnection shown in Figure 2.6 is an example of a row where all modules are connected in series. Other parallel and series connections are possible between modules within the pack and Section 5.5.2 covers these options in more detail. In addition, the module interconnects appear metallic in the image but are insulated within the pack. The row rack also contains a cooling system comprised of coolant panels, an inlet, an outlet, and connecting tubes between the panels. BatPaC assumes the coolant panels are made of

stainless steel to provide structural support and resistance to corrosion from the coolant. Note that BatPaC v5.0 assumes all packs are liquid cooled. A structural support system is also included in the row rack, which contains top and bottom support channels, side rails, and restraint plates. BatPaC assumes these components are made from stainless steel. The restraint plates are used to provide compression on the cells. The cells are oriented within the modules to force compression on the largest faces of the cells. The structural support system encompasses the coolant panels and the modules to form the row rack. Note that Figure 2.6 is meant to show the major systems within the row rack and has no indication on the expected order of assembly.

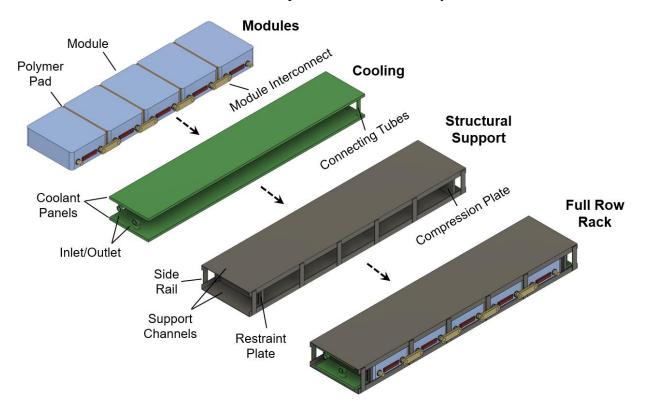


Figure 2.6. Breakdown of the components which go into the row rack of modules.

2.5 Pack Design

The pack is constructed with all the module row racks and includes additional components for battery and thermal management. A breakdown of the main components can be found in Figure 2.7. The additional components outside the module row racks consist of bus bars, main tubing for the coolant, and pack terminals. The bus bar included in the figure is explicit for the generic pack design shown in this section. The number and location of bus bars will depend on the pack configuration (*i.e.*, number of module rows and series/parallel connections). Details on how BatPaC handles these design variations can be found in Section 5.5. The main tubing shown in Figure 2.7 is used to bring coolant in and out of the row racks.

The components in the figure are all enclosed in a pack jacket. The structure of the pack jacket is more detailed than what is shown in the figure. The jacket is comprised of insulation sandwiched

between two metal layers. The top and sides of the jacket use aluminum as the interior and exterior metal. The bottom base uses aluminum for the interior and steel for the exterior. Steel is used at the exterior to prevent puncturing on the undercarriage of the vehicle. The jacket also includes a steel perimeter frame (not shown) that goes around the outside of the base and has a lip which extends slightly up the sides to provide additional support. The size and inclusion of the steel frame depends on the size of the pack (see Section 5.5 for details).

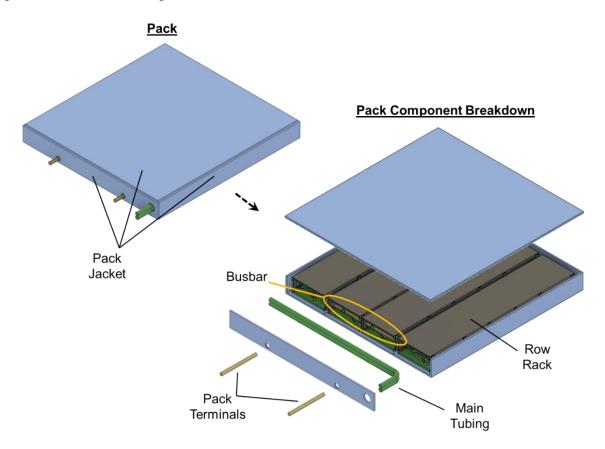


Figure 2.7. Breakdown of main components in battery pack.

The pack in BatPaC also contains additional elements for the battery and thermal management systems, which are not shown in the figure (see Sections 7 and 8 for details). Some elements, such as disconnects, power electronics, pumps and coolant mixing equipment, are assumed to exist outside the main pack. Their mass and volume are accounted for in the calculations, but BatPaC does not specify their locations. Their locations will depend on the exact design of the vehicle and how the pack is situated amongst other vehicle components. There are also additional, smaller components (wiring, fuses, circuit boards, etc.) that exist within the main pack. Their mass is included in the calculation, but their volume is not. They are assumed to reside within the void space left between the other pack components. They are not shown in Figure 2.7 to prevent over-cluttering of the image with small components. Their locations will also depend on manufacturer preference and are not provided by BatPaC.

3. DESCRIPTION OF THE SPREADSHEET MODEL AND INSTRUCTIONS FOR USE

3.1 Background and General Instructions

The model is based on the use of Microsoft[®] Office Excel spreadsheets. The following subsections provide an explanation on how to operate the spreadsheet-based model. **The user is advised to save the original document separately as a back-up copy**. Corruption of the calculations is possible and will likely occur during use by someone unfamiliar with the model.

This Microsoft[®] Office Excel workbook requires the use of iteration. The iterative function may be enabled by going to File > Options > Formulas. Check the box next to "Iteration" and change the maximum number of iterations to 1000 (Figure 3.1). (The latter change is less important for this version than in the past because the calculations almost always come to the final answer in well under the default Excel value of 100 iterations.) If the iteration setting is not turned on, the software will present an error complaining about circular references. If the model is opened while a different Excel spreadsheet is in use, the software may also warn of an error.

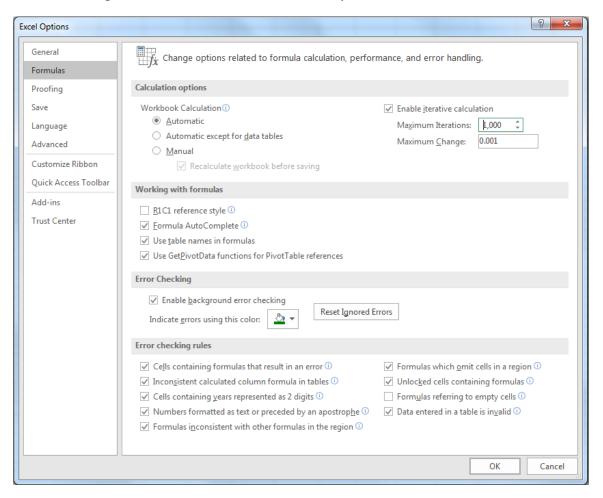


Figure 3.1. Automatic iteration must be enabled for the spreadsheet model to function

In addition, several features and tools require macros to be enabled in the workbook. While they are not required to run the model, they improve the functionality. To enable macros in Excel, select "Developer" in the ribbon (Figure 3.2). Then choose "Macro Security" and make sure "Enable all macros" is selected in the pop-up window that appears. Click "OK" once this is confirmed.

File Home Insert	Add Excel COM Insert Design View Code Source	E Import
Trust Center Trusted Publishers Trusted Locations Trusted Documents Trusted Add-in Catalogs Add-ins	Macro Settings Disable all macros without notification Disable all macros with notification Disable all macros with notification Disable all macros (not recommended; potentially dangerous code can run)	? ×
ActiveX Settings Macro Settings Protected View Message Bar External Content File Block Settings Privacy Options Form-based Sign-in	Developer Macro Settings □ Trust access to the ¥BA project object model	
	OK	Cancel

Figure 3.2. Image showing how to enable macros in Microsoft Excel.

3.2 Dashboard Worksheet

Most of the functionality of BatPaC can be controlled through the 'Dashboard' worksheet. This worksheet includes commonly altered user inputs, a summary of key outputs, and possible error warnings associated with the battery design. This section provides a description of 'Dashboard' with information on how to alter the inputs and read the results.

3.2.1 Dashboard Ribbon

The top ribbon of 'Dashboard' is frozen in place (Figure 3.3). One of the most important features of the ribbon is the ability to reset the calculation, which is located at the bottom. A reset of the calculation is recommended after changing design inputs. It is also required to re-converge the model if the output cells show a #N/A error. To reset the calculator:

If Macros are Enabled: CTRL + SHIFT + R

If Macros are NOT Enabled: Set the cell to the right of "Restart 0/1" in the 'Dashboard' ribbon to 0, then change back to 1

Dashboard							
EV with NMC811-G (Energy) Electrodes							
Applied inpu	t (can only be changed using overrides)	Default input values (may	be changed) Required input by user		Optional override input		
Reset Calculation							
	Restart (0/1)	1	OR	OR CTRL+ SHIFT + R if Macro Enabled to Reconverge Calculation			

Figure 3.3. Top ribbon of dashboard showing cell color-coating key and how to reset calcualtion.

The ribbon also provides a description of the vehicle and electrode couple under investigation. For instance, "EV with NMC811-G (Energy) Electrodes" is shown in Figure 3.3. This indicates the model is being solved for an all-electric vehicle, EV (*i.e.*, not hybrid), with cells designed for energy applications that contain $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$ (NMC811) as the positive electrode and graphite (G) as the negative electrode. Directions on how to change these values are provided later in this section. The ribbon also describes the four types of input cells in BatPaC. These four input types are:

Applied Input Cells – Purple cells are applied values that will be used for your simulation. These cells **should not be changed directly**; To change their value, use one of the other input cells. This is important because these cells contain information on default values that could be over-ridden (and lost) if changed directly.

Default Input Values (may be changed) – Yellow cells contain defaults that are generally applicable, but the user may alter directly. The default value of these cells is often listed at the end of the row label for reference. It is preferred that these cells are only changed by expert users who have read the full user manual and understand the interactions of the workbook.

Required Input by User – Blue cells contain default values that the user may accept or change. They represent the key design and manufacturing parameters for the battery pack. These include the chemistry, type of battery, battery configuration, manufacturing strategy, etc. Several of these cells use drop down lists, while others require direct input. For example, there is a drop-down menu to choose the vehicle type – *i.e.*, electric vehicle (EV), plug-in hybrid-electric vehicle (PHEV), high-power hybrid-electric vehicle (HEV-HP), or mild hybrid-electric vehicle (mildHEV).

Optional Override Input – Green cells are optional overrides. They are left blank by default. When a user inputs a value into a green cell, it will override the default value in the adjacent purple cell.

The ribbon in 'Dashboard' also includes a table of contents (Figure 3.4). Users can quickly jump to the main worksheets in the workbook using the links in the table of contents. Most worksheets in BatPaC contain a ribbon with the vehicle and electrode descriptions, the cell-input guide, and

the table of contents. Only the 'Dashboard' ribbon contains the calculation restart cell; however, the calculation can be restarted on any tab using the macro-enabled method (Crtl+Shift+R).

Table of Contents (jump to worksheet)				
Dashboard	Manufacturing Costs			
Summary of Results	Cost Input			
<u>Chem</u>	Cost Breakdown			
Battery Design	Recycle			
BMS	<u>Thermal</u>			

Figure 3.4. Table of contents at the top of the 'Dashboard' (and other) worksheets for quick navigation.

3.2.2 Dashboard Inputs

1

3.2.2.1 Chemistry Inputs

The inputs in 'Dashboard' are separated into three main categories: chemistry, battery design, and manufacturing costs. Figure 3.5 shows a screenshot of the chemistry-related inputs that can be changed on 'Dashboard.' Details on how these inputs influence the battery design can be found in Section 5. The first input is the electrode couple, which can be selected using the drop-down menu in the blue cell. The menu contains all the default electrode couples available in BatPaC. The first part of the electrode couple label (before the dash) corresponds to the positive electrode active material. The second part of the label (after the dash) corresponds to the negative electrode active material. The description in the parentheses defines whether a power or energy couple was selected.

The designation of power and energy couples is a new feature in BatPaC v5.0. For every default electrode couple, a power and energy couple are provided which have different electrode designs tailored to high-power or high-energy applications, respectively. Power couples typically provide more favorable designs when the power-to-energy ratio of the pack is greater than 15. Table 3.1 provides an overview of the property differences between the two couples. The power couples are better suited at high-power because they have lower area-specific impedances (ASI), which correspond to lower voltage losses during high-current (*i.e.*, high-power) discharges. The energy couples are better suited for high-energy applications because they are more energy-dense, resulting in more compact cell designs. See the overview of the 'Chem' worksheet in Section 3.4 for more information.

istry	Drop-down menu			
	Current Selection	Choose		
Electrode Couple	NMC811-G (Energy)	NMC811-G (Energy)		
Positive Electrode: Li(Ni0.8Mn0.1Co0.1)O2		Override		
Positive active material specific capacity, mAh/g	214			
Void volume fraction, % of positive electrode	25			
Positive foil thickness, µm	15			
Maximum positive electrode thickness, µm	120			
Negative Electrode: Graphite				
Negative active material specific capacity, mAh/g	360			
N/P capacity ratio after formation	1.10			
Void volume fraction, % of negative electrode	25			
Negative current collector thickness, µm	10			
Separator thickness, µm	15			

Figure 3.5. Chemistry inputs on 'Dashboard'

Table 3.1. Overview of	f electrode desig	gn changes for	r default pow	er and energy couples

	Power	Energy
Positive active material particle radius, µm		
Manganese spinel and layered oxides [†]	1.00	2.00
Lithium-iron-phosphate (LFP)	0.25	0.50
Negative active material particle radius, µm		
Graphite	4.00	6.00
Lithium-titanate (LTO)	0.25	0.50
Porosity (both electrodes)	0.25	0.35
Current collector thickness, µm		
Positive (aluminum)	20	15
Negative (copper) ^{††}	15	10
Positive wt.% (active:carbon:binder)	94:4:2	96:2:2
Negative wt.% (active:carbon:binder)		
Graphite	96:2:2	98:0:2
Lithium-titanate (LTO)	94:4:2	96:2:2

[†] nickel-cobalt-aluminum oxide (NCA), nickel-manganese-cobalt oxide (NMC), and lithium manganese oxide (LMO)

^{††} aluminum used for LTO

The chemistry inputs in Figure 3.5 (purple cells) automatically update when an electrode couple is selected. The values can be overridden by entering values into the green cells. 'Dashboard' provides the most-commonly adjusted properties -i.e., the specific capacities of the electrodes in mAh/g, the thicknesses of the current collectors and separator, the porosity of both electrodes, and the negative-to-positive capacity ratio after formation (N/P or N:P). 'Dashboard' also includes the

maximum allowable positive electrode thickness. This value impacts the battery design and is discussed in detail in Section 5. All other chemistry-related values (including several in Table 3.1) can be overridden in the 'Chem' worksheet.

3.2.2.2 Battery Design Inputs

The battery design section (Figure 3.6) on 'Dashboard' provides all the input parameters for designing the battery. The first section is general information, where the user can change the vehicle type, modify the cutoff states of charge (SOCs), and turn on charging requirements. The vehicle type can be changed using the drop-down menu in the blue cell labeled "Vehicle Type." Changing the vehicle type will impact default design choices described in detail in Sections 4 and 5. This includes the default upper and lower cutoff SOCs. The ability to turn on charging requirements is only available when an all-electric vehicle (EV) is selected. Figure 3.7a shows that, when this cell is set to "Yes," an additional set of inputs become available under "Extras" in "Power and Storage Requirements." These extra inputs allow the user to specify the minimum time to recharge the pack from 15% to 95% SOC. Details on how this impacts the battery design are provided in Section 6.

The second section in battery design is power and storage requirements. For most of the inputs in this section (and all remaining input sections), values can be provided for up to seven batteries (in columns). BatPaC performs the cost and size calculations simultaneously for all seven batteries, which are included to allow for quick comparisons between batteries with different inputs. Parameterization across the seven batteries is available for most inputs in battery design and manufacturing. Note that chemistry-dependent inputs like material properties and costs are not adjustable and the same value is applied across all seven batteries.

The first part of the second section is power requirements, which includes the rated peak power of the pack, the duration at rated power, and the operating initial SOC at rated power. The first is a required user input. The latter two are typically default values that change with vehicle type. The user can modify their values by setting "Use default power requirements for vehicle" to "No" (see Figure 3.7b). The battery is designed to achieve the rated power for the entirety of a power-pulse that is started at the input, initial SOC and lasts the input duration.

The second part of the power and storage requirements section is the storage requirements, which are set through either the pack capacity (Ah) or the pack energy (kWh). A value should only be specified for the capacity or the energy. Specifying a value for both over constrains the model (see Section 5) and will produce inaccurate results.

The third part of this section is extra requirements, which include the time to recharge (discussed previously), an optional override for the positive electrode thickness (which sets the positive electrode thickness as an input value), and the average operating temperature during discharge. Caution should be taken when using the override feature for the positive electrode since setting this value may prevent the model from meeting other inputs such as power or charging time.

al								
		Current Selection	Choose			OEM Upper Cuttoff SOC	95	
	Vehicle Type	EV	EV	🔨 D	rop	OEM Lower Cutoff SOC	10	
	Calculate Charging Requirements?	No	No		own	Useable battery energy, % of total (EV)	85	
an	d Storage Requirements							
	Pawer							
		Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Batte
	Target pack rated peak power, kW	300	300	300	300	300	300	30
	Use default power requirements for vehicle				Yes			
	Duration at rated power, s	10	10	10	10	10	10	10
	Barakarrakhatesponer, s	~						10
	Operating initial SOC for rated peak power, %	20	20	20	20	20	20	20
					non d			
				υ	rop a	own me	enu —	
	Storage							
	Fill in value for either capacity or energy	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Batte
	Total pack capacity, 0-100% SOC (Ah)							
	Total pack energy, 0-100% SDC (kWh)	100.0	100.0	100.0	100.0	100.0	100.0	100.
	Extras							-
		Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Batte
	To select time to recharge, fast charge must be enable							
	Optional positive electrode thickness override, µm							
	Australia Australia di vica di sebuara							
	Average temperature during discharge (default = 30°C), °C	30	30	30	30	30	30	30
	Pack Configuration	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Batte
	Number of cells per module	Battery 1 12	Battery Z 12	Battery 3	20 Battery 4	Battery 5 20	Battery 6	Batte 12
	Number of cells in parallel	4	2	3	20	20	3	4
			5	6	5	4	5	6
		5		0				
	Number of modules in row	5		4	4	4	4	4
	Number of modules in row Number of rows of modules per pack	4	4	4	4	4	4	4
	Number of modules in row Number of rows of modules per pack Number of modules in parallel		4	1	2	4	4	4
	Number of modules in row Number of rows of modules per pack	4	4	1	2			

Figure 3.6. Battery design section for the inputs on 'Dashboard'

The final part of this section is pack configuration, which contains inputs for the cell and module configurations in the pack. This includes the number of cells per module, the number of cells in parallel, the number of modules in a row, the number of module rows in the pack, and the number of modules in parallel.

Finally, there is a button at the bottom of the power and storage requirement section labeled "Add set of default pack designs (power, energy, pack configurations)." Macros must be enabled to use the button. If clicked, the button will cycle through default conditions and load their values in the appropriate inputs for all seven batteries. Different default conditions are available for each vehicle type. Information on how to add default sets is provided in Section 4.

		Current Selection	Choose			OEM Upper Cuttoff SOC	95			
	Vehicle Type	EV	EV	<<< Fast Ch usable for se	arging only lect vehicles	OEM Lower Cutoff SOC	10			
a)	Calculate Charging Requirements?	Yes	Yes			Useable battery energy, % of total (EV)	85			
Power and storage requirements										
	Pawer									
_	Target pack rated peak power, kW	Battery 1 300	Battery 2 300	Battery 3 300	Battery 4 300	Battery 5 300	Battery 6 300	Battery 7 300		
b)	Use default power requirements for vehicle				No					
	Duration at rated nower is	10	10	10	10	10	10	10		
	Override duration at rated peak power, s									
	Uperating initial SUC for rated peak power. %	20	20	20	20	20	20	20		
	Override for operating initial SDC for rated peak power, %									
Δn	pears when "Use def	ault pov					hicle"	= No		
γp	Fill in value for either capacity or energy	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7		
γp										
γp	Total pack capacity, 0-100% SOC (Ah)									
ΛP		100.0	100.0	100.0	100.0	100.0	100.0	100.0		
ΛP	Total pack capacity, 0-100% SOC (Ah)									
	Total pack capacity, 0-100% SOC (Ah) Total pack energy, 0-100% SOC (kWh) <i>Entras</i>	100.0 Battery 1					100.0 Batterv 6			
	Total pack capacity, 0-100% SOC (Åh) Total pack energy, 0-100% SOC (kWh)									

Appears when "Calculate Charging Requirements" = Yes

Figure 3.7. Modifications to battery design inputs upon selection of non-default values from pulldown menus. a) When "Calculate Charging Requirements" is set to "Yes," "Time to recharge" becomes available. b) When "Use default power requirements for vehicle" is set to "No," override options for duration and initial SOC at rated power become available.

3.2.2.3 Manufacturing and Cost Inputs

The final input section is for manufacturing and cost inputs (Figure 3.8). The first sub-section is for the main material costs. Default values are provided for the active materials, carbon additives, binders, and solvents in both the positive and negative electrodes. Costs for the aluminum current collector foil, copper current collector, separator, and electrolyte are also provided. The cost basis (*e.g.*, $\frac{k}{g}$, $\frac{m^2}{r}$, or $\frac{k}{L}$) for each value is included in the label to the left of the cell. The default values will change when different electrode couples are selected. The user can override the cost values using the green cells. The same set of data and override options exist in the 'Chem' worksheet. Other purchased items included in the cell, module, and pack – like terminals, interconnects, and enclosures – are found in the 'Cost Input' worksheet. See Section 9 for more detail on these items.

								_
Positive Electrode, \$/kg		Override						+
Active material, \$/kg	\$26.00	Override						+
Carbon additive, \$/kg	\$26.00							+
Binder, S/kg	\$7.00							+
Solvent (NMP), \$/kg	\$15.00							+
Solvent (NMP), s/kg	\$2.70							
Negative electrode, \$/kg		Override			No	t availa	able for	r
Active material, \$/kg	\$10.00	CTOTTING .						
Carbon additive, S/kg	\$7.00				— pia	ant utili	zation	
Binder, \$/kg	\$10.00							-
Solvent (Water), \$/kg	\$0.00					Metho	u I	
AI foil, \$/m ²	\$0.20							T
Cu foil, \$/m ²	\$1.20							
Separator, \$/m ²	\$0.90							
Electrolyte, \$/L	\$10.00							
pecifications								_
pecifications	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7	
	Battery 1 500,000	Battery 2 500,000	Battery 3 500,000	Battery 4 500,000	Battery 5 500,000	Battery 6 500,000	Battery 7 500,000	
Number of packs manufactured per year	500,000	500,000	500,000	500,000	500,000	500,000	500,000	
pecifications	500,000		500,000	500,000	500,000	500,000	500,000	
Decifications Number of packs manufactured per year Method to calculate plant utilization	500,000 Method 2: Purch	500,000 nase land and building for 100	500,000	500,000	500,000	500,000	500,000 levels	
Decifications Number of packs manufactured per year Method to calculate plant utilization In addition, fill in values for one of the two below	500,000	500,000	500,000	500,000	500,000	500,000	500,000	
Number of packs manufactured per year Method to calculate plant utilization In addition, fill in vulues for one of the two below Packs manufactured at 100% utilization (pack/year)	500,000 Method 2: Purch	500,000 nase land and building for 100	500,000 0% utilization, bu	500,000 t only purchase e	500,000 quipment for curre	500,000 ent production	500,000 levels	
Number of packs manufactured per year Method to calculate plant utilization In addition, fill in values for one of the two below Packs manufactured at 100% utilization (pack/year) Percent plant utilization (%)	500,000 Method 2: Purch 100%	500,000 nase land and building for 100	500,000 0% utilization, bu 100%	500,000 t only purchase e	500,000 quipment for curre	500,000 ent production	500,000 levels	
Decifications Number of packs manufactured per year Method to calculate plant utilization In addition, fill in values for one of the two below Packs manufactured at 100% utilization (pack/year) Percent plant utilization (%) Cell yield, % of built cells that pass inspection	500,000 Method 2: Purch 100%	500,000 nase land and building for 100 100%	500,000 0% utilization, bu 100%	500,000 t only purchase e	500,000 quipment for curre	500,000 ent production	500,000 levels	
Decifications Number of packs manufactured per year Method to calculate plant utilization In addition, fill in values for one of the two below Packs manufactured at 100% utilization (pack/year) Percent plant utilization (%) Cell yield, % of built cells that pass inspection	500,000 Method 2: Purch 100%	500,000 nase land and building for 100 100% Dwn menus	500,000 0% utilization, bu 100%	500,000 t only purchase e 100%	500,000 quipment for curre	500,000 ent production	500,000 levels	
Decifications Number of packs manufactured per year Method to calculate plant utilization In addition, fill in values for one of the two below Packs manufactured at 100% utilization (pack/year) Percent plant utilization (%) Cell yield, % of built cells that pass inspection Ianufacturing Method and Cost Options	500,000 Method 2: Purch 100%	500,000 hase land and building for 100 100% Nown menus All m	500,000 1% utilization, bu 100% 95 anu facturing in-	500,000 t only purchase e 100%	500,000 quipment for curre 100%	500,000 ent production	500,000 levels	

Figure 3.8. Manufacturing and cost inputs in 'Dashboard.'

The next subsection is plant specifications, where the user can specify the number of packs manufactured per year for each of the seven batteries. The user can also choose from three methods for the plant utilization using a pull-down menu. The chosen method is applied to all seven batteries. Method one assumes the plant is operating at 100% utilization. Method two assumes the space has been built to operate at 100% utilization (*i.e.*, land and building costs are sized for full capacity), but the equipment inside the plant has only been purchased to match current production levels at <100%. Method three assumes that the land, building, and equipment have been purchased to match full production capacity, but the plant is operating at <100%. If method two or three is selected, two additional lines appear to specify the degree of utilization for the seven batteries (see Figure 3.8). Two options are provided. The user should only specify one of the two. The utilization can be specified by inputting i) the number of packs produced if the plant were to operate at 100% utilization or *ii*) the percent utilization of the plant. The user input for number of packs manufactured per year is the actual number of packs manufactured. For example, 100,000 packs manufactured per year at a 50% utilization will cause BatPaC to size a plant for 200,000 packs per year. Details on how the utilization methods impact the calculated manufacturing cost can be found in Section 9.5.2. Finally, the last input in this subsection is the cell yield defined as the percentage of built cells that pass inspection. This value is applied to all seven batteries.

The final subsection provides two drop-down menus for modifying the pack manufacturing method and cost options. Three options are provided for the manufacturing method: i) all manufacturing from cells to modules to packs is done in-house, ii) the cells are purchased from a battery manufacturer and used to manufacture the modules and packs, and iii) the modules are purchased from a battery manufacturer and used to manufacture the packs. Option one is the

default in BatPaC. It reflects the business practice whereby battery manufacturers and vehicle makers have a joint effort to assemble the full vehicle pack at one facility. Options two and three reflect practices where vehicle makers buy most of the components from battery manufacturers. These options include additional mark-ups for profits and warranty on the cells modules. Further details on how these scenarios impact the calculated manufacturing cost can be found in Section 9.6.4. Two options are also provided for determining the pack cost: *i*) "Cost to consumer" which includes profits and warranty on the total pack and *ii*) "Cost to build" which does not include additions for profits and warranty. BatPaC's default conditions assume all manufacturing is done in house and the cost includes profits and warranty.

3.2.3 Dashboard Results

3.2.3.1 Calculation and Validation Results

The first section of the results in 'Dashboard' provides validation of the calculation (Figure 3.9a). It starts with configuration errors and warnings, which appear if BatPaC detects issues in the inputs. If an issue is detected, a number will appear in either the errors or warnings row. The number correlates to an error message described in a table located to the right of this section. The table is reproduced in Figure 3.9b. This table can be moved anywhere within 'Dashboard' for the user's convenience. Errors (#1 to #4) correspond to physical issues with the pack which must be addressed by changing the inputs. The first two correspond to improper configurations where either the number of cells is not divisible by the number of cells in parallel or the number of modules is not divisible by the number of modules in parallel. The third error occurs if the SOC during the pulse at rated power goes below the lower SOC cutoff. This may occur if the default power requirements are modified as shown in Section 3.2.2.2. The fourth error occurs if the electrode thickness calculated by BatPaC to meet the power/energy requirements is below the minimum allowable thickness. The minimum allowable thickness is set in the 'Chem' worksheet and usually correlates to manufacturing limitations. The fourth error usually occurs when the power-to-energy ratio is too high.

Warnings (#5 to #12) correspond to minor issues with the pack design which the user may want to address. Some of these issues cause slight inaccuracies in the sizing of supporting components. Others lead to poorly designed packs. The first warning (#5) triggers when the number of rows of modules is not 1, 2, or 4. Configurations outside these values require additional bus bars, which increase the size and mass of the pack (refer to Section 5.5.1). The second warning (#6) triggers if the number of modules in parallel is greater than two, which may cause BatPaC to underestimate the number and mass of module-to-module interconnects. Higher levels of parallelization should be handled amongst the cell-to-cell connections (*i.e.*, increase the number of cells in parallel). See Section 5.5.2 for details. The third warning (#7) triggers if the pulse at rated power goes below the reserve safety margin. This can only happen if non-default power requirements are used. Each vehicle type has a set safety margin, defined as a certain SOC above the SOC lower limit, that should be avoided to ensure reliable operation of the battery. BatPaC includes default values for each vehicle type, which are discussed in more detail in Section 4.

Warnings #8 and #9 trigger if a power or energy electrode couple are selected, but the other couple may be more suited for the vehicle type under consideration. For example, high-power hybridelectric vehicles (HEV-HP) and all-electric vehicles (EVs) are typically better served by power and energy couples, respectively. Power couples typically provide more favorable designs when the pack power-to-energy ratio is greater than 15. Warning #10 triggers if multiple pack dimensions exceed five feet because the pack may not be able to fit within a vehicle. Warning #11 triggers if the pack voltage exceeds 1000 V because this will cause underestimations in the battery management system (see Section 7). High voltages also introduce additional safety concerns which pack designers may want to avoid. Warnings #10 and #11 can be addressed by modifying the pack configuration. The final warning (#12) occurs if the power required to meet the set charging time is larger than the charger specifications. This may occur if the pack energy is too high, relative to the desired charge time. This warning is only active for EVs with "Calculate Charging Requirements?" set to "Yes" (see Section 3.2.2.2). The default value of 150 kW can be overridden in the "Electrode Thickness Calculations" portion of the 'Battery Design' worksheet.

	Results									
Calculation and Validation										
	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7			
Configuration Errors (see table to right)	None									
Configuration Warnings (see table to right)	None									
Plant Size, GWh	50.0	50.0	50.0	50.0	50.0	50.0	50.0			
Power-to-energy ratio	3.00	3.00	3.00	3.00	3.00	3.00	3.00			
Adequacy of cooling	Excellent									
	Max									
Cathode thickness limited by	Thickness									

b) (

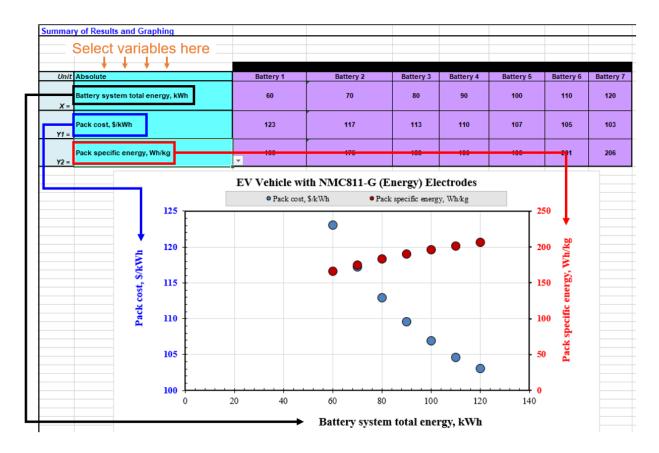
	Warnings and Errors								
Number	Error								
1	Error: Number or cells not divisible by number of cells in parallel								
2	Error: Number of modules not divisible by number of modules in parallel								
3	Error: Pulse goes below lower operating SOC window								
4	4 Error: Electrode thickness smaller than minimum allowable thickness								
	Warnings								
5	Warning: Number of modules rows not 1, 2 or 4 (number and size of busbars may become excessive)								
6	Warning: Number of modules in parallel should be 1 or 2 (number and mass of interconnects may be underestimated)								
7	Warning: Pulse ends in reserve safety margin (voltage drops too low)								
8	Warning: Power couple selected but energy couple may be more suitable for selected vehicle								
9	Warning: Energy couple selected but power couple may be more suitable for selected vehicle								
10	Warning: Pack size exceeds 5 ft in multiple dimensions (may exceed dimensions of vehicle)								
11	Warning: Pack voltage exceeds 1000 V (BMS cost and size will be underestimated)								
12	Warning: Desired charge time requires a charging power which exceeds input charger power								

Figure 3.9. a) Calculation and validation sub-section in results section of 'Dashboard.' b) Table on 'Dashboard' located to the right of the calculation and validation sub-section, which describes the errors and warnings.

The Calculation and Validation Results section also includes the plant size in GWh and the powerto-energy ratio. These values serve as quick checks on the manufacturing and battery design inputs to ensure they produce results with desired expectations. An adequacy of cooling check is also performed in this section. Values of "Excellent," "Good," "Fair," or "Poor" appear depending on the internal temperature of the cell calculated in the 'Thermal' worksheet. See Section 8 for details on the cooling check and suggestions for addressing poor grades. The calculation and validation section also displays which condition sets the thickness of the positive electrode in the present simulation. Note that the positive electrode thickness in BatPaC can be set by five conditions (see Section 5 for details). The five conditions are *i*) the power requirements, *iii*) the energy requirements, *iiii*) charging limits (see Section 6), *iv*) the maximum allowable thickness input, and *v*) the optional positive electrode thickness override input.

3.2.3.2 Summary of Results and Graphing

The final section in 'Dashboard' contains a summary of the results along with a feature for graphing trends between the seven batteries. The graphing function appears first in this section and is shown in Figure 3.10. The table above the graph can be used to select the variables for plotting using pull-down menus in the blue cells. The values in the purple cells will update automatically when a new variable is selected. The plotted data and labels will also update automatically on the graph. The variables available for plotting are contained in the results table below the graph (see Figure 3.11). The variables in this table can be updated using the 'Summary of Results' worksheet. Details on using the 'Summary of Results' worksheet are provided in the next section. The results table automatically includes any errors and warnings for the seven batteries. If an error occurs, the corresponding column will display red. The table also has a color coating scheme, whereby the minimum and maximum values between batteries 1 to 7 for each variable are highlighted in light orange or light purple, respectively.



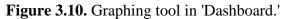


	Table of Res	Minimum Value Between batteries 1-7 Maximum Value Between Batteries 1-7						
System	EV Vehicle with NMC811-G (Energy) Electrode	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7
	Configuration Errors	None	None	None	None	None	None	None
	Configuration Warnings	None	None	None	None	None	None	None
1	Battery system total energy, kWh	60	70	80	90	100	110	120
2	Battery system capacity, Ah	163	191	218	245	273	300	327
3	Battery system rated power, kW	300	300	300	300	300	300	300
4	Battery system nominal voltage (average OCV), V	371	371	371	371	371	371	371
5	Pack power to energy ratio (with respect to rated powe	5.0	4.3	3.8	3.3	3.0	2.7	2.5
6	Pack energy density, Wh/L	270	288	305	320	334	346	357
7	Pack specific energy, Wh/kg	166	175	183	190	196	201	206
8	Number of modules per pack	20	20	20	20	20	20	20
9	Number of cells per pack	400	400	400	400	400	400	400
10	Pack volume, L	222	243	262	281	300	318	336
11	Pack total mass, kg	361	399	437	474	510	546	582
12	Cell capacity, Ah	41	48	55	61	68	75	82
13	Cell nominal voltage (average OCV), V	3.71	3.71	3.71	3.71	3.71	3.71	3.71
14	Positive electrode thickness, µm	115	120	120	120	120	120	120
15	Positive electode areal capacity, mAh/cm ²	8.0	8.4	8.4	8.4	8.4	8.4	8.4
16	Negative electrode thickness, µm	146	153	153	153	153	153	153
17	Negative electrode areal capacity, mAh/cm ²	8.6	9.1	9.1	9.1	9.1	9.1	9.1
18	Cell energy density, Wh/L	590	607	622	635	647	657	665
19	Cell specific energy, Wh/kg	328	332	333	335	336	337	338
20	Pack cost, \$/pack	7,386	8,204	9,036	9,864	10,688	11,511	12,363
21	Pack cost, \$/kWh	123	117	113	110	107	105	103
22	Pack cost, \$/kWh(Useable)	145	138	133	129	126	123	121
23	Cell cost, \$/kWh	79	77	76	75	75	74	74
24	Plant Size, GWh	30	35	40	45	50	55	60
25	Packs manufactured per year (packs/year)	500,000	500,000	500,000	500,000	500,000	500,000	500,000

Figure 3.11. Summary results table on 'Dashboard.'

3.3 Summary of Results Worksheet

The major results across all worksheets in BatPaC are compiled and listed in the 'Summary of Results' worksheet for all seven batteries. This includes calculated parameters with information on the size, mass, and configuration of the battery. It also includes manufacturing information and calculated costs. The calculated parameters and costs are given at four levels: the cell, module, pack, and battery system. The battery system is one level above the pack and includes masses and costs of cooling systems exterior to the pack that are added to the vehicle to operate the battery properly. The battery system also includes any additional packs in multi-pack designs, which can be modeled by adjusting inputs at the top of the 'Battery Design' worksheet.

Column 'A' in the 'Summary of Results' worksheet is used to control the variables in the summary of results table. The table appears at the bottom of 'Dashboard' (see Figure 3.11). It also exists as a moveable table in most worksheets within BatPaC. An image of the default, moveable table is shown in Figure 3.12. Variables are added to the summary of results table by placing a number in column 'A' of the 'Summary of Results' worksheet next to the variable label. The number will correspond to the variable's row in the summary of results table. If the same row is provided for two variables, both values are highlighted in red to indicate an error (see Figure 3.13).

Su	mmary Box (Can be mo	ved/dragged	l around)				
Name	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7
Configuration Errors	None	None	None	None	None	None	None
Configuration Warnings	None	None	None	None	None	None	None
Battery system total energy, kWh	100	100	100	100	100	100	100
Battery system capacity, Ah	271	271	271	271	271	271	271
Battery system rated power, kW	300	300	300	300	300	300	300
Battery system nominal voltage (average OCV), V	371	371	371	371	371	371	371
Pack power to energy ratio (with respect to rated power)	3.00	3.00	3.00	3.00	3.00	3.00	3.00
Pack energy density, Wh/L	323	323	323	323	323	323	323
Pack specific energy, Wh/kg	183	183	183	183	183	183	183
Number of modules per pack	20.00	20.00	20.00	20.00	20.00	20.00	20.00
Number of cells per pack	400	400	400	400	400	400	400
Pack volume, L	309	309	309	309	309	309	309
Pack total mass, kg	546	546	546	546	546	546	546
Cell capacity, Ah	67.83	67.83	67.83	67.83	67.83	67.83	67.83
Cell nominal voltage (average OCV), V	3.71	3.71	3.71	3.71	3.71	3.71	3.71
Positive electrode thickness, µm	70.00	70.00	70.00	70.00	70.00	70.00	70.00
Positive electode areal capacity, mAh/cm²	4.90	4.90	4.90	4.90	4.90	4.90	4.90
Negative electrode thickness, μm	89.07	89.07	89.07	89.07	89.07	89.07	89.07
Negative electrode areal capacity, mAh/cm²	5.28	5.28	5.28	5.28	5.28	5.28	5.28
Cell energy density, Wh/L	618	618	618	618	618	618	618
Cell specific energy, Wh/kg	314	314	314	314	314	314	314
Pack cost, \$/pack	\$12,525	\$12,288	\$12,001	\$11,802	\$11,618	\$11,150	\$11,091
Pack cost, \$/kWh	\$125	\$123	\$120	\$118	\$116	\$112	\$111
Pack cost, \$/kWh(Useable)	\$147	\$145	\$141	\$139	\$137	\$131	\$130
Cell cost, \$/kWh	\$87	\$86	\$84	\$83	\$82	\$80	\$79
Plant Size, GWh	0.50	1.00	2.50	5.00	10.00	75.00	100
Packs manufactured per year (packs/year)	5000	10000	25000	50000	100000	750000	1000000

Figure 3.12. Default summary box which includes the summary of results table. This box is moveable and exists on most worksheets in the BatPaC.

As an example, note that the value "1" in Figure 3.13 is to the left of "Battery system total energy, kWh". The number and label are in columns 'A' and 'B' in the 'Summary of Results' worksheet, respectively. As such, "Battery system total energy, kWh" is included as the first variable listed in the summary of results table (after the configuration errors and warnings) in Figure 3.11 and Figure 3.12. A maximum of 46 variables can be plotted in the summary of results table. The variables are limited to 46 to prevent visualization problems in the moveable summary box.

Error notification

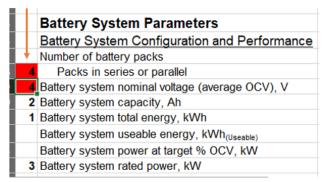


Figure 3.13. Demonstration of error warning that occurs when two variables are given the same row assignment in the summary of results table.

The final section of the 'Summary of Results' worksheet contains a dynamic table to add extra variables from throughout BatPaC into the worksheet. Extra variables can be added by placing an "x" in column 'A' to the left of the variable label in its respective worksheet. The "x" may be used to import any variable from the 'Chem,' 'Battery Design,' 'BMS,' 'Manufacturing Costs,' 'Cost Breakdown,' 'Recycling,' and 'Thermal' worksheets. New variables are automatically added to the dynamic table and are organized by worksheet. The dynamic table lists the worksheet/tab name and the location, which is the row number for that variable in its respective worksheet. Note that with this feature, users can add new variables to the summary of results table by first importing the new variable into the 'Summary of Results' worksheet next to the variable that should be included in the summary of results table. The dynamic table can also be used to summarize single value constants, such as those in the 'Chem' worksheet. Note that single values cannot be plotted in 'Dashboard' (as they are a single value).

3.4 Chem Worksheet

The 'Chem' worksheet provides input values and optional overrides for the costs and properties (both physical and electrochemical) of the electrodes, current collectors, separator, and electrolyte. It is likely the next most important worksheet for BatPaC users, behind 'Dashboard' and 'Summary of Results.' Figure 3.14 provides an example of the physical and electrochemical properties for the negative electrode region on the worksheet. 'Chem' follows the same cell-key as the rest of BatPaC, whereby purple cells are the automatic inputs which can be overridden using the green cells. This worksheet also includes a "BatPaC Default" column which is populated based on the

electrode couple selected on 'Dashboard.' This column remains unchanged when values are overridden to provide reference.

'Chem' is also the repository for the properties and costs of the default electrode couples. This data can be found on the right-hand-side of the worksheet. Each couple contains a unique panel, which is populated into the "BatPaC Default" column when selected on 'Dashboard.' Within each panel, input values derived from calculations are highlighted in green (see Figure 3.15). Information on how to add a new couple into 'Chem' is provided in Section 4.

Property	Applied Value	BatPaC Default	Override	Notes
Couple Name	Li(Ni0.8Mn0.1Co0.1)O2	2 / Graphite	Drop do	
Negative Electrode				wn menu
Add 5% silicon to negative electrode?	No	No		
Negative Electrode Active Material	G	G		Note to
Negative-to-positive capacity ratio after formation	1.10	1.10		consult
Negative electrode active material capacity, mAh/g:	360	360		consuit
				'Chem
Negative Electrode Composition, Weight %				Couplo
Negative electrode active weight %	98.0	98.0		Couple
Negative electrode carbon addtive weight %	0.0	0.0		Tool'
Negative electrode binder weight %	2.0	2.0		
Binder solvent for negative electrode	Water	Water		
Negative Material Density, g/cm ³				
Negative electrode active material density, g/cm ³	2.24	2.24		
Negative electrode carbon additive density, g/cm ³	1.95	1.95		
Negative electrode binder density, g/cm³	1.10	1.10		
Negative Electrode Structural/Kinetic Properties				Note to
Negative electrode porosity, volume % of void space	25	25.0		consult
Negative electrode active material particle radius, µm	6	6.0		default
Negative electrode specific area "a", cm²/cm³	3,600	3600.4		
Negative electrode active material exchange current, i_{0} mA/cm^{2}	0.50	0.5		couples
Negative Foil Properties				
Negative foil material	Copper	Copper		
Negative foil thickness, µm	10	10.0		

Figure 3.14. Screenshot of negative electrode inputs in the 'Chem' worksheet. Figure highlights features and notes with additional information.

3.4.1 Chem Inputs

This section provides an overview of the main inputs in 'Chem.' The 'Chem' worksheet provides the weight percentages and densities of the components in both electrodes (*i.e.*, active materials, carbon additives, and binders), the electrode structures (*i.e.*, porosities and specific surface areas), and the electrochemical properties of the couple (*i.e.*, specific capacities, exchange current densities, default area-specific impedances, and open circuit voltages). Similar properties for the separator (*i.e.*, porosity, density, and thickness), the electrolyte (*i.e.*, density), and current collectors (*i.e.*, thickness and material type) are also provided. Details on how these properties translate to the cell, module, and pack design can be found in Section 5. 'Chem' also contains the cost inputs from 'Dashboard' for these components. Note that both the 'Chem' worksheet and 'Dashboard' contain override features for the same inputs. The 'Dashboard' override always takes precedent over the 'Chem' override in BatPaC.

Almost all the default inputs can be overridden; however, caution is advised since many input parameters in the worksheet are coupled. These couplings are often complex and can vary depending on the exact materials and manufacturing processes. Therefore, while some assumptions on coupled inputs have been made in the generation of the default values, these assumptions are not imbedded into BatPaC. Several important examples are highlighted below.

First, for BatPaC to successfully simulate a wide range of power requirements, 'Chem' provides the area-specific impedances (ASIs) of the electrode couple at 2 and 10 seconds into a discharge pulse. The default ASIs were determined from simulations of the electrochemical performance of a single cell layer (*i.e.*, positive electrode-separator-negative electrode, no current collectors) using porous electrode theory [13]. The inputs into the model were derived from experiments and literature. The ASI depends on many of the default properties mentioned above - e.g., porosities, particle sizes, electrolyte, exchange current densities, weight percentages, etc. When overriding any of these values, the values listed for the ASI should also be re-considered.

Second, the default ASIs depend on the electrode thicknesses and C-rate (*i.e.*, current density) used in the simulated discharge pulses. The values/conditions used to obtain the default ASIs are provided in the "BatPaC Default" column for reference and cannot be overridden. All ASIs in the worksheet, including the amount of interfacial ASI in the total ASI, will depend on the conditions used for the default pulse. The interfacial ASI at the default conditions is an input parameter. Its value should also be changed if the default ASIs are overridden with data from a pulse obtained at different conditions. The default approximation used to determine the interfacial ASI is available in Section 5.2.2.2 and example calculations are included in the default chemistry couples on the right-hand side of the 'Chem' worksheet. At present, the interfacial ASI and the electrode thicknesses and C-rate during the default pulse are left uncoupled to provide flexibility by not restricting users to the default approximation used by BatPaC. Note that the interfacial ASI also depends on the exchange current densities, specific surface areas, and limiting currents assumed in the 'Chem' worksheet. Recall that all ASI inputs (including the interfacial ASIs) should be reconsidered upon changing of properties.

Third, the particle radii inputs have a similar structure to the pulse conditions, whereby the default values are shown for reference but cannot be overridden. This is highlighted in Figure 3.14. The default particle radii were used for determining the specific surface area of the electrodes. Some users may prefer other methods for approximating the specific surface area, such as BET. Therefore, the specific surface areas and particle radii are left uncoupled. Note that the specific surface areas and exchange current densities are often fit together to match experimental data. Users should consider this fact when overriding the specific surface area.

Finally, there is a coupling associated with the specific capacities of the two electrode active materials, the negative-to-positive capacity ratio in the cell, and the open circuit voltage. All three are required to properly size the battery. All three are also coupled based on the initial amounts of materials added to the cell, the cut-off voltages during cycling, and the losses during formation. Small changes to these properties will not invalidate the results. Large changes without direct experimental evidence should be considered carefully. BatPaC offers a tool for generating these

three parameters in a self-consistent manner based on assumptions for formation losses and experimental open-circuit voltage data. The tool is in the 'Tool-Generate Chem Couple' worksheet and details are presented in Section 4. Notes directing users to the tool are included in the 'Chem' worksheet (see Figure 3.14).

3.4.2 Additional Features in Chem

The 'Chem' worksheet includes several built-in features that increase the functionality of BatPaC. First, when graphite electrodes are selected, a drop-down menu becomes active in the worksheet where the user can add 5% silicon to the negative electrode (see Figure 3.14). Selecting "Yes" will increase the capacity of the negative active material. All other properties remain the same.

Other additives can be included in the electrodes and electrolyte using the "Additives" section of the worksheet. All default chemistry couples assume zero additives. To include an additive, the user must specify the weight percent of the additive with respect to the component (*i.e.*, positive electrode, negative electrode, or electrolyte). The user should also specify the lithium mass fraction in the additive, which is used for keeping track of recoverable materials (see Section 10). Lithium-containing additives are commonly used for pre-lithiation. A cost for the additive in \$/kg is also required. Note that additives are assumed to be small fractions of the total component mass with negligible volumes. Their mass is included in the total mass of the cell but effects on the cell volume are neglected.

The final feature in the 'Chem' worksheet involves the final default electrode couple at the far right-hand side of the worksheet. This couple lets the user simulate electrodes with blended cathodes. Two electrode couples from the list of default couples can be selected using the drop-down menus in the "Mixing Values" section of the last default couple (see Figure 3.15). The section also includes an input for the weight percent of the cathode material in the first couple. The properties of the blended cathode are calculated using a weighted average of the properties of the two cathodes. Note that the blending is only done on the cathodes. For the calculation to work, both selected couples must have the same anode. BatPaC performs an anode check and returns a value of "Good" or "Anode couples don't match" depending on the results (see Figure 3.15). Finally, note that the chemistry name and notes for the couple and the label in the chemistry couple drop-down menu on 'Dashboard' are automatically updated when the couples and/or weight percentages are changed.

Text automatically updates

Chemistry	50%/50% NMC532/LMO - G	ID #	17					
Notes	Default is 50/50 NMC532 and L	MO, % is mass based						
This data set considers a mix of two positive electrodes. Change values in Description Chem!CQ7:CQ9								
Property	Default Value	Notes						
Green in	dicates	Drop-down menu	IS					
Positive Electrode calculate	d value	Mixing Values						
Active material	50%/50% NMC532/LMO	Positive Electrode 1 Source	NMC532-G (Energy)					
Active material capacity, mAh/g:	152.85	% Positive electrode 1	50%					
		Positive Electrode 2 Source	LMO-G (Energy)					
Positive Electrode Composition		Positive electrode 1 Col Val	28					
Active material weight %	96	Positive electrode 2 Col Val	78					
Carbon additive weight %	2	Anode Check	J Good					

Check to make sure anodes are same

Figure 3.15. Screenshot of the final, default electrode couple which is used to generate couples with mixed cathode composition. The user can modify the electrodes and weight percentages using the green boxes in the "Mixing Values" section.

3.5 Remaining Worksheets

The remaining worksheets in BatPaC contain the detailed calculations, less-frequently adjusted inputs, additional results breakdowns, and tools for adding new default options. An overview of these worksheets is provided in this section with references to other parts of the manual for details.

3.5.1 Battery Design Worksheet

The bulk of the calculation is done in the 'Battery Design' worksheet, which determines the size, mass, and dimensions of the battery system. Details on the calculation are provided in Section 5 of this manual, which includes significant reference to the cell, module, and pack layouts described in Section 2. The 'Battery Design' worksheet is divided into six parts:

<u>Battery System Parameters</u>: The first part lists key pack inputs and battery design outputs (*i.e.*, number of cells, number of cells in parallel, vehicle type, power, energy, voltage, capacity, etc.). The main pack configuration and performance inputs are only adjustable in 'Dashboard.' There are additional inputs only available in this part of the worksheet for the number of packs per vehicle and whether these packs are in series or parallel.

<u>Mass Balance</u>: The second part contains the calculations used to determine the amounts of materials in the cells. It also contains adjustable, default inputs for the cell container, length-to-width ratio, and terminal design.

<u>Electrode Thickness Calculations</u>: The third part determines the thickness of the electrodes based on the power, energy, and charging requirements of the pack. Default inputs for the design of interconnects, terminals, and bus bars in the cell, module, and pack are also included in this part. These design features are used to determine the area-specific impedance in the calculation. This part also includes adjustable, default inputs for the charger and allowable temperature during charging. Note that these inputs only impact the calculation when "Calculate Charging Requirements" is set to "Yes" for EVs in 'Dashboard' (see Section 6 for details).

<u>Cell, Module, and Pack Construction</u>: The fourth part of the worksheet sizes all the components in the pack. It also contains adjustable, default inputs for the cell, module, and pack dimensions – e.g., module enclosure, rack support in pack, pack cooling systems, etc. The calculation is supported by inputs from the 'BMS' (Section 7) and 'Thermal' (Section 8) worksheets to help size the battery management system and cooling system, respectively.

<u>Battery System Values:</u> The fifth part summarizes some of the main results of the worksheet, including the power and energy densities (volumetric and gravimetric) of the pack and cells. These results can also be found in the 'Summary of Results' worksheet.

<u>Calculation Warnings and Errors:</u> The sixth part contains the calculation of the error and warning handling that is also displayed on 'Dashboard.'

3.5.2 BMS, Thermal, and Recycle Worksheets

The 'BMS' worksheet contains the calculations for determining the volume, mass, and cost of the battery management system. Details on the calculations can be found in Section 7. The top portion of the worksheet contains data from other parts of BatPaC that are included as convenience and referenced in the calculation. The middle portion contains the main calculation. The final portion contains reference cost values used in the calculation.

The 'Thermal' worksheet contains calculations for determining the cooling and heating requirements of the pack. The cooling requirements are determined for maintaining the internal temperature of the cells at a safe value during sustained driving on a hot day. The heating requirements are determined for heating up to the operating temperature on cold days. Details on the calculations can be found in Section 8.

The 'Recycle' worksheet calculates the amounts of recoverable materials in the pack at the end of life. It also keeps track of recoverable materials that are rejected from the plant. This includes both scrap materials (*i.e.*, from electrode slitting, coating, etc.) and from rejected cells that did not pass quality control tests. Further details can be found in Section 10.

3.5.3 Cost Worksheets

There are four cost worksheets in BatPaC: 'Cost Input,' 'Manufacturing Costs,' 'Cost Breakdown,' and 'Detailed Cost Breakdown.' They correspond to the inputs, calculation, main results, and

detailed results for the cost of the battery, respectively. Details on the cost calculations are provided in Section 9.

In short, the 'Cost Inputs' worksheet contains adjustable, default inputs for the cost of purchased materials (*i.e.*, terminals, bus bars, cooling panels, etc.), cost rates for manufacturing and cost breakdowns (*i.e.*, labor rates, depreciation rates, warranty cost, etc.), and battery assembly costs. The battery assembly costs contain the direct labor, capital equipment, and plant area for each step of the manufacturing process in a baseline plant (50 GWh/yr). It also contains p-factors which are used to scale these costs for different plant sizes. Cell materials costs are also shown in this worksheet, but they should only be changed in 'Dashboard' or 'Chem.' Finally, the 'Cost Input' worksheet contains yields for each step of the manufacturing process.

The 'Manufacturing Costs' worksheet starts by determining the direct materials costs of all components in the pack, including raw materials (*i.e.*, electrodes, separators, etc.), terminals, BMS, heating system, cooling panels, etc. It then determines the battery assembly costs based on the inputs from the 'Cost Input' worksheet for direct labor, capital equipment, and plant area and the manufacturing rates and plant utilization specified on 'Dashboard.' This information is combined with the direct materials costs to determine the entire cost (materials + manufacturing) of the cells, module(s), pack(s), and battery system. The final costs also depend on the pack manufacturing strategy (*i.e.*, all in-house versus purchasing cells or modules from the battery manufacturer) and pack cost options (*i.e.*, with or without profits and warranty) selected in 'Dashboard.'

The 'Cost Breakdown' worksheet provides several detailed breakdowns of the pack cost. Unless specified, all values are reported in units of pack. The first is the breakdown of materials and purchased item costs. This includes the costs of individual cell components (*i.e.*, active materials, carbon additive, current collectors, etc.), purchased items, and BMS. It does not include any manufacturing costs. The second is a breakdown of the total cost. This includes active materials, purchased items, BMS, direct labor, variable overhead, GSA (general, sales, and administration), R&D (research and development), depreciation, and profits/warranty (if selected by the user in 'Dashboard'). The final breakdown is of the total cost with overhead items distributed into the manufacturing processes – *i.e.*, labor, capital depreciation, building overhead, GSA, and R&D are distributed into electrode processing, cell assembly, formation, etc. This final breakdown helps show which processes are most expensive in the battery assembly. Finally, the bottom of 'Cost Breakdown' includes pie-charts graphing some of these breakdowns for batteries 1 and 7. Additional default charts can be added at the user's discretion.

The 'Detailed Cost Breakdown' worksheet is a more granular version of the 'Cost Breakdown' worksheet. For instance, 'Cost Breakdown' provides the costs of purchased items as one value per level (*i.e.*, one value each for cell, module, and pack purchased items), while 'Detailed Cost Breakdown' provides the cost of each purchased item separately. The detailed worksheet also provides more information when breaking down the costs with overhead items distributed into the manufacturing steps. For example, 'Cost Breakdown' provides the cost of electrode processing, while 'Detailed Cost Breakdown' lists the contributions from electrode mixing, coating, calendering, notching, and drying separately for both the positive and negative electrodes (see Section 9). The 'Detailed Cost Breakdown' also provides percent contributions of each item to the total pack cost.

3.5.4 Other Worksheets

There are five additional worksheets that are not directly involved in the calculation. The 'USABC Data' worksheet provides the mass, volume, and cost of the pack in a format that is consistent with publications from the United States Advanced Battery Consortium (USABC). Note that, for the cost breakdown to work properly, the "Method for manufacturing pack" and "Option for pack cost" on 'Dashboard' should be set to "All manufacturing in-house (Default)" and "Cost to build – excludes profit/warranty," respectively. A warning message is provided above the cost table in this worksheet to remind the user.

The next three worksheets – 'Tool-Generate Chem Couple,' 'Vehicle Considerations,' and 'Default Vehicle Configurations' – provide methods for modifying and adding default electrode chemistry couples, vehicle types, and vehicle configurations. Details on these worksheets are covered in the next section (Section 4).

The 'Lists' worksheet is the final worksheet in BatPaC. It is the "junk drawer" of the program. It contains lists and tables of properties, calculation flags, and some default cost inputs called by other worksheets in the program. Editing of this worksheet is highly discouraged.

3.6 Explanation of Iterative Solver

The calculations in BatPaC involve many interdependent variables whose values must be determined to solve the sets of equations that define the battery performance. The main calculations that require iteration are organized in the 'Battery Design' worksheet at the bottom of the "Cell, module, and pack construction" section, under the header "Iterative Calculations." BatPaC uses convergence constants to iteratively (and simultaneously) solve for the pack capacity, electrode thickness, and cell thickness adjustment (see Section 5 for details). All other results in BatPaC are calculated from the converged solution of these three parameters. Note that during the iterations, variables affected by these parameters also iterate.

To arrive at a solution in a moderate number of iterations, it is important to start with a reasonable estimate of the final answer. All three parameters have built-in initial estimates, which have proven sufficient over the range of operating conditions, vehicle types, and chemistries in BatPaC. A similar statement can be made about the convergence constants. These are provided by BatPaC and two of the three are calculated from other variables within BatPaC to provide a seamless convergence.

It is possible, although highly unlikely, that the user may select a set of input variables that does not immediately lead to a solution. In that case, the user should consider adjusting the convergence constants and initial estimates for that study. Recall that most issues with BatPaC can be solved by resetting the calculation (refer to Section 3.2.1). When the calculation is reset, BatPaC sets the three parameters to their initial estimates. Then, the iterative solver in excel (see Section 3.1) automatically converges towards a solution.

4. ADDING NEW CHEMISTRIES AND VEHICLES

BatPaC has three, main, built-in datasets, which contain options for designing a battery pack for an electric vehicle. Options from all three datasets can be selected using the input fields on 'Dashboard' (see Section 3.2.2) The first dataset contains default chemistry couples. The second dataset contains vehicle types. The third dataset contains default vehicle configurations. This section provides information for modifying and adding to the default datasets. When appropriate, additional descriptions of the items in the datasets are also provided.

4.1 New Electrode/Chemistry Couples

BatPaC designs vehicle batteries for a range of positive and negative electrode couples. Different couples have different electrochemical, physical, and cost properties for the components in the cells. See Section 3.4 in this manual for details. BatPaC offers two methods for generating new electrode/chemistry couples that can be added to the drop-down menu in 'Dashboard.' Note that electrode couple and chemistry couple are often used synonymously within BatPaC and this text. The first method is within the 'Chem' worksheet. The second method employs macros in the 'Tool-Generate Chem Couple' worksheet. Both methods are described below.

4.1.1 New Couples from Chem Worksheet

As mentioned in Section 3.4, the 'Chem' worksheet contains the property values for the selected chemistry couple and serves as the database for all default couples. Each default couple is included as a unique pane on the right-hand side of the worksheet. The panes are organized from left to right, with the left-most pane appearing at the top of the "Electrode Couple" drop-down menu in 'Dashboard' and the right-most pane appearing at the bottom. The user is welcome to adjust the default properties listed in any pane for their personal use. A new default couple can also be added by copying an existing chemistry couple pane (4 columns) and pasting it to the right of all other couple panes (see Figure 4.1). The number of columns between two couple panes does not matter. The new couple is automatically populated into the "Electrode Couple" drop-down menu on 'Dashboard.' The new couple is listed in the drop-down menu based on the name provided in the yellow cell next to the "Chemistry" cell. No other changes are required to start using the couple. Please refer to Section 3.4.1 for guidance on modifying the properties.

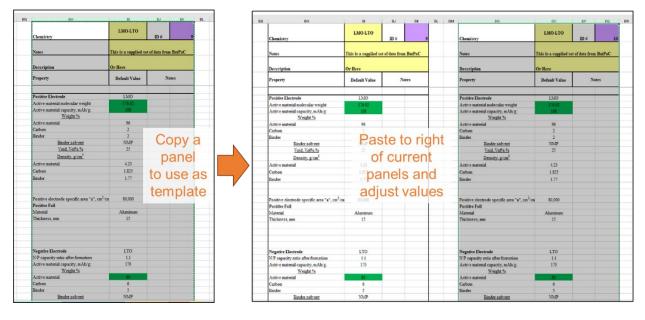


Figure 4.1. Screenshots showing how to create a new default couple in the 'Chem' worksheet by copying an existing couple and pasting it to the right of the current panels. New couples will automatically populate at the bottom of the drop-down menu in 'Dashboard.'

4.1.2 Tool-Generate Chem Couple Worksheet

The 'Tool-Generate Chem Couple' worksheet provides a tool for generating the properties – *i.e.*, reversible gravimetric capacities of the active materials (mAh/g) and open circuit voltage (OCV) versus state of charge (SOC) – of new chemistry couples that can be modeled with BatPaC. The tool guarantees the capacity and OCV values are self-consistent with the desired negative-to-positive capacity ratio and voltage window set by the user. This section provides a how-to-guide for using the worksheet. Note that macros must be enabled to use these tools (see Section 3.1).

4.1.2.1 Step 1: Choose couple and formation information

First, the active materials in the new couple must be chosen from an existing database in BatPaC. This can be accomplished either by taking the values from the currently selected chemistry couple, which was selected on 'Dashboard' (Figure 4.2a) or by creating a new couple from the database of active materials provided by BatPaC (Figure 4.2b). Use the drop-down menu next to the "Select Method" cell to choose one of the two options. If the first option is chosen, the positive and negative electrode chemistries are automatically taken from the currently selected values on 'Dashboard.' If the second option is chosen, two drop-down boxes appear, which must be used to select the chemistries from a database of values. Results are only guaranteed when graphite (G) or lithium titanate (LTO) are used as the negative electrode. If any other chemistry is selected as the negative electrode or either of the two are chosen as the positive, a warning message shows up in the "Check for compatibility" rows.

Drop-down	menu			Drop-down menus					
	1	Step 1: Choos	b)		A	S	tep 1: Choo		
Select Method	Use Currently Selected	Chemistry Couple		Select Method	Create	New Cou	ple		
					Positive		Negative		
				Select chemistries	NMC811	¥	G		
Positive Electrode				Positive Electrode	NMC333 NMC532	^			
Chosen Chemistry		NMC811		Chosen Chemistry	NMC622 NMC611		NMC811		
ID for the material (if NA, the material is not in th	e database)	4		ID for the material (if NA, the material is not in the		_	4		
Check for compatability		good		Check for compatability	LFP		good		
Positive half-cell losses during formation, %		5%		Positive half-cell losses during formation, %	LMO	~	5%		
Negative Electrode				Negative Electrode					
Chosen Chemistry		G		Chosen Chemistry			G		
ID for the material (if NA, the material is not in th	e database)	9		ID for the material (if NA, the material is not in the	database)	_	9		
Check for compatability		good		Check for compatability			good		
Negative half-cell losses during formation, %		1%		Negative half-cell losses during formation, %		1	1%		
Lithium inventory loss from SEI formation, mAh j		20.0		Lithium inventory loss from SEI formation, mAh p	er g of negative		20.0		
Negative half-cell cutoff voltage during formation,	V vs. Li/Li*	0.01		Negative half-cell cutoff voltage during formation, V	/ vs. Li/Li*		0.01		
Full Cell				Full Cell					
Target N:P ratio after formation		1.05		Target N:P ratio after formation		1	1.05		
Upper cutoff voltage at 100% SOC		4.25		Upper cutoff voltage at 100% SOC			4.25		

Figure 4.2. Screenshots showing two ways to choose the new chemistry couple when using the tool: a) by using the currently selected chemistry couple from 'Dashboard' and b) by creating a new couple from the database. Use the first drop-down menu to choose between the two methods.

Next, input information for the three types of capacity loss during formation. The first is the positive half-cell losses during formation, which reflects the loss in active sites of the positive material during formation and has units of percent of first cycle capacity. The second is the negative half-cell losses during formation, which reflects the loss in active sites of the negative material during formation and has units of percent of first cycle capacity. Both values should be provided without regards to lithium inventory loss. They should reflect the losses observed during formation of half-cells with excess Li-metal, where the voltage windows for either electrode are identical to the voltage windows observed during operation of the full cell when measured with respect to a Li/Li^+ reference electrode. The third loss is the lithium inventory loss from SEI formation. It has units of mAh of lithium lost per gram of negative active material. The description assumes all lithium inventory loss occurs at the negative electrode SEI, which was done for simplicity. Other forms of lithium inventory loss (*e.g.*, cathode-electrolyte interphase, CEI) can be incorporated by increasing the value of this term.

In addition to formation losses, specify the desired negative half-cell cutoff voltage during formation. This sets the lowest voltage seen by the negative electrode when the full cell is at 0% SOC. The upper cutoff voltage of the full cell at 100% SOC must also be provided to set the voltage window. Finally, specify the target negative-to-positive (N/P) capacity ratio in the full cell after formation. The N/P capacity ratio has units of mAh/mAh or mAh cm⁻²/mAh cm⁻² since the tool assumes identical areas for the positive and negative half-cells. Table 4.1 provides the assumptions used to derive the properties (mAh/g and OCV) for the default chemistry couples available in the 'Chem' worksheet.

Positive active material	NCA	NMC 333	NMC 532	NMC 622	NMC 811	LFP	LMO	LMO
Negative active material	G	G	G	G	G	G	G	LTO
Positive half-cell losses	5%	5%	5%	5%	5%	5%	5%	5%
Negative half-cell losses	1%	1%	1%	1%	1%	1%	1%	0%
Li inventory losses, mAh/g _{neg}	20	20	20	20	20	20	20	0
Negative half-cell cutoff, V	0.01	0.01	0.01	0.01	0.01	0.01	0.01	1.2
Full cell upper cutoff, V	4.25	4.25	4.25	4.25	4.25	3.80	4.25	3.00
N/P ratio	1.1	1.1	1.1	1.1	1.1	1.1	1.1	1.02

Table 4.1. Assumptions used to derive properties (mAh/g and OCV) for default chemistry couples.

4.1.2.2 Step 2: Run Calculation

Click the "Run Calculation" button to initiate the macro and run the calculation (Figure 4.3).

	Step 2: Run Calculation				
Run Calculation					

Figure 4.3. Screenshot showing the button to run the calculation

4.1.2.3 Step 3: Verify/modify output data

The results of the calculation (*i.e.*, gravimetric capacities, N:P ratio, and OCV vs. SOC) will appear in the table as shown in Figure 4.4. This section also includes a graph of the OCV vs. SOC for the full cell. Verify the results and repeat steps 1 and 2 until satisfied. If necessary, override the calculated voltage using the "Override" column. This is only advised for minor changes (*e.g.*, adjusting the calculated OCV at 0% SOC from 3.01 to 3.00 to yield a more typical lower cutoff voltage).

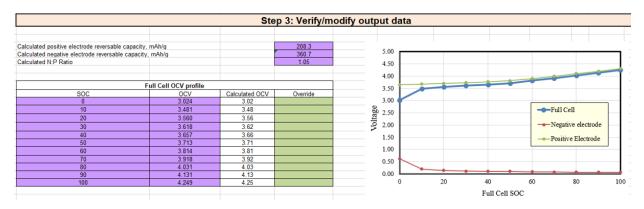


Figure 4.4. Screenshot showing the results of the calculation.

4.1.2.4 Step 4: Export to Chem Tab

Two options are provided for transferring the results to the 'Chem' worksheet so they can be used by BatPaC for the battery design calculation (Figure 4.5). For the first option, click the button labeled "Add Values to Current." This will add the new values to the "Override" column in the 'Chem' worksheet. All other properties come from the existing, default electrode couple selected in 'Dashboard', unless overridden previously. This option does <u>not</u> save the new values as a new default chemistry couple.

The second option is to create a new default chemistry couple that will be added to the list of selectable chemistry couples in the electrode couple drop-down menu on 'Dashboard.' First, use the drop-down menu under "Select a Chemistry Couple to Use to Serve as Template" to select a pre-existing default couple to serve as template. Next, provide a name for the new couple under "Create Name for New Electrode Couple." An error will appear if the name already exists. After that, click the button "Create New Electrode Chemistry Couple" to add the new couple to the default list. The couple will be created by combining the calculated results above with all other properties from the template couple (*e.g.*, ASI, densities, porosities, etc.). Finally, to use the new couple in the BatPaC calculations, return to 'Dashboard' and select the new couple in the electrode couple pull-down menu.

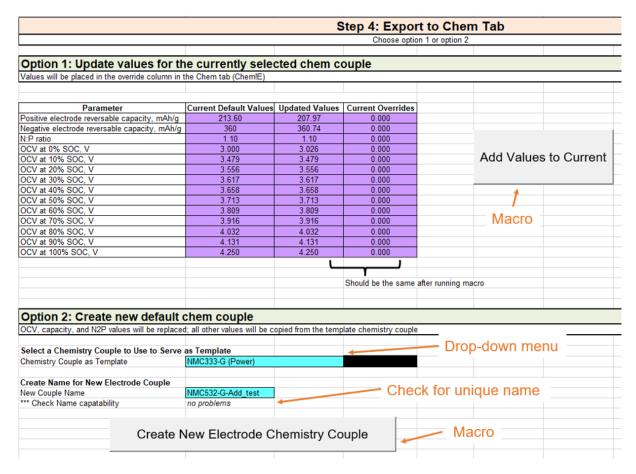
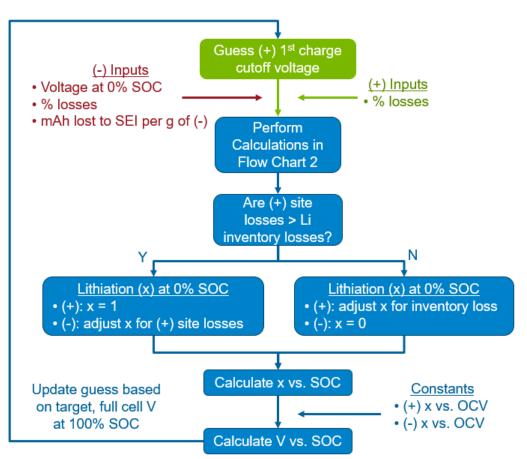


Figure 4.5. Screenshot showing the two options for exporting the results to the Chem tab.

4.1.2.5 Explanation of Calculation

The calculation is solved using two, nested, iterative loops to guarantee self-consistency between all parameters. Two flow charts are provided below to describe the calculation. The full calculation is contained at the end of the spreadsheet and should not be modified.

The outer iterative loop is shown by the flow chart in Figure 4.6. Here, the positive, first-charge, cutoff voltage is iteratively updated until the full cell voltage at 100% state of charge (SOC) converges to the target value. The positive, first-charge, cutoff voltage is used to determine the gravimetric capacity of the positive material. It is used in combination with the user-specified formation losses and the negative voltage at 0% SOC (see input arrows in Figure 4.6) to solve the inner, iterative loop shown by Flow Chart 2 in Figure 4.7.



<u>New Chem Couple Flow Chart 1</u>

Figure 4.6. Flow chart describing the outer iterative loop in the calculation. The positive firstcharge cutoff voltage is updated iteratively in the calculation until the full cell voltage at 100% state of charge converges to the target value. OCV, SOC, (+), and (-) correspond to the open circuit voltage, state of charge, positive active material, and negative active material, respectively. Green, red, and blue boxes/text reflect calculations/inputs involving the positive electrode, the negative electrode, or both, respectively. The inner loop (Figure 4.7) iteratively updates the negative-to-positive (N:P) mass ratio until the N:P capacity ratio converges to the target value. At first, the user-specified, positive site losses; the positive, first-charge cutoff voltage specified by the outer loop; and the positive mAh_{theory}/g vs. OCV (i.e., no losses) are used to determine the positive reversible, half-cell capacity. Next, the total number of positive sites lost (in mAh) is calculated using this value and the N:P mass ratio. This is compared to the Li inventory losses (in mAh) calculated from the N:P mass ratio and the user-specified mAh lost per gram of negative. The relative size of the positive losses and Li inventory losses determines the course of action for calculating the real capacity of each material in the full cell. If the positive site losses are larger, the negative capacity is adjusted to account for the fact some lithium will reside in the negative upon discharge because it has no "home" in the positive. If the Li inventory losses are greater, the positive capacity is adjusted to account for a lack of Li to fill all its vacant sites upon discharge. Simultaneously, the reversible, half-cell capacity of the negative material is calculated using the user-specified, negative site losses; the user-specified negative voltage at 0% SOC; and the BatPaC-provided mAhtheory/g vs. OCV. Both reversible capacities are combined with the adjustments to determine the mAh/g. The calculated mAh/g are then combined with the N:P mass ratio to determine the N:P capacity ratio. Finally, this value is compared with the target and the N:P mass ratio is updated.

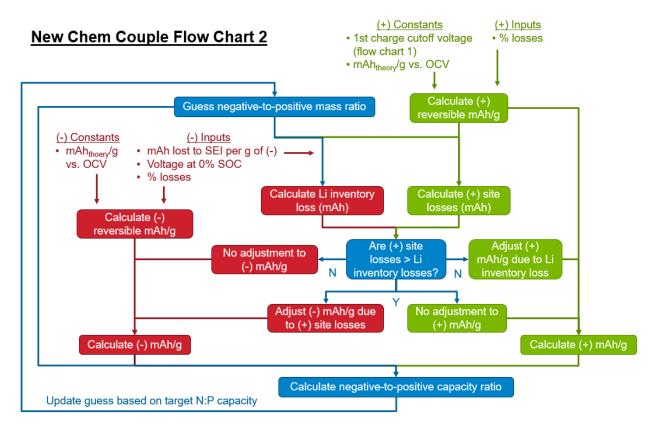


Figure 4.7. Flow chart describing the inner iterative loop in the calculation. The negative-topositive (N:P) mass ratio is updated iteratively in the calculation until the N:P capacity ratio converges to the target value. OCV, SOC, (+), and (-) correspond to the open circuit voltage, state of charge, positive active material, and negative active material, respectively. Green, red, and blue boxes reflect calculations involving the positive electrode, the negative electrode, or both, respectively.

Results from the inner loop are used to complete the calculation on the outer loop. For instance, the formation losses calculated in the inner loop are used to determine the course of action in the outer loop for determining the degree of lithiation in the materials at 0% SOC (see Figure 4.6). The course of action depends on whether the total positive site losses (mAh) are greater than the lithium inventory losses. Next, the degree of lithiation (x, where x = 1 corresponds to all sites filled) in both materials is calculated as a function of SOC. After that, the voltage of each electrode versus Li/Li⁺ is determined by interpolating values from the database of x versus open circuit voltage (OCV) provided by BatPaC. The full cell voltage at 100% SOC is then compared to the target voltage and the positive, first-charge, cutoff voltage is updated.

4.2 Vehicle Considerations

The vehicle type impacts the design requirements of the battery. BatPaC offers four default vehicle types: mild hybrid-electric vehicles (mildHEV), high-power hybrid-electric vehicles (HEV-HP), plug-in hybrid-electric vehicles (PHEV), and all-electric vehicles (EV). The vehicle type is a required user input and can be selected from the drop-down menu on 'Dashboard' (see Section 3.2.2.2). Changing the vehicle type changes battery design constraints related to the power, state of charge window (SOC), charging options, battery management system, and thermal considerations.

The 'Vehicle Considerations' worksheet in BatPaC provides the properties of the four default vehicles (Figure 4.8). It also provides space to the right of the table (shaded region) where users can create new vehicle types. To create a new vehicle type, populate the new values in the next empty column in the shaded region to the right of the table. Note that all fields must be completed and maintain the same format as similar rows in the table. All numbers must remain numbers. All Boolean must remain TRUE or FALSE. All text should choose from previous inputs in the table – *i.e.* "Ideal chemistry couple" should be Power, Energy, or Either. A unique vehicle name should also be provided in the "Vehicle" row. This is the same name that will automatically appear in the "Vehicle Type" drop-down menu on 'Dashboard.' In addition, the "Configuration Number" at the top of the table should be in numerical order from left to right. The importance of this number is described in the next section (Section 4.3). The remainder of this section provides a description of the vehicle considerations. Detailed discussions for some considerations are left to specific sections in this manual to provide more context.

The first set of vehicle considerations are associated with the battery design properties. A detailed discussion on the first six is provided in Section 5.7. In short, the first item is a default cell thickness, which is based on industry standards observed by the BatPaC group. The next five are related to the power requirements and state of charge (SOC) window of the vehicle.

The seventh item is the reserve safety limit defined as the percentage of SOC above the lower SOC limit. Vehicles typically try to avoid operating below this SOC to guarantee consistent performance of the battery. Power pulses that cause the battery to go below the reserve safety limit trigger a warning in BatPaC (see Section 3.2.3.1). The next consideration determines whether

charging requirements can be included in the design process. It is only TRUE for EVs. Ramifications of charging requirements are discussed in Section 6. Item 10, "Ideal chemistry couple," provides guidance for the type of electrode couple best suited for the vehicle (see Section 3.2.2.1). A warning is triggered if a different couple type is selected (see Section 3.2.3.1). The final consideration in this set determines the added cost for multiple packs in the battery system.

The second set of vehicle considerations are associated with the battery management system (see Section 7 for details). Both considerations (charger fuse and main contactor) are included for high current vehicles that can be charged from an external source.

The final set of vehicle considerations are associated with the thermal management system. The first consideration in this set determines whether BatPaC should assume the refrigerant with the highest cooling capacity. This assumption is required when including charging requirements in the design process (see Section 6). The next item ("Size cooling system for sustained speed") is a relic from a previous version of BatPaC. It does not impact the present calculation. It was left to allow for potential re-introduction in a later version of BatPaC. Considerations three and four determine the cost of additions to the pack and vehicle for thermal components. Considerations five and six are both used for determining the rate of heat generation in the pack during driving (see Section 8). The final consideration sets the thickness of the aluminum conductors. The conductors for mildHEVs are thinner because they are rated for 2-second power pulses where heat generation is less than the 10-second pulse for the other vehicles.

	Selected Vehicle					Default Paramete
Vehicle	EV	mildHEV	HEV-HP	PHEV	EV	
Configuration Number	4	1	2	3	4	
Design Properties						Other configuration
Default Cell Thickness	20	10	12	16	20	
Default time for power pulses	10	2	10	10	10	
SOC for full power	20	80	50	80	20	I I
SOC at average operation	50	80	80	50	50	
Upper SOC Limit	95	95	90	90	95	
Lower SOC Limit	10	70	30	20	10	
% of SOC above lower SOC for reserve safety limit	5	2	2	2	5	
Allow for charging considerations	TRUE	FALSE	FALSE	FALSE	TRUE	
deal chemistry couple	Energy	Power	Power	Either	Energy	۸dd
Additional for multiple packs, \$/additional pack	150	50	100	150	150	Add
BMS Considerations						new
Add Charger Fuse	TRUE	FALSE	FALSE	TRUE	TRUE	vehicles
Add Main Contactor	TRUE	FALSE	FALSE	TRUE	TRUE	
						here
Thermal Considerations						1 C C C C C C C C C C C C C C C C C C C
Require refridge 4 system when fast charge is enabled	TRUE	FALSE	FALSE	FALSE	TRUE	
Size cooling system from sustained speed	TRUE	FALSE	FALSE	TRUE	TRUE	
Additions to AC system, \$/battery system	40	20	40	40	40	
Heating system, \$/pack	20	0	20	20	20	
Maximum sustained vehicle speed at maximum cell temperature	70	0	35	70	70	L
Energy requirement for pack on UDDS, Wh/mile	250	250	250	250	250	•
Default thickness of aluminum conductors, cm	0.04	0.02	0.04	0.04	0.04	

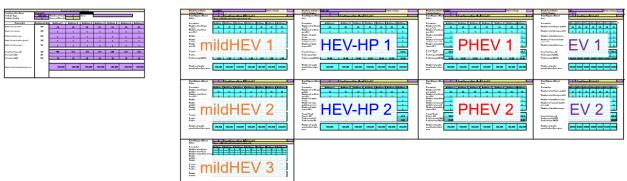
Figure 4.8. Default parameter table in 'Vehicle Considerations' worksheet. Users can add new default vehicle types using the columns to the right of the existing table.

4.3 Vehicle Configurations

Each vehicle type contains a dataset of default configurations which can be selected using the macro button on 'Dashboard' (see Section 3.2.2.2). Each default configuration has unique power and storage requirements for all seven battery packs (*i.e.*, target power, target energy, number of cells per module, number of cells in parallel, etc.). The 'Default Vehicle Configurations' worksheet stores the default vehicle configuration datasets that are interchanged when the macro button "Add set of default pack designs (power, energy, pack configurations)" on 'Dashboard' is clicked. This section will describe the worksheet and explain how to add default vehicle configurations for new and existing vehicles.

The 'Default Vehicle Configurations' worksheet contains several tables, with each table representing a single set of configuration data for all seven batteries (Figure 4.9). The first, left-most table in the worksheet contains the current selection by the default configuration macro. This table should <u>not</u> be modified. As a reminder, most of the cells are purple indicating they are automatic inputs that should not be adjusted directly (see Section 3.2.1). All other tables to the right contain configurations for each vehicle type. Each vehicle type has its own set (*i.e.*, columns) of configuration tables. BatPaC has several built-in configurations, and additional configurations can be added for all vehicles (see details below). The built-in configurations represent example designs for each vehicle.

Clicking the macro button on 'Dashboard' will cycle through the default vehicle configurations for a given vehicle type and update the appropriate values on 'Dashboard.' The "Current selection" table on the 'Default Vehicle Configurations' worksheet will be updated too. The macro only cycles through vehicle configurations for the vehicle type selected on 'Dashboard.'



Current selection

Figure 4.9. Default layout of 'Vehicle Configurations' worksheet in BatPaC 5.

Figure 4.10 provides a screenshot of the first configuration for the mildHEVs as an example. The table has two main components: i) the vehicle header which only exists once per vehicle and ii) the configuration table. The vehicle header contains the vehicle name and number, which are automatically imported from the 'Vehicle Considerations' worksheet. It also includes the number of configurations, which is used by the macro. The vehicle configuration table contains

information about the configuration and corresponding BatPaC inputs. Each new configuration for a given vehicle will only include the configuration table (excluding the vehicle header). At the top of the table are two cells which are calculated automatically and used by the macro. Each configuration contains inputs related to the pack configuration, pack power, pack energy, and manufacturing capacity. Most of the default, built-in configurations provide a comparison of the power-to-energy ratio across all seven batteries. Some configurations are also included to demonstrate how the pack configurations (*i.e.*, arrangement and number of cells and modules) impact the size and cost of the battery, even for the same power and energy requirements.

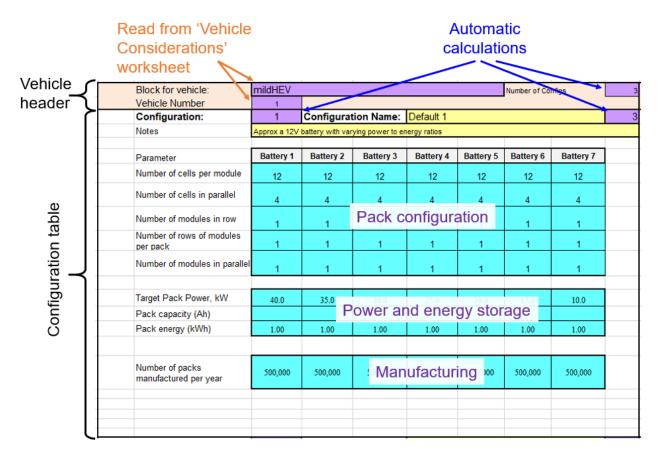


Figure 4.10. Example vehicle configuration table for a mild HEV

Figure 4.11 shows how to add vehicle configurations for a new vehicle type and new vehicle configurations for an existing vehicle type. To add configurations for a new vehicle, copy the first, full table for any existing configuration (including vehicle header) and paste it in the blank space to the right of the current tables. The table should be placed in the next available space, with no blank columns in between vehicle types. All header data will be automatically updated. If a vehicle has not yet been added in the 'Vehicle Considerations' worksheet, a #REF! error will appear in the "Block for vehicle:" cell in the header. Note that the vehicle numbers in the 'Vehicle Consideration' worksheet should be in numerical order from left to right for the default configurations macro to work correctly.

To add a new configuration to an existing vehicle, copy any configuration table and paste it at the bottom of the desired vehicle column. Do not include the vehicle header in the new table. The new table should be pasted directly below the other tables with no white space in between. The macro in BatPaC will automatically recognize the new configuration as part of the configurations for the desired vehicle type. Note that BatPaC provides a single, blank configuration table for a fifth, unused vehicle type as a template. This table becomes active once a fifth vehicle is added in the 'Vehicle Considerations' worksheet (after EV). All other additional configurations in BatPaC must be added with the copy and paste method described herein.

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Figure 4.11. Image showing how to add vehicle configurations for a new vehicle type and new vehicle configurations for an existing vehicle type.

5. MODELING OF BATTERY DESIGN AND PERFORMANCE

This section presents the model used to design the cell, module, and pack. In detail, Section 5.1 provides an overview of the battery design model. Section 5.2 provides the governing equations and algorithm for determining the cell design that satisfies the user inputs. Section 5.3 and 5.4 describe the calculation of the module and pack dimensions, respectively. Section 5.6 describes how the connections between modules and packs are sized. Section 5.7 provides information on how the vehicle type impacts the default input parameters used in the calculation.

5.1 Overview of Battery Design

Figure 5.1 shows a schematic of the user-defined inputs and battery design outputs from the BatPaC model. BatPaC uses an iterative process to generate a cell design that satisfies all user inputs. The resulting cell design is used to calculate the dimensions and performance of the module(s) and pack(s). The goal of the model is to quantify how the various components of a specific battery design sum to make the mass and volume of the pack. In this way, a true energy and power density can be calculated as well as the exact materials requirement to meet the design.

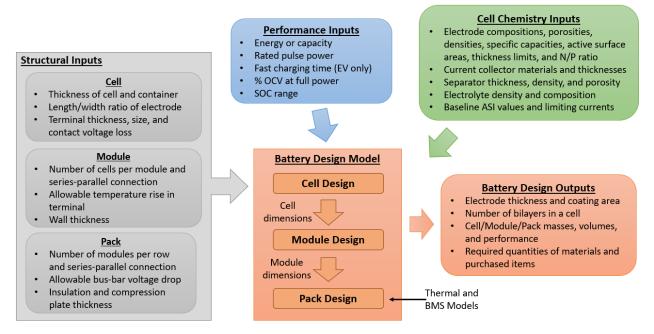


Figure 5.1. Schematic summary of the battery design model.

In the figure, the user-defined inputs are broken into three main categories: performance, cell chemistry, and structural. First, the performance inputs provide the target values used by the BatPaC model to design the battery. The two main performance inputs are the energy and power of the pack. The energy can be specified from either the total capacity or total energy. Defining one of these values will determine the value of the other, when the cell chemistry (cell voltage) is defined. The model uses the energy to guide the total amount of active material in the pack. The power input guides how that material is distributed in the cells (e.g., electrode thickness and total electrode area). In addition to the energy and power, there are also performance inputs related to

fast charging constraints (Section 6), the state of charge range of the battery, and the target voltage at full power (Section 5.7).

The second category corresponds to cell chemistry inputs. These inputs are used by the model to translate the power and energy requirements into the structure of the electrodes in the cell. These inputs include the compositions and properties of the electrodes, electrolyte, current collectors, and separator. For instance, the density, specific capacity, and porosity of the electrodes help determine the size and weight of the material required to meet the energy demand. In addition, the volumetric surface area of the electrode, the conductivity of the materials, and baseline performance data (*e.g.*, area-specific resistance and limiting currents) are used to determine the electrode thickness and area required to meet the power demand. The chemistry inputs also help determine the size of the pack. For example, the densities and thicknesses of all the materials are required to determine the pack volume and weight.

Third, structural inputs are used by the model to help calculate the size, weight, internal connections, and packaging of the battery pack. The structural inputs reflect the battery design presented in Section 2.1. They refer to physical constraints at the cell-, module-, and pack-level. Cell constraints set the design of the non-electrochemically active portion of the cell – e.g., thicknesses of the container, length-to-width ratio of the electrodes, and size of the cell terminals. The module constraints determine how the cells are packaged together – e.g., number of cells per module, the series-parallel connection of the cells, and the thickness of the module walls. The pack constraints determine how the modules are packaged together – e.g., number of modules per pack, series-parallel connection of the modules, and thicknesses of the insulation and compression plates.

BatPaC provides default values for the inputs based on industry practice, as well as a wide variety of chemistry selections with their properties measured at Argonne National Laboratory. Sections 3 and 4 provide instructions on how to select and modify the default inputs. Additional detail on several main inputs is left to Section 5.7. Note that BatPaC is developed to allow many customizations, and users can override the values to design their own battery using their parameter sets.

5.2 Cell Design

The first step in the battery design model is the calculation of the cell design that meets the performance inputs. The main design outputs are the thickness of the electrodes, the electrode area, and the number of bi-cell layers per cell. These values set the total dimensions of the cell (Section 5.2.5), which, in turn, set the dimensions of the module (Section 5.3) and pack (Section 5.4).

5.2.1 Governing Equations

The cell design model consists of five coupled equations that translate the cell geometry (*i.e.*, surface area, A_{pos} , and electrode thickness, δ_{pos}) into the power and energy of the battery pack. Here we present the expressions of the equations and explain how the unknowns are determined. First, the total energy of the pack, E_{pack} (Wh), is defined as the product of the capacity (Ah) and the

average voltage (V) during discharge. In this work, the average voltage is calculated assuming discharge at a C/3 rate. This assumption leads to the following equation:

$$E_{pack} = N_{cell} C_{cell} \left(U_E - \left(\frac{C_{cell}}{3} \right) \frac{ASI_E}{A_{pos}} \right)$$
(5.1)

where, N_{cell} and U_E are user-defined inputs corresponding to the number of cells in the pack and the single-cell open circuit voltage (OCV) taken at the average state of charge (SOC) during operation, respectively. C_{cell} , A_{pos} , and ASI_E are calculated quantities from the model and refer to the capacity (Ah), positive electrode area (cm²), and area-specific impedance for energy (Ω cm²), respectively, of a single cell. C_{cell} is defined using equation 5.2:

$$C_{cell} = Q\rho\varepsilon_{act}A_{pos}\delta_{pos} \tag{5.2}$$

In Eq. 5.2, Q, ρ , and ε_{act} are user-defined chemistry inputs that correspond to the specific capacity (Ah g⁻¹), density (g cm⁻³) and volume fraction of the active material, respectively. δ_{pos} (cm) is the thickness of the positive electrode, another unknown. A_{pos} is determined by satisfying the basic power equation (power = current × voltage). To accomplish this, BatPaC requires the user to specify the beginning of life (BOL) voltage drop for rated power, $[V/U]_P$, where V is the total voltage during the power pulse and U is the OCV at the SOC at the start of the pulse. The value of $[V/U]_P$, usually >0.8, is selected to reflect the allowable degradation rate of the battery. It has a default value of 0.8 in BatPaC. A detailed discussion on this parameter can be found in the previous version of the manual [12]. Using this value results in the following equation for power:

$$P_{pack} = N_{cell} A_{pos} I_P U_P \left[\frac{V}{U}\right]_P$$
(5.3)

where P_{pack} (W) is the user-defined, rated power of the battery, and U_P (V) is the OCV of a single cell at the SOC at the start of the power pulse (a chemistry-related input). Details on the selection of U_P (and U_E) for different vehicle types are provided in Section 5.7. In Eq. 5.3, I_P is the calculated current density of a single cell at the rated power. It is determined using Ohm's law as follows:

$$I_P = \frac{U_P \left(1 - \left[\frac{V}{U}\right]_P\right)}{ASI_P} \tag{5.4}$$

where ASI_P is the area-specific impedance ($\Omega \text{ cm}^2$) of the cell at rated power. The ASIs (ASI_P and ASI_E) depend on the electrode thickness (δ_{pos}), electrode area (A_{pos}), and applied current density (I) of the cell. The calculation is described in detail in Section 5.2.2. For now, it is represented using the following expression:

$$ASI = f(\delta_{pos}, A_{pos}, I)$$
(5.5)

Equations 5.1 to 5.5 represent a set of six algebraic equations (Eq. 5.5 is used twice) with six unknowns: C_{cell} , A_{pos} , δ_{pos} , I_p , ASI_P , and ASI_E . To properly bound these equations, recall that BatPaC requires the user to input the total pack energy (E_{pack} , Wh) or the total pack capacity (C_{pack} , Ah) to define the size of the pack. If E_{batt} is specified, the formulation above is unchanged and equations 5.1 to 5.5 can be solved to calculate the unknowns, with Eq. 5.5 used twice for ASI_P and ASI_E . If C_{pack} is specified, equation 5.1 is replaced by equation 5.6.

$$C_{pack} = C_{cell} N_{mod,||} N_{cells,||}$$
(5.6)

where $N_{mod,||}$ and $N_{cells,||}$ are the number of modules in parallel within the pack and the number of cells in parallel within a module, respectively. Both are user-defined inputs. Note that, in this case, Eq. 5.1 is still used by BatPaC to output the calculated energy, but it is no longer required to solve the coupled equations.

5.2.2 ASI Model

As noted in the previous section, area-specific impedance (ASI) is an important characteristic of a battery that determines the energy and power. However, ASI is not an inherent constant of a specific battery chemistry or cell design. Rather, it is a complex combination of resistances within the battery resulting from the physical processes occurring at different length and time scales. ASI is, therefore, a function of many factors (*e.g.*, state of charge, charge/discharge pulse length, current density, particle size, transport and kinetic parameters, etc.). BatPaC employs a model for the ASI in calculations associated with the rated power and energy. This section introduces the ASI model employed in BatPaC and explains the physical meanings of the model components and approximations. Detailed derivation of the model, as well as its validation against experiments, can be found in [5].

5.2.2.1 Experimental Definition of ASI

ASI is the impedance per unit area of electrode coating, generalized as a function of time, current density, and SOC. To ground the discussion, this work assumes the ASI is measured by a current pulse from an unperturbed state, followed by a rest period. Equation 5.7 shows the definition of ASI employed in BatPaC.

$$ASI = \frac{V_{t2} - V_{t1}}{I_{t1} - I_{t2}}$$
(5.7)

In Eq. 5.7, *I* and *V* correspond to the current and voltage, respectively, of the battery at times t1 and t2 during the pulse current experiment. Time t1 corresponds to the time just before the pulse ends, and time t2 corresponds to the time long after the current pulse, when the battery is assumed to be resting at open circuit voltage without polarization. I_{t1} is a positive valued current density for a discharge pulse. I_{t2} is equal to zero since there is no applied current at rest. Note that this definition for the experimentally determined ASI is slightly different than the one presented in [5]. In [5], the rest period before the pulse (not after) is used as the reference state. Using the rest period before the pulse adds an extra component to the ASI related to the thermodynamic changes in the

OCV. The thermodynamic changes result for increased intercalation concentration during the pulse. The definition in Eq. 5.7 neglects the thermodynamic component, resulting in a slightly smaller value for the ASI when compared to the ASI in [5]. One advantage of Eq. 5.7 is that it can be estimated theoretically without detailed information on the OCV with respect to SOC. This is an important feature for BatPaC because it facilitates the comparison of different battery chemistries without the need for detailed experimental results.

5.2.2.2 Theoretical Treatment of ASI

In this model, the ASI of a cell is expressed theoretically as follows:

$$ASI = ASI_{echem} + ASI_{cc} + ASI_{term,cell} + \frac{R_{cnct}A_{pos}}{N_{cell}}$$
(5.8)

where the subscripts *echem*, *cc*, and *term*,*cell* correspond to the ASI of the electrochemical charge/discharge processes, the cell current collectors, and the terminals of the cell, respectively. The fourth term in the equation accounts for resistances associated with electrical connections at the cell, module, and pack levels. These values are distributed on a per-cell basis to facilitate the calculation.

The ASI for the electrochemical processes (ASI_{echem}) is calculated using an Arrhenius-type equation to account for changes in resistance due to operating temperature.

$$ASI_{echem} = ASI_{echem, ref} exp\left[\frac{E_{a, eff}}{\bar{R}} \left(\frac{1}{T_{ref}} - \frac{1}{T}\right)\right]$$
(5.9)

In Eq. 5.9, T_{ref} is the reference temperature (298.15 K), T is the operating temperature, \overline{R} is the universal gas constant (8.314 J mol⁻¹ K⁻¹), and $E_{a,eff}$ is an effective activation energy. $E_{a,eff}$ is typically negative and accounts for decreases in ASI with increased temperature. A default value of -30 kJ/mol was determined from experiments conducted on coin cells containing graphite negative electrodes with NCA, NMC333, NMC532, NMC622, and NMC811 positive electrodes [14]. *ASI_{echem,ref}* is the reference ASI calculated at 298.15 K. It is composed of three terms in the model, as shown in Equation 5.10. The first two terms account for impedance that arises from the interfacial charge transfer and ion transport. The third factor is a lumped parameter used to capture the remaining impedance. Contributions to this term includes the potential drop across the separator and the porous electrodes and any error introduced by the simplified electrode models. Details on its determination are provided in Section 5.2.2.3.

$$ASI_{echem,ref} = ASI_{intf,neg} + ASI_{intf,pos} + ASI_{const}$$
(5.10)

The interfacial ASIs of the negative ($ASI_{intf,neg}$) and positive ($ASI_{intf,pos}$) electrodes are modeled using the interfacial charge transfer resistance $\bar{R}T/i_oa\delta F$, as shown in Equations 5.11 and 5.12. This formulation assumes the battery operates within the linear kinetics regime. Detailed derivation is provided in [5].

$$ASI_{intf,neg} = \frac{\bar{R}T_{ref}}{i_o a\delta_{neg}F}$$
(5.11)

$$ASI_{intf,pos} = \frac{\bar{R}T_{ref}}{i_o a\delta_{pos}F} \left\{ \left(1 - \frac{I}{I_{ionic,lim}}\right) \left[1 - \left(\frac{r_c}{r_{c,lim}}\right)^2\right] \right\}^{-0.5}$$
(5.12)

In equations 5.11 and 5.12, i_o is the exchange current density (A m⁻²) related to the interfacial area and *a* is the ratio of interfacial area to electrode volume (*i.e.*, specific surface area, m² m⁻³). An approximation often used for *a* relates the parameter to the volume fraction of the active material and the particle radius, $a = 3\varepsilon_{act}/r_p$. The variables i_o and *a* should be specified relative to the same area as they are usually determined together. *F* is Faraday's constant (96,485 C mol⁻¹).

Note that the positive electrode interfacial impedance in Eq. 5.12 includes two additional factors that account for transport limitations in the cell. The first term accounts for depletion of lithium ions in the electrolyte due to transport resistances in the separator between the electrodes. It is governed by $I_{ionic,lim}$, the limiting ionic current for lithium cation transport through the porous separator. The second term corresponds to transport limitations associated with solid state diffusion from the surface of the particles in the electrode. It is governed by $r_{c,lim}$, the limiting C-rate for solid state diffusion of lithium. The C-rate is related to the current density of the cell as follows:

$$r_c = \frac{I}{Q\rho\varepsilon_{act}\delta_{pos}} \tag{5.13}$$

 $I_{ionic,lim}$ and $r_{c,lim}$ are both user-defined inputs. The values of these terms can be estimated using diffusion coefficients and diffusion lengths in the separator and active material particles, respectively, as shown in [5]. Verification of the values may be done with detailed models based on concentrated solution theory and/or with experimental measurements.

The second term in Eq. 5.8, the current collector foil impedance (ASI_{cc}) , is determined from the analytical expression in Eq. 5.14. This expression accounts for the coated and uncoated region of the foil, represented by the subscripts *act*, for active, and *tab*, for tab connection, respectively. The resistance factor, R_f , and the resistance of the current collector foils, R_{cc} , are also shown for clarity in equations 5.15 and 5.16.

$$ASI_{cc} = L_{act}W_{act}R_{cc} = R_f\left(\frac{(L_{act})^2}{3} + L_{act}L_{tab}\right)$$
(5.14)

$$R_f = \left(\frac{2}{\sigma_{cc,neg}\delta_{cc,neg}} + \frac{2}{\sigma_{cc,pos}\delta_{cc,pos}}\right)$$
(5.15)

$$R_{cc} = R_f \left(\frac{L_{act}}{3W_{act}} + \frac{L_{tab}}{W_{tab}} \right)$$
(5.16)

In the equations, L_{act} and W_{act} refer to the length and width of the active portion of the electrode area. They are calculated using A_{pos} according to equation 5.34 in the cell dimension Section 5.2.5 and correspond to the length (L_{pos}) and width (W_{pos}) of the positive active area. The tab length (L_{tab}) is 120% of the cell thickness ($1.2 \times \delta_{cell}$). This definition provides excess foil so all tabs can reach the center of the cell for welding to the terminal without the risk of tearing. The current collector foil conductivities (σ_{cc}) and thicknesses (δ_{cc}) are user-defined inputs. Note that the factor of 2 in the R_f term (Eq. 5.15) accounts for the assumption that the foils are double side coated, and half of the foil thickness (δ_{cc}) carries the current produced on one side of the foil. Another assumption is the use of L/3 as an equivalent length for the resistance in Eq 5.16. The equivalent length is determined so that multiplication of the equivalent length by the total cell current gives the correct ohmic drop in the foil. This assumption accounts for the fact that the current varies along the length of the coated foil as the reaction area continually contributes current to the foil. The equivalent length is L/3 if the current density is relatively constant over the entire length of the foil. Previous work has shown this is a reasonable assumption for the cells under consideration [12].

The third term in Eq. 5.8, ASI of the cell terminals ($ASI_{term,cell}$), includes the resistance of the positive and negative cell terminals as shown in Eq. 5.17. The dimensions for these terminals are set by the width of the exterior portion of the terminal ($W_{term,ext}$, see Figure 5.5 for details), the user defined terminal thicknesses ($\delta_{term,i}$, default equals 1.2 mm for the positive and 0.8 mm for the negative), and the length of the terminal ($L_{term,cell}$). The length of the terminal is multiplied by 1.2 to produce an effective length which includes an extra 20% to account for contact resistances.

$$ASI_{term,cell} = \left(\frac{1}{\delta_{term,pos}\sigma_{cc,pos}} + \frac{1}{\delta_{term,neg}\sigma_{cc,neg}}\right) \frac{1.2L_{term,cell}}{W_{term,ext}} A_{pos}$$
(5.17)

The ASI for connectors is the last term in the ASI summation stated in Eq. 5.8. This ASI depends on R_{cnct} , which includes the resistances for the cell, module, and pack connections. In Eq. 5.8, the positive electrode area per cell (A_{pos}) and number of cells (N_{cell}) are included to distribute this resistance amongst all cells, thereby converting the total system losses from carrying the electric current onto a per-cell basis. The calculation of R_{cnct} is detailed in Equation 5.18 with the individual sources of connection losses shown as follows:

$$R_{cnct} = R_{cnct,cell} + R_{cnct,mod} + R_{cnct,pack}$$
(5.18)

In Eq 5.18, the subscripts *cell*, *mod*, and *pack* denote the connection resistance on the cell, module, and pack level, respectively. $R_{cnct,cell}$ is the total cell-to-cell interconnect resistance and is calculated as follows:

$$R_{cnct,cell} = \frac{\ell_{icnct,cell}}{\sigma_{Cu}A_{icnct,cell}} \left(\frac{N_{cell/mod}}{N_{cell,||}} - 1\right) N_{cell,||} N_{mod}$$
(5.19)

where σ_{Cu} , $A_{icnct,cell}$, and $\ell_{icnct,cell}$ are the conductivity, area, and effective length of the copper cell interconnects, respectively. $N_{cell/mod}$, $N_{cell,//}$, and N_{mod} are the number of cells in a module, the number of cells in parallel, and the number of modules in the pack, respectively. The effective

length and area of the cell interconnects depend on the cell and terminal dimensions according to Equations 5.20 and 5.21:

$$\ell_{icnct,cell} = \delta_{cell} + L_{term,ext} \tag{5.20}$$

$$A_{icnct,cell} = \delta_{cnct,cell} W_{term,ext}$$
(5.21)

where δ_{cell} is the cell thickness, $L_{term,ext}$ is the length of the cell terminal external of the cell pouch, and $\delta_{cnct,cell}$ is the thickness of the cell interconnect (default = 1 mm). See Figure 5.5 in Section 5.2.5 for details on the cell terminal dimensions.

The module connection resistance accounts for resistances in the tabs connecting the cells to the module terminals (including extra cell interconnects), resistances in the module terminals, and resistances in the interconnects between modules. It is calculated using the following equations:

$$R_{cnct,mod} = R_{tab,mod} + R_{term,mod} + R_{icnt,mod}$$
(5.22)

$$R_{tab,mod} = \left(\frac{\ell_{tab,mod}}{\sigma_{cu}A_{tab,mod}} + \frac{f_{icnct,cell}\ell_{icnct,cell}}{\sigma_{cu}A_{icnct,cell}}\right)2N_{mod}$$
(5.23)

$$R_{term,mod} = \frac{\ell_{term,mod}}{\sigma_{Cu}A_{term,mod}} 2N_{mod}$$
(5.24)

$$R_{icnt,mod} = \frac{\ell_{icnct,mod}}{\sigma_{cu}A_{icnct,mod}} (N_{mod/row} + 1) N_{rows of mods}$$
(5.25)

In equations 5.23 to 5.25, ℓ and A refer to the effective length and area, respectively, while the subscripts tab, mod; term, mod; and icnct, mod refer to the module tabs, terminals, and interconnects respectively. Copper is assumed for all components. In Eq. 5.23, the second term in the parentheses accounts for extra cell interconnects required to make the connection with the tab, which are not accounted for in Eq. 5.19. ficnet, cell is a factor accounting for series and parallel cell connections. It has a value of 1/4 if $N_{cell,||}$ equals three, 5/16 if $N_{cell,||}$ equals four, and zero for all other values of $N_{cell,//}$. Connections of greater than four cells in parallel are not anticipated. In Eq. 5.25, $N_{mod/row}$ is the number of modules per row, and $N_{rows of mods}$ is the number of rows of modules in the pack. The module tab, terminal, and interconnect areas are determined from a calculation based on a predetermined allowable rate of temperature rise for the conductor. This approach is explained in more detail in Section 5.6. The effective length of the module tabs ($\ell_{tab,mod}$) is equal to half the tab length ($0.5 \times L_{tab,mod}$). The effective length of the module terminals ($\ell_{term,mod}$) is 10 mm less than the terminal length ($L_{term,mod}$). The effective lengths ($\ell_{tab,mod}$ and $\ell_{term,mod}$) are less than the actual lengths to account for the fact that parts of the tabs and terminals are inserted into each other and are not a part of the conduction path. The effective length of the module interconnects ($\ell_{icnct,mod}$) is an input parameter with a default value of 6 cm. See Section 5.3.2 for details on module component sizing.

The final set of resistances in Eq. 5.18 are for the pack connections. These are composed of bus bar and terminal resistances, which are calculated as follows:

$$R_{cnct,pack} = \frac{\ell_{BB,term}}{\sigma_{Cu}A_{BB,term}} N_{BB,term} + \frac{\ell_{BB,mod}}{\sigma_{Cu}A_{BB,mod}} N_{BB,mod} + \frac{2\ell_{term,pack}}{\sigma_{Cu}A_{term,pack}}$$
(5.26)

where the subscripts *BB,term*; *BB,mod*; and *term,pack* refer to the bus bar connected to the terminal, the bus bar connecting modules, and the pack terminals, respectively. The number of bus bars ($N_{BB, term}$ and $N_{BB,mod}$) depend on the module configuration, and their calculation is described in Section 5.5.1. The effective lengths of the bus bars are equal to their total length ($L_{BB,term}$ and $L_{BB,mod}$). The effective length of the pack terminal is an input with a default value of 12 cm. The areas of the bus bars and terminals are calculated using the same rate of temperature rise considerations for the modules, which is presented in Section 5.6.

5.2.2.3 Determination of ASI_P and ASI_E

In the cell design model, there are two separate versions of the ASI used in equations 5.1 and 5.4 relating to the ASI for energy, ASI_E , and power, ASI_P , respectively. ASI_E refers to the resistance during a constant C/3 discharge, while ASI_P refers to the resistance during a high-power pulse. Both are calculated using Eq. 5.8 but with different values for $ASI_{echem,ref}$, which appears in Eq. 5.9.

ASIechem, ref is determined for ASIP and ASIE from user-input data for the ASI of the cell during a discharge pulse. BatPaC requires three sets of default ASI data as input in the 'Chem' worksheet: i) ASI_{echem, ref} at two seconds into a high-power pulse (ASI_{2s,0}), ii) ASI_{echem, ref} at ten seconds into a high-power pulse (ASI105,0), and iii) the interfacial resistances (ASI105,0 and ASI105,0) calculated using equations 5.11 and 5.12 for the default case. ASI_{2s,0} and ASI_{10s,0} are required from 0-100% SOC, in increments of 10%, and correspond to ASIechem, ref for cells with the default properties listed in the 'Chem' worksheet. $ASI_{2s,0}$ and $ASI_{10s,0}$ values may be determined experimentally or through simulation. For the default chemistry couples in BatPaC, they were determined using a continuumlevel model of a Li-ion cell formulated with concentrated solution theory. An example of the model for a NMC532-graphite cell can be found in this recent publication [15]. The default interfacial resistances ($ASI_{intf,pos,0}$ and $ASI_{intf,neg,0}$) were calculated from inputs for the default case -i.e., default electrode thicknesses, electrode specific surface areas, active material exchange current densities, pulse C-rate, limiting current, and limiting C-rate. Calculations are provided for the default chemistry couples in the 'Chem' worksheet to show how changing these parameters should impact the interfacial resistances. Caution should be taken when updating or overriding the default ASI values to make sure all coupled parameters are updated. For instance, note that the default ASI values provided in the 'Chem' worksheet correspond to adiabatic operation with an initial temperature of 25 °C.

*ASI*_{2s,0} and *ASI*_{10s,0} from 0 to 100% SOC and *ASI*_{intf,pos,0} and *ASI*_{intf,neg,0} are required for BatPaC to provide the ASI at all user-defined pulse lengths and starting SOCs. Recall from Section 3 that the user can override the default power requirements in 'Dashboard' to design for unique pulse durations and SOCs. For BatPaC to handle all possible cases, a correlation was developed using a simulated dataset of a Li-ion cell that was discharged under adiabatic conditions across a wide range of operating and design parameters. Initial SOCs ranged from 20% to 90%. C-rates ranged from 1 to 12C. Electrode loadings ranged from 1 to 4 mAh cm⁻². To increase the diversity of the

dataset, simulations were conducted for fast and sluggish mass transport by using either Bruggeman exponents of 1.5 for the electrodes and separator or exponents from Colclasure et al. (which range from 2 to 2.5), respectively [16,17]. In addition, three lithium-ion chemistry couples were simulated (NMC532-graphite, LFP-graphite, and LFP-LTO). These chemistry couples varied in their electrode porosities, particle sizes, kinetic properties, electrode conductivities, and thermodynamic behavior. The dataset was used to develop a correlation for predicting the default electrochemical ASI (*ASI_{echem,0}*) as a function of SOC and pulse duration. It is given as follows:

$$ASI_{echem,0} = ASI_{2s,SOC} - \left(1 - \frac{1}{2\sqrt{2}}\right) ASI_{intf,0} + \frac{4(ASI_{10s,SOC} - ASI_{2s,SOC} + ASI_{intf,0})}{10\sqrt{10}}\sqrt{t} + ASI_{10s,SOCe} - ASI_{10s,SOC}$$
(5.27)

1

where $ASI_{2s,SOC}$ and $ASI_{10s,SOC}$ refer to the default two- and ten-second ASIs, respectively, at the SOC at the start of the pulse. They are determined by interpolating the $ASI_{2s,0}$ versus SOC and $ASI_{10s,0}$ versus SOC data provided in the 'Chem' worksheet, respectively. $ASI_{intf,0}$ is the combined interfacial resistances of the positive ($ASI_{intf,pos,0}$) and negative ($ASI_{intf,neg,0}$) electrodes at the default case. Its value does not depend on SOC. *t* is the duration of the pulse in seconds. $ASI_{10s,SOCe}$ is the default, ten-second ASI taken at the SOC at the end of the pulse. It is calculated by first determining the end SOC based on the initial SOC, the pulse duration, and the C-rate. Then, $ASI_{10s,SOCe}$ is determined by interpolating the $ASI_{10s,SOCe}$ and $ASI_{10s,SOCe}$ is included in Eq 5.27 to capture the increases in ASI due to shifts in OCV during the pulse. Figure 5.2 demonstrates the good agreement between Eq 5.27 and the simulated pulses.

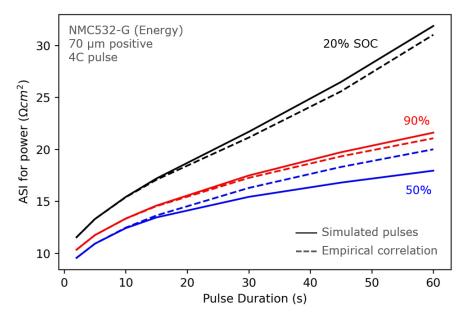


Figure 5.2. Comparison of the ASI from simulated pulses and the empirical correlation (Eq. 5.27) for three pulses from NMC532/graphite cells at different initial states of charge (SOC): 90% (red), 50% (blue), and 20% (black). The solid lines represent the simulated pulses, and the dashed lines represent the estimated values from the correlation.

Eq. 5.27 was developed by first using Pearson and Kendall correlations to isolate which BatPaC parameters best correlated to the simulated ASI. This included testing both linear and non-linear correlations. Trial equations were developed with various combinations and functional forms of the isolated parameters. These equations included weighted constants whose values were determined from a combination of trial and error and physical intuition. Care was taken to ensure the equations accurately reproduced the two- and ten-second ASI and captured the sharp increases in ASI at long times and low SOCs. Eq. 5.27 above was selected because it provided the most accurate results with the least amount of data.

For ASI_P, ASI_{echem,ref} is determined using Eq 5.10, where ASI_{const} is defined as follows:

$$ASI_{const,P} = ASI_{echem,0} - ASI_{intf,pos,0} - ASI_{int,neg,0}$$
(5.28)

All terms are calculated at the default electrode thickness at the duration and SOC for rated power. For ASI_E , Eq. 5.10 is ignored and $ASI_{echem,ref}$ is calculated using a multiplier on the ten-second, default ASI, which is calculated at the SOC for energy (see Section 5.7).

$$ASI_{echem, ref, E} = 1.3 \cdot ASI_{10s, SOC}$$
(5.29)

A factor of 1.3 was determined from analysis of the discharge dataset used to determine the correlation for $ASI_{echem,0}$. It provides a reasonable approximation of the steady-state ASI at C/3.

5.2.3 Model Solution

Once the five governing equations are set (equations 5.1 to 5.5, where Eq. 5.5 arises from equations 5.8 to 5.29), BatPaC solves the model using an iterative process that adjusts the positive electrode thickness (δ_{pos}) and cell capacity (C_{cell}) until all five governing equations are satisfied. The results of the model are then used to determine all other output parameters for the cell design. For instance, note that equations 5.1 to 5.5 all depend on the properties of the positive electrode. The properties of the negative electrode are calculated from these output values. The negative electrode area is calculated by assuming it is 1 mm larger than the positive electrode in both length and width to alleviate concerns of lithium plating during charge pulses. In addition, the separator area is slightly larger than the negative electrode to prevent the electrical shorting of the two electrodes.

Furthermore, the negative electrode thickness (δ_{neg}) is determined by its specific reversiblecapacity and the designed excess-capacity to prevent lithium plating during charging. A ratio of 1.1 negative to positive reversible capacity (N/P ratio) has been chosen for the default value for all cells. With the dimensions of the active portions of the cell set, the total size and weight of the cell are designed using the formulation in Section 5.2.5.

5.2.4 Additional Constraints

Finally, note that there are two additional constraints placed on the cell design formulation. The first is an integer constraint on the number of bilayers in a cell, which is discussed in Section 5.2.5. The second is a constraint on the maximum electrode thickness, which can occur in two ways. The

first way is by setting it as a user-defined input in "Dashboard." This limitation may be set by manufacturing capabilities, ionic and electronic current transport within the porous electrode, or aging characteristics related to adhesion to the current collector. Detailed discussion of these challenges can be found in [12,18]. The second way is through calculation of the maximum allowable thickness to prevent plating during fast charging of an electric vehicle. This method is only valid when EVs are selected as the vehicle type. Details on the calculation are provided in Section 6. If both constraints are set, BatPaC will take the thinnest as the maximum allowable value.

When the maximum electrode thickness, δ_{max} , has been reached on either the positive or negative electrode, the electrode area equation is modified as shown in Equation 5.30.

$$A_{pos,\delta_{max}} = \frac{\delta_{tgt}}{\delta_{max}} A_{pos}$$
(5.30)

where the electrode thickness, δ_{tgt} , is the largest electrode thickness, negative or positive, determined by solving the governing equations (5.1 to 5.5). The area of the electrode is now determined by the cell capacity requirement to meet the battery energy demands and not the rated power. To elaborate, if $\delta_{tgt} > \delta_{max}$, the model completes one more design iteration. For the final iteration, Eq. 5.30 replaces equations 5.3 and 5.4 with δ_{tgt} and A_{pos} as constants. The model then reduces to a set of four governing equations (5.1, 5.2, 5.5, and 5.30) with four unknowns (C_{cell} , $A_{pos,\delta_{max}}$, ASI_E , and I_E).

Consequently, to maintain the same input power rating, the designed battery will operate at a smaller voltage drop than the maximum allowed by the user. The new $[V/U]_P$ may then be calculated from Equation 5.31, which is the solution to the quadratic in Equation 5.32.

$$\left[\frac{V}{U}\right]_{P} = \frac{1}{2U_{P}} \left(U_{P} + \sqrt{(U_{P})^{2} - 4\frac{P_{pack}ASI_{P}}{N_{cell}A_{pos}}}\right)$$
(5.31)

$$V_{cell} = U_P - \frac{P_{pack}ASI_P}{V_{cell}N_{cell}A_{pos}}$$
(5.32)

5.2.5 Cell Dimensions

Solution of the cell design model provides outputs that are used to determine the size of the cell. Figure 5.3 provides an image of a bi-cell layer within the cell and highlights important nomenclature for understanding the cell design. First, the number of bi-cell layers, N_{layers} , in each cell is determined in Equation 5.33 by accounting for the packing density ($X_{packing}$) and the individual thicknesses of the current collector foils (δ_{cc}), electrodes (δ_{pos} and δ_{neg}), separator (δ_{sep}), and container (δ_{cont}). $X_{packing}$ accounts for inefficiencies in the packing of the electrode stack within the pouch cell is taken to be 0.97. All these values are user-defined inputs except the electrode thicknesses. The Li-ion battery chemistries in BatPaC v5.0 are assumed to undergo negligible volume change at the cell level.

$$N_{layer} = X_{packing} \frac{\delta_{cell} - 2\delta_{cont} - \delta_{cc,neg}}{\delta_{cc,neg} + \delta_{cc,pos} + 2(\delta_{neg} + \delta_{sep} + \delta_{pos})}$$
(5.33)

The term in the denominator of Eq. 5.33 corresponds to one bi-cell layer (see Figure 5.3b). $\delta_{cc,neg}$ is included in the numerator to correct for an extra component in the cell that is not part of a standard bi-cell layer. Its value arises from the assumption that the first and last layers in the cell are negative current collectors with single-sided electrodes that face internally towards the separators. Note that N_{layers} is a natural number, which results in Equation 5.33 introducing an integer constraint to the governing equations 5.1 to 5.5. BatPaC finds a solution that satisfies the constraint by iteration. If the thickness of the bi-cell layers does not permit a whole number of layers to fit into the set thickness of the cell, the cell thickness is slightly altered until there is an exact fit. Note that the set thickness of the cell is a user-defined input that will be discussed in Section 5.7.

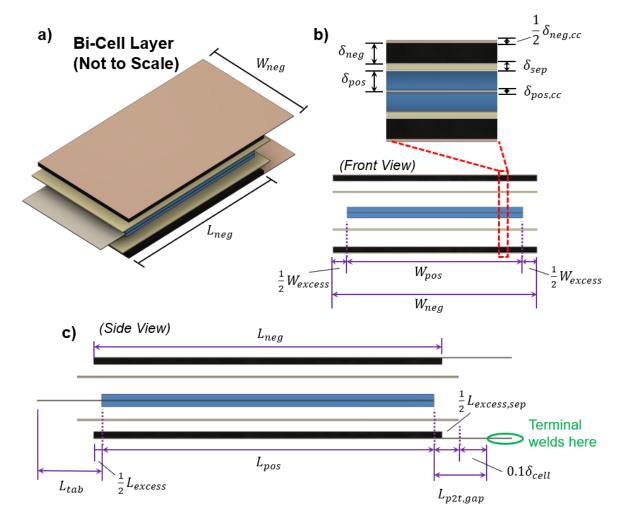


Figure 5.3. Images of a bi-cell layer within the cell highlighting important dimensions for understanding cell design: a) profile of a bi-cell layer, b) front view, and c) side view. Dimensions of layers are exaggerated to improve their visibility and are not drawn to scale.

The width of the positive electrode is determined using the calculated electrode area, A_{pos} , N_{layers} , and the user-defined electrode aspect ratio, [L/W], as follows:

$$W_{pos} = \sqrt{\frac{A_{pos}}{2\left[\frac{L}{W}\right]N_{layers}}}$$
(5.34)

The factor of 2 enters the denominator as both sides of the foil are assumed to be coated. Note that determination of the width also determines the length using the electrode aspect ratio, [L/W]. The default [L/W] is set at 3. The negative electrodes are assumed to have an excess width (W_{excess}) and length (L_{excess}) to guarantee full overlap between the positive and negative active materials (see Figure 5.3b and Figure 5.3c. Both values are 2 mm by default (1 mm on all sides). The separator is assumed to have the same excess width as the negative electrode but a slightly larger excess length (default $L_{excess,sep} = 4$ mm) to prevent short circuiting with the current collectors. Recall from the discussion of equation 5.14 that the current collector tabs (uncoated regions of the foils) are assumed to extend 120% of the cell thickness ($1.2 \times \delta_{cell}$) past the edge of the positive electrode. Note that by this definition, the uncoated region of the negative foil is shorter than the uncoated region of the positive by $0.5 \times L_{excess}$.

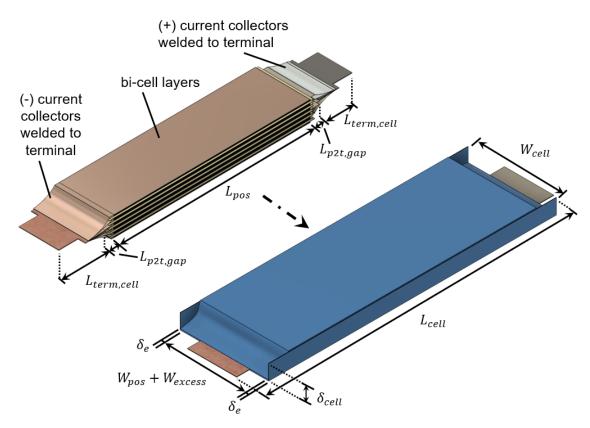


Figure 5.4. Schematic of full stack of bi-cell layers and pouch cell showing dimensions. Thicknesses of components are exaggerated to improve their visibility and are not drawn to scale.

Once these terms are calculated, the rest of the cell dimensions are calculated using Equations 5.35 and 5.36 for the cell width and length, respectively. These dimensions are also shown schematically in Figure 5.4.

$$W_{cell} = W_{pos} + W_{excess} + 2\delta_e \tag{5.35}$$

$$L_{cell} = L_{pos} + 2(L_{term,cell} + L_{p2t,gap})$$
(5.36)

In Eq. 5.36, δ_e is the thickness of the folded edge, which arises because the seals on the sides of the pouch are folded up, pressing along the inside wall of the module casing. It has a default value of 1 mm. The length of the cell, L_{cell} , is the length of the positive electrode (L_{pos}) with additions for the length of the terminals ($L_{term,cell}$) and the gaps between the positive electrode and the start of the terminal ($L_{p2t,gap}$). Note that perceived differences in $L_{term,cell}$ between the positive and negative terminals in Figure 5.4 is only an artifact of the image's perspective and is not a reality. Both terminals have the same length. The length of the terminals is the sum of the three terms shown in Figure 5.5: $L_{term,ext}$ is the exterior portion of the tab protruding out from the pouch for cell-to-cell connection; $L_{term,fr}$ is the feedthrough portion of the terminal, on which the pouch is sealed; and $L_{term,int}$ is the interior portion of the terminal welded to the current collectors of the electrodes (see welded region in Figure 5.4). $L_{term,ext}$ and $L_{term,fr}$ have default values of 8 and 5 mm, respectively. $L_{term,int}$ is assumed to extend from $L_{p2t,gap}$ to the edge of the current collector tab. $L_{p2t,gap}$ is the distance between the edge of the positive electrode and the edge of the separator ($0.5 \times L_{excess,sep}$) plus $0.1 \times \delta_{cell}$ to provide some flexibility before the weld (see Figure 5.3c).

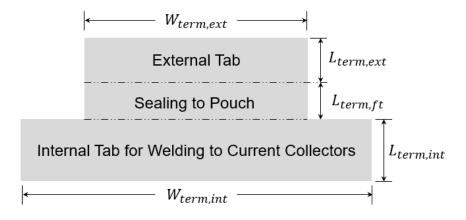


Figure 5.5. Schematic of cell terminals

Figure 5.5 also shows the width of the external ($W_{term,ext}$) and internal ($W_{term,int}$) portions of the terminal. BatPaC assumes $W_{term,ext}$ is equal to 40 mm if W_{pos} is less than 85 mm and 50 mm for larger W_{pos} . $W_{term,int}$ is equal to W_{pos} minus a buffer region (default = 2 mm on either side) so the tab does not extend directly to the end of the current collector.

5.3 Module Design

The modules are designed to contain all the cells, along with supporting components for thermal and electrical control. This section explains the dimensions of the module and the design of the individual components. As a refresher from Section 2.3, Figure 5.6 shows the main components in the module.

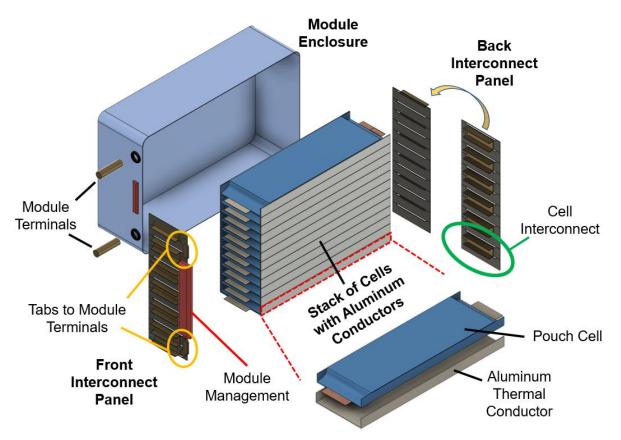


Figure 5.6. Breakdown of main components in the module.

5.3.1 Module Dimensions

Figure 5.7 provides a schematic of the module and its dimensions. The module dimensions are defined by Equations 5.37 to 5.39. BatPaC assumes the module is equal to the length of the cell plus additional lengths at the front ($L_{excess,front}$) and back ($L_{excess,back}$) to account for the gas release provisions, the module management system, and the enclosure walls (see Figure 5.7c). $L_{excess,front}$ and $L_{excess,back}$ have default values of 6 and 2 mm, respectively. Note that the length of the terminals extruding from the module are not included in its length.

$$L_{mod} = L_{cell} + L_{excess,front} + L_{excess,back}$$
(5.37)

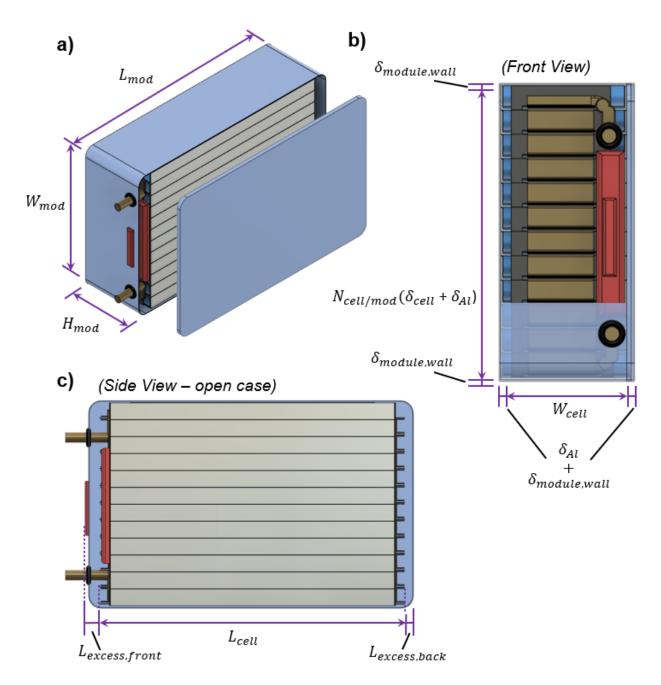


Figure 5.7. Schematic of the module showing important dimensions for understanding the module design: a) profile, b) front view without the case on 80% of the image, and c) side view with the top portion of the case open to show the items inside. Thicknesses of components are exaggerated to improve their visibility and are not drawn to scale.

The height of the module (Figure 5.7b) is equal to the width of the cell plus the thicknesses of the module walls and aluminum conductors. Recall that the aluminum thermal conductors extend up the sides of the cells, which increases their width when assembled in the module (see Figure 5.6).

$$H_{mod} = W_{cell} + 2(\delta_{wall} + \delta_{Al})$$
(5.38)

In Eq. 5.39, δ_{Al} is the thickness of the aluminum conductor (default = 0.2 mm for mildHEV and 0.4 mm for all other vehicles), and δ_{wall} is the thickness of the steel module wall (0.3 mm). The width of the module is related to the total thickness from all the cells, aluminum conductors, and module walls (Figure 5.7b). It is calculated as follows:

$$W_{mod} = N_{cell/mod}(\delta_{cell} + \delta_{Al}) + 2\delta_{wall}$$
(5.39)

5.3.2 Module Component Design

Recall that the module is comprised of the cells, aluminum thermal conductors between each cell, cell interconnect panels, cell interconnects, module tabs, a module management system, module terminals, and the module enclosure. This section provides their dimensions, which are used in the mass and ASI calculations. See Figure 5.6 and Figure 5.7 for references to the components. First, the interconnect panels are polymers, and their length is equal to the sum of all the cells and aluminum conductors, as shown in equation 5.40:

$$L_{inct,panel} = N_{cell/mod}(\delta_{cell} + \delta_{Al}) - 0.5\delta_{cell}$$
(5.40)

In this equation, the $-0.5\delta_{cell}$ is a correction factor to account for the fact the panel does not need to extend to the top of the stack. The panel widths ($W_{inct,panel}$) are equal to 90% of the cell width (W_{cell}). The panels have a default thickness ($\delta_{inct,panel}$) of 2 mm.

The cell interconnects are made of copper. Their area is provided in equation 5.21, and their length is calculated as follows:

$$L_{inct,cell} = \delta_{cell} + \delta_{Al} + 2(L_{ext,term} - \delta_{inct,panel})$$
(5.41)

The length of the module tabs connecting the terminals to the cells ($L_{tab,mod}$) is equal to $W_{ext,term}$ plus 20 mm to extend up the side of the cell stack (see Figure 5.6). The length of the module terminals ($L_{term,mod}$) has a default value of 35 mm. The areas of the tabs and terminals are calculated using the procedure described in Section 5.6.

The volumes for the module management system and gas release are accounted for in $L_{excess,front}$ and $L_{excess,back}$, while their masses are assumed to equal 46 g and 5 g per module, respectively. The length and width of the aluminum thermal conductors are given as follows:

$$L_{Al} = L_{pos} + 6mm \tag{5.42}$$

$$W_{Al} = W_{cell} + 2\delta_{Al} + 0.95 * 2 * \delta_{cell}$$
(5.43)

where the length includes an extra 6 mm past the positive electrode length to increase the cooling area, and the width assumes the lips of the thermal conductor cover 95% of the cell thickness.

5.4 Module Row Rack Design

The packs in BatPaC are constructed from rows of modules, which are initially assembled into row racks with structural and thermal support. Figure 2.6 shows all the components of the row rack: modules with polymer pads in between, module interconnects, stainless steel cooling panels, and steel structural support. Figure 5.8 provides a schematic demonstrating how those components control the size of the module row rack (MRR). The length of the row rack, Eq. 5.44, is the width of all the modules and thicknesses of the polymer pads (δ_{pad}) plus extra lengths for the restraint ($L_{add,rstrnt}$), coolant ($L_{add,clnt}$), and bus bars ($L_{add,BB}$).

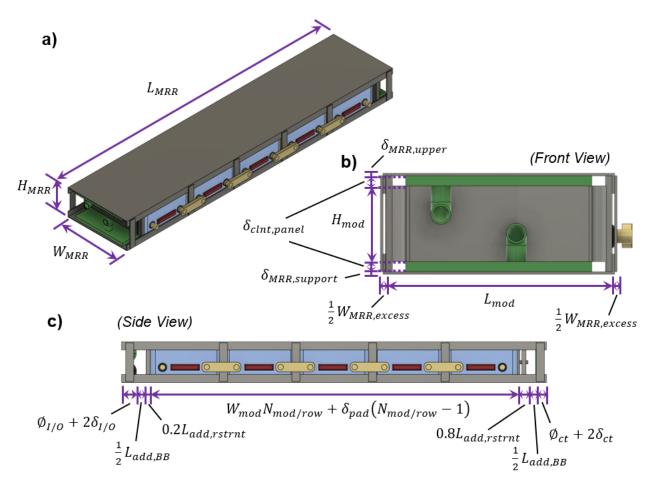


Figure 5.8. a) Profile, b) front, and c) side view of the module row rack (MRR) highlighting its dimensions. Thicknesses of some components are exaggerated to improve their visibility and are not drawn to scale.

$$L_{MRR} = W_{mod}N_{mod/row} + \delta_{pad}(N_{mod/row} - 1) + L_{add,rstrnt} + L_{add,clnt} + L_{add,BB}$$
(5.44)

 $L_{add,rstrnt}$ and $L_{add,BB}$ have default values of 15 and 10 mm, respectively. $L_{add,rstnt}$ accounts for the additional length needed to accommodate the restraint plates at the front and back of the rack (2 mm-thick default) and the compression system at the back. The majority of $L_{add,rstrnt}$ is in the back

of the rack with the compression system. $L_{add,BB}$ provides excess room at the front and back of the row rack for potential bus bar connections (see Section 5.5.1) $L_{add,clnt}$ depends on the dimensions of the inlet/outlet manifolds in the front of the rack and the coolant connecting tubes in the back. It is calculated as follows:

$$L_{add,clnt} = \phi_{I/O} + \phi_{ct} + 2(\delta_{wall,I/O} + \delta_{wall,ct})$$
(5.45)

where the subscripts I/O and ct refer to the inlet/outlet manifolds and the connecting tubes, respectively. \emptyset is the diameter (default values of 25 and 12 mm for I/O and ct, respectively), and δ_{wall} is the wall thickness (default values of 0.5 and 0.4 mm for I/O and ct, respectively).

Equation 5.46 shows that the width of the MRR is equal to the length of a module plus an excess width (default = 5 mm) for the assembly of the steel support structures. Note that the module interconnect thickness is not included in this calculation. It will be added when the total pack dimensions are calculated.

$$W_{MRR} = L_{mod} + W_{MRR,excess} \tag{5.46}$$

The height of the module row rack is calculated in Eq. 5.47. It is equal to the height of a module, the thickness of both coolant panels, the thickness of the upper steel channel (default = 1 mm), and the thickness of the supporting steel channel at the bottom (default = 1 mm). The thickness of the coolant panel is equal to the thickness of the coolant channel (default = 5 mm) plus twice the thickness of the panel walls (default = 0.3 mm). The coolant panel dimensions also influence the coolant pumping power and adequacy of cooling calculations described in Section 8.

$$H_{MRR} = H_{mod} + 2\delta_{clnt,panel} + \delta_{MRR,upper} + \delta_{MRR,support}$$
(5.47)

The upper and support channels both have side rails/lips which extend down the side of the module row rack. The default extension is 10 mm. The support system also has vertical rack members, which attach the upper and support channels. BatPaC assumes there is one vertical member at each corner and two additional members between all modules (one at the front and back of the module). BatPaC also includes four diagonal members in rows with more than one module (not shown in Figure 5.8 to improve image clarity) for increased structural stability. The default cross-sectional area for all vertical members is 15 mm².

5.5 Pack Design

5.5.1 Bus Bars

Packs may require internal bus bars depending on the number of module rows. This section describes the two bus bar types and outlines when BatPaC includes them in the pack. Figure 5.9 shows schematics of module configurations in the pack with a) one, b) two, and c) four rows. BatPaC assumes both terminals (positive and negative) exist on the same side of the pack. As a result, packs with only one row of modules (Figure 5.9a) require a bus bar to connect the module

at the back of the pack to the terminal. The same is true for all packs with an odd number of modules (not shown).

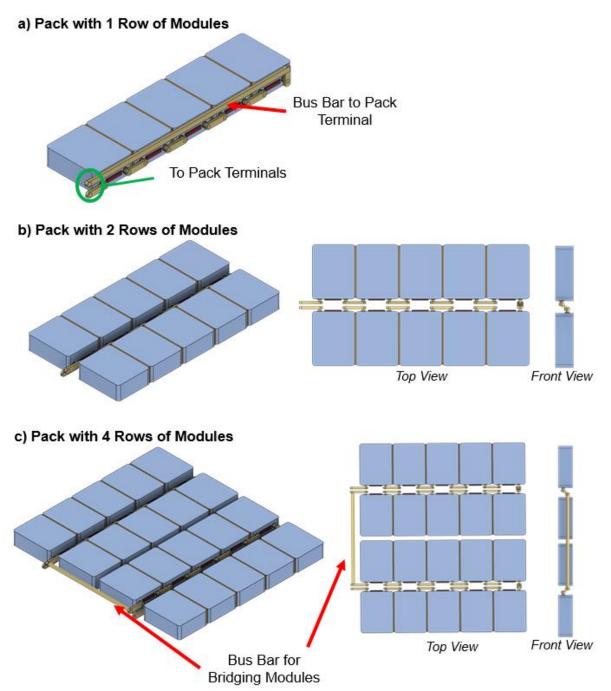


Figure 5.9. Bus bar and module configurations within a pack with a) one, b) two, and c) four rows of modules. Images demonstrate two types of bus bars in BatPaC: 1) to pack terminals and 2) between modules.

Packs with two rows of modules (Figure 5.9b) do not require this bus bar since one string of modules carries the current from the front to the back of the pack and the other string of modules carries the current from the back to the front. Packs with four rows of modules (Figure 5.9c) also do not require this bus bar. However, they require another bus bar which bridges one row of modules to another. This occurs because the most efficient way to connect two rows of modules is to have their terminals face each other. When there are four rows of modules, there are two sets of module rows facing each other. This produces a gap between the two sets, which must be bridged with a bus bar. All packs with greater than two rows require at least one bus bar for bridging module rows.

Section 3.2.3.1 mentioned that BatPaC provides a warning when the number of rows is not 1, 2, or 4. The above discussion provides the basis for this warning. For instance, three rows of modules require both types of bus bars: one bus bar to bridge rows one and two with the modules in row three and one bus bar to connect the back of row three with the front of the pack. Five rows of modules require the same bus bars as three rows plus an additional bus bar to bridge rows. Packs with six rows of modules, do not require a bus bar to connect to the pack terminal, but they do require two bus bars for bridging modules. As a result, packs with 1, 2, or 4 rows of modules are the most efficient because they require 1, 0, or 1 bus bars, respectively. All other configurations require at least two, which adds excess mass and volume to the pack.

In addition to determining the number of bus bars, BatPaC also determines their size. Their length is straightforward, as it corresponds to the distance that needs connection. The cross-sectional area is calculated to accommodate an allowable temperature rise at rated power. This is detailed in Section 5.6, which discusses sizing of all electrically connecting components at the module and pack level.

5.5.2 Module-to-Module Connections

The schematics in Figure 5.9 all show examples of series connections between modules -i.e., one module in parallel. BatPaC determines the number and size of the module interconnects assuming all modules are connected in series, regardless of the configuration input on 'Dashboard.' The configuration of the modules (*i.e.*, series and parallel connections) impact the voltage and current of the pack, but the calculation for the interconnects does not rely on this data. This is done to simplify the calculation as the exact orientation of modules, module terminals, and module interconnects may be considered an open-ended optimization problem.

For all packs, the number of interconnects between modules is equal to the number of modules plus an additional interconnect for each row of modules. This additional interconnect accounts for extra connection distances between bus bars and pack terminals. Note that, although BatPaC assumes one module in parallel, the calculation also provides a reasonable estimate for the mass, cost, and ASI of the interconnects for two modules in parallel. The length of the interconnects increases when going from one to two modules in parallel to account for connections across multiple modules. However, the area of most interconnects decreases because the current passing through is lower (see Section 5.6). These factors cancel each other out to produce similar interconnect masses for one and two modules in parallel. This logic does not hold true for greater than two modules in parallel. Accommodating greater than two modules in parallel in the present

design may require re-orientation of the modules and/or excess interconnects. Therefore, it is recommended to handle higher degrees of parallel connections within the pack at the cell-to-cell level (*i.e.*, increase the number of cells in parallel). BatPaC v5.0 includes a warning to flag errant configurations with more than two modules in parallel.

5.5.3 Pack Dimensions

The battery pack volume includes all the module row racks (MRRs), spacing for connections between modules and module row racks ($W_{icnct,gap}$), the battery pack jacket (δ_{jack}), and extra tolerances for assembly (δ_{tol}). Figure 5.10 provides schematics of the pack which highlight these dimensions. The pack length is calculated as follows:

$$L_{pack} = L_{MRR} + 2\delta_{jack,side} + \delta_{tol}$$
(5.48)

where δ_{tol} has a default value of 2 mm in all dimensions. The jacket is composed of insulation sandwiched between two metal sheets. Its thicknesses are calculated using Eq. 5.49 and 5.50.

$$\delta_{jack,side} = \delta_{jack,top} = \delta_{Al,int} + \delta_{insulation} + \delta_{Al,ext}$$
(5.49)

$$\delta_{jack,base} = \delta_{Al,int} + \delta_{insulation} + \delta_{steel,ext}$$
(5.50)

In Eq. 5.49, the subscripts Al, *int*; Al, *ext*; *steel*, *ext*; and *insulation* refer to interior aluminum (default = 1 mm), exterior aluminum (default = 1 mm for packs less than 10 kWh, 1.5 mm for packs between 10 and 20 kWh, and 2 mm for all other packs), exterior steel (default = 1 mm), and insulation (default = 10 mm), respectively. Steel is used at the exterior base of the jacket to protect against punctures. Note in Figure 5.10a that the terminals and coolant tubes extruding from the main pack are not included in this length or the volume since they will be incorporated by other portions of the vehicle.

The width and height of the pack are calculated as follows:

$$W_{pack} = N_{row}W_{MRR} + W_{icnct,gap} + 2\delta_{jack,side} + \delta_{tol}$$
(5.51)

$$H_{pack} = H_{MRR} + \delta_{jack,top} + \delta_{jack,base} + \delta_{tol}$$
(5.52)

 $W_{icnct,gap}$ refers to the spacing between modules needed for connections. Referring to Figure 5.9, there are three types of spacings within BatPaC's design: *i*) spacing when module interconnects are next to the pack wall (this would occur in Figure 5.9a), *ii*) spacing when module interconnects are next to module interconnects from another row (Figure 5.9b and c), and *iii*) when two module rows are back-to-back (Figure 5.9c). Figure 5.10c demonstrates a scenario with a back-to-back spacing in the center (*iii*) and two interconnect-to-interconnect spacings (*ii*) on either side. BatPaC assumes default spacings of 10, 15, and 5 mm for spacing types *i*), *ii*), and *iii*), respectively. The number of each spacing type is calculated based on the number of rows and bus bars in the pack.

The final volume of the main battery pack is the product of the three dimensions (equations 5.48, 5.51, and 5.52). The mass of the main pack is the sum of the mass of the individual components.

This includes the mass of the coolant within the cooling system. The mass of the pack also includes the mass of an angle iron frame around the bottom perimeter of the jacket for structural stability (not shown in Figure 5.10). The dimensions of the angle iron depend on the volume of the pack. No angle iron is used for packs <20 L. An angle iron with dimensions $30 \times 30 \times 3$ is used for packs between 20 and 40 L, where the first two dimensions refer to the extensions of the angle iron along the side and base of the jacket and the third refers to the thickness of the steel. A $40 \times 40 \times 4$ angle iron is assumed for packs >40 L. The total mass of the angle iron can be overridden. The volume of the angle iron is not included in the volume of the pack in BatPaC.

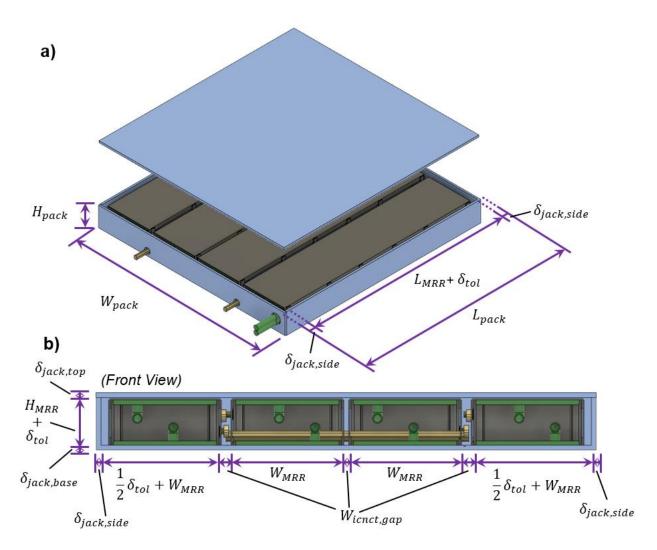


Figure 5.10. a) Profile and b) front view of generic pack containing four module row racks, which highlights important dimensions for understanding the pack volume calculations. Thicknesses of the jacket are exaggerated to improve their visibility and are not drawn to scale.

The total battery pack volume and mass also contain additional elements for the battery and thermal management systems, which are shown in Figure 5.11 (see Sections 7 and 8 for details). Their masses and volumes are included in the total results, but no assumptions are made for their

precise location within the vehicle. These excess components include disconnects, power electronics, pumps, and coolant mixing equipment.

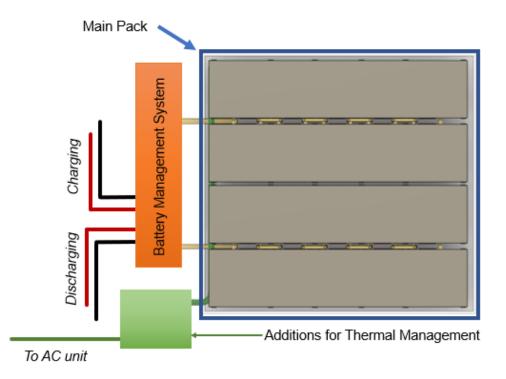


Figure 5.11. Schematic of total battery pack highlighting additional components for the battery management and thermal management systems. These components are included in the total pack mass and volume, but their location is not specified within the vehicle.

5.6 Sizing Module and Pack Connections

Recall from Sections 2, 5.2.2.2, 5.3, 5.4, and 5.5 that the modules and pack have various forms of connectors for managing the electrical connections between components. The module has tabs for connecting the cells to the module terminals, terminals to provide connections outside the module encloser, and interconnects for connecting modules to other modules. The pack has bus bars and terminals. An important factor in the module and pack design is the sizing of these connectors to accommodate an allowable rate of temperature rise in the conductor at the rated power. BatPaC sets the acceptable rate of temperature rise, dT/dt, for all connections. The default rate ranges from 0.04 to 0.4 °C/sec, depending on the connector and whether EV charging is considered. The default value is 0.4 °C/sec for the module tabs and 0.2 °C/sec for the module terminals and interconnects. For the pack bus bars and terminals, the acceptable temperature rise is 0.04 °C/sec with EV charging and 0.1 °C/sec without. The heating rate, q, is combined with these values to determine the mass, m, of the connection required for the designed battery, as follows:

$$q = mC_{p,cnct} \left(\frac{dT}{dt}\right)_{cnct}$$
(5.53)

where $C_{p,cnct}$ is the specific heat capacity of the connector material. In this equation, connector refers to the tabs, terminals, interconnects, or bus bars. The heating rate is also a function of the length, L_{cnct} , and area, A_{cnct} of the connector based on the joule heating equation, which produces the following equation:

$$q = \frac{L_{cnct}}{A_{cnct}\sigma_{Cu}} \left(I_P A_{pos} \right)^2 \tag{5.54}$$

Equations 5.53 and 5.54 can be combined to determine the area of the connector as shown in Equation 5.55.

$$A_{cnct} = I_P A_{pos} \left(\rho_{Cu} \sigma_{Cu} C_{p,cnct} \left(\frac{dT}{dt} \right)_{cnct} \right)^{-\frac{1}{2}}$$
(5.55)

In this way, the area of each connector is redesigned during each simulation to meet the specified power requirements and allowable temperature rise. Along with helping to determine the size and weight of the module, recall that A_{cnct} for each of these connectors is also used to determine the connector resistances in the modules and packs according to Equation 5.22 to 5.26.

5.7 Influence of Vehicle Type

The values of the input parameters used to calculate the power and energy of the battery pack depend on the vehicle type being simulated. The values change because the different vehicle types are operated at different states of charge and have different power requirements. BatPaC provides default values for these input parameters based on the operating conditions of the vehicle.

Table 5.1 summarizes the operating conditions assumed by the model for the four vehicle types: mild hybrid-electric vehicle (mild-HEV), high-power hybrid-electric vehicle (HEV-HP), plug-in hybrid-electric vehicle (PHEV), and electric vehicle (EV). The table also lists which input parameters are impacted by the assumed operating conditions. In addition, a default cell thickness for each vehicle type is included in

Table 5.1, which is based on industry standards observed by the BatPaC group. In general, cells become thinner for vehicles with higher power to energy ratios where thermal management is more of a concern. The remainder of this section provides a brief description of the rationale behind the values.

The first two driving conditions are the upper and lower SOC limits during operation. These values are also highlighted in Figure 5.12, which provides a schematic of the SOC window. The upper and lower SOC values are determined to provide the desired pack performance and degradation rate for each vehicle type. These values do not directly impact the calculation; however, they are used by BatPaC to calculate the useable pack energy (*i.e.*, energy between SOC limits, see Figure 5.12). This is an important metric for pack design. For packs where range is important (PHEVs and EVs), the useable energy can be combined with the Wh/mile of the vehicle to determine the total pack size required to reach a certain driving range. The total pack size is a key input parameter

in 'Dashboard.' The lower SOC limit is also used by BatPaC to guide user design when the SOC and duration at full power are overridden. BatPaC provides a check to make sure the pack does not go below the SOC limit during the pulse and provides an error if this occurs. BatPaC also provides a less severe warning if the SOC goes below a reserve safety limit (see Figure 5.12). The reserve safety limit is included in most vehicles to guarantee consistent performance of the vehicle. Note that the default lower SOC limits correspond to graphite negative electrodes, where the risk of lithium metal plating restricts the useable battery energy. For other materials, like lithium titanate spinel (Li₄Ti₅O₁₂, LTO), it may be prudent to lower this number for PHEVs and EVs.

Vehicle Type	Mild-HEV	HEV-HP	PHEV	EV	Impacted Input
Upper SOC limit	95	90	90	95	-
Lower SOC limit	70	30	20	10	-
SOC at average operation, %	80	80	50	50	U_E , ASI_E
SOC for at rated power, %	80	50	80	20	U_P, ASI_P
Duration at rated power, sec	2	10	10	10	ASI_P
Cell Thickness, mm	6	12	16	20	δ_{cell}

Table 5.1. Default operating conditions and input parameters for pre-defined vehicle types

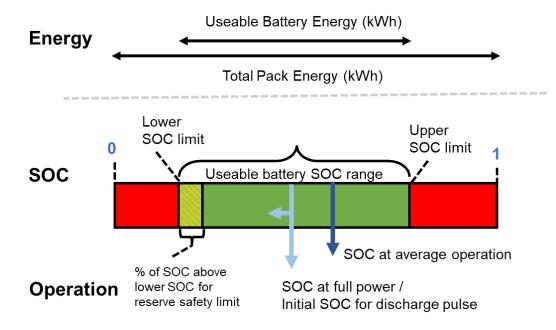


Figure 5.12 Schematic of the usable energy for a battery and the locations of the state of charge (SOC) for average operation and the SOC at full power. The locations of the SOCs do not correspond to a specific vehicle type.

The second driving condition that impacts the model inputs is the state of charge at average operation, which is also the SOC for rated energy. This condition impacts the default, user-defined inputs for the open circuit voltage (U_E) and area-specific resistance (ASI_E) used to determine the

battery energy in Eq. 5.1. For PHEVs and EVs, these inputs are taken at 50% SOC. For mild-HEVs and HEV-HPs, the battery operates at a higher state of charge, where the cell voltage and ASI are favorable for operation at high power. Therefore, the values of U_E and ASI_E are taken at 80% SOC for these vehicles.

The final two driving conditions are the SOC and duration for rated power. The SOC for rated power impacts the default, user-defined input for the open circuit voltage (U_P) and the area-specific resistance (ASI_P) used to determine the battery power in equations 5.3 and 5.4. The duration for rated power impacts the value of ASI_P . BatPaC assumes that the mild-HEV is designed to reach the power rating at 80% SOC after a 2 second pulse, reflecting the short assist from the electric powertrain. For the HEV-HP, the battery is assumed to provide the rated power for a full 10 seconds. Note that the SOC for the rated power to account for occasional hill climbing, where the HEV-HP battery may be discharged to a low SOC. The PHEV power is rated at 80% SOC because, at this state of charge, the battery will likely provide all the power for the vehicle. The power performance of the battery will be assisted by the internal combustion engine. EV batteries must provide the rated power near the end of discharge. Therefore, U_P and ASI_P are taken at 20% SOC after a full 10 second pulse for this vehicle.

6. CHARGING OF ELECTRIC VEHICLE BATTERIES

In the previous chapter, estimating the thickness of the electrodes was based on power requirements for discharge. This assumed that charging was not a limiting factor, which is generally true for vehicles that are charged over several hours (such is the case with home chargers). However, the desire for full-electric vehicles to be charged quickly creates another means for limiting the thickness of the electrode.

This section provides the methodology used by BatPaC to estimate the maximum allowable thickness of an electrode for a given charge time. The methodology relies on results from an electrochemical-thermal model of a lithium-ion pouch cell published previously by the BatPaC group [15]. An empirical correlation is developed which calculates the maximum electrode thickness that can achieve the desired charged time without exceeding operational limits in the cell (*i.e.*, maximum current, maximum allowable temperature, and lithium-plating potential). The methodology and correlation have been tested and verified for the range of default electrode couples and default conditions provided in BatPaC.

6.1 Description of Charging Model

The correlation for electrode thickness was developed from data generated by a coupled electrochemical-thermal model. The model is composed of a 3-D thermal model of a lithium-ion pouch cell with aluminum thermal conductors, which is coupled to two, 1-D electrochemical models. The 3-D model predicts the temperature distribution in the cell assuming the cell is cooled from coolant in contact with the aluminum thermal conductors. The 3-D model is based off BatPaC's default cell and thermal conductor designs (see Figure 5.6). The first, 1-D, electrochemical model is solved at the average cell temperature and is used to determine the heat generation rate within the 3-D thermal model. The results of this 1-D model also determine the overall electrochemistry of the cell. The second, 1-D, electrochemical model is solved at the anode overpotential at the negative electrode/separator interface. Details on the equations and solving methodology can be found in [15].

The data used for the correlation was developed using a constant risk charging protocol, which determines the practical limits of fast charging based on thermal and electrochemical control. The protocol controls the charging current and the coolant flow to minimize the charging time, while preventing lithium plating and avoiding excessive temperatures. The protocol charges the cell at the maximum allowable C-rate unless the potential at the negative electrode/separator interface approaches the onset of lithium plating or the cell approaches the maximum allowable temperature. In these cases, the current is reduced and/or thermal intervention is employed. The protocol employs an active thermal management strategy, whereby coolant flow is turned on or off depending on the maximum temperature in the cell.

Figure 6.1 shows an example of the data obtained from this model for a cell containing $LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ (NMC532) as the positive electrode and graphite (G) as the negative electrode, with a negative-to-positive capacity ratio of 1.1. The figure shows the maximum

electrode thickness that can achieve the desired charge time while maintaining the cell with the operational limits. The maximum allowable C-rate was set at 12 C for all cases, and the minimum allowable overpotential to prevent lithium plating was set at 10 mV above Li/Li⁺. The coolant was set at 15 °C, and a cell voltage limit of 4.2 V was employed. The graph shows results for different maximum allowable temperatures in the cell. The time corresponds to charging from 15% to 95% state of charge (SOC). The graph shows how higher allowable temperatures facilitate faster charging times for electrodes with the same thickness. The data from this figure and similar data for other electrode couples was used to generate the correlation used by BatPaC. All simulations assumed the same maximum allowable C-rate, Li plating limit, and coolant temperature. The cell voltage limit was equal to the voltage at 100% state of charge for each electrode couple. Constant voltage operation is assumed at the voltage limit.

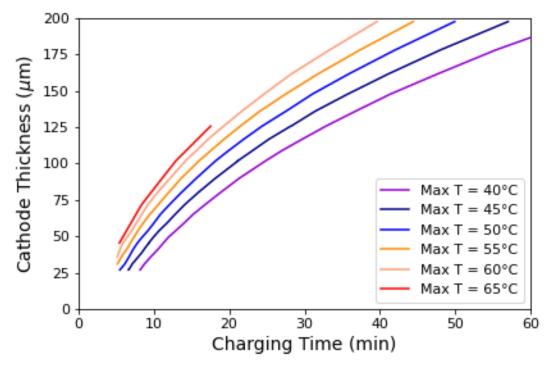


Figure 6.1. Example of fast charge results from previous work for NMC532-G pouch cells [15]. The figure provides the maximum cathode (*i.e.*, positive electrode) thickness that can achieve the desired charge time using the constant risk protocol without exceeding the operation limits of lithium plating potential (10 mV vs. Li/Li⁺), maximum C-rate (12 C), and maximum allowable temperature (variable). All results were obtained from a coupled thermal-electrochemical model.

6.2 Parameter Space of Simulations

The variable space for this problem is extensive. As such, the model was not exercised over all possible scenarios. The correlation used in BatPaC provides the most accurate results by maintaining the following sets of parameters within the given values and/or ranges:

<u>Vehicle Type:</u> Valid only for all-electric (EV)

<u>Cell Thickness:</u> Keep at the default value of 2 cm

Positive Electrode Length-to-Width Ratio: Keep at the default value of 3

<u>Maximum Allowable Temperature (T_{max})</u>: Fittings were performed between 40 °C and 70 °C, thus the validity is uncertain beyond this range (mainly below the lower limit)

Charging Time: Keep above 5 minutes

<u>Electrode Couples:</u> The model has been tested with the default couples. It is possible that breakdowns will occur with novel chemistries.

<u>State of Charge Range:</u> Keep at the default values of 95% to 10% for the upper and lower SOC limits, respectively (these are the default value for an EV)

6.3 Correlation for Estimating the Positive Electrode Thickness

A dataset was generated by exercising the model for the default electrode couples and the range of maximum allowable temperatures listed above. This dataset was diverse and included power and energy couples; lithium titanate and graphite negative electrodes; and layered oxide and spinel positive electrodes (see Sections 3.2.2.1, 4.1.2, and 9.2.1). An analysis of the dataset found that the following expression linearized the charge time with respect to the positive electrode (*i.e.*, cathode) thickness:

$$\delta_{pos} = \frac{\alpha ln^2(t_{chg}) + \beta}{Q\rho_{act/etrode}}$$
(6.1)

where Q is the specific capacity of the active material (mAh/g), and $\rho_{act/etrode}$ is the density of the active material within the electrode ($g_{active}/cm^3_{electrode}$). The term in the numerator is the electrode loading (mAh/cm²), where the slope (α) and intercept (β) are functions of the design parameters. t_{chg} is the desired charge time (minutes). The linearization of the data with this expression is demonstrated in Figure 6.2 for a cell with NMC532-G electrodes. Figure 6.2 highlights that Eq. 6.1 holds for a range of maximum allowable temperatures (T_{max}); however, the value of T_{max} changes the value of α and β , as observed by the differences in the slopes and intercepts of the lines in the figure.

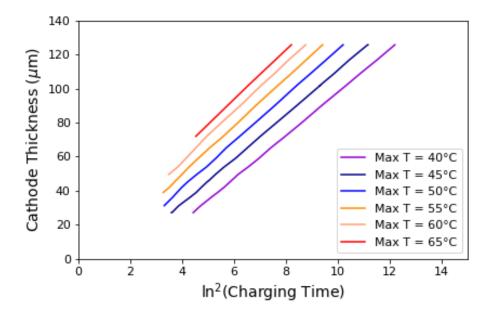


Figure 6.2. The linearization of cathode (*i.e.*, positive electrode) thickness with respect to charging time per Equation 6.1 for a NMC532-Graphite (Energy) couple at a fixed cell capacity.

A series of Pearson and Kendall correlations were used to determine the dominate inputs that effect the slope (α) and intercept (β) parameters. These are given as follows:

$$\alpha, \beta = f(L, T_{max}, ASI_{10s, 50\%}) \tag{6.2}$$

where *L* is the cell length, and $ASI_{10s,50\%}$ is the reference area specific resistance of the cell at ten seconds and 50% state of charge (SOC). The functional forms of α and β were determined using data from the NMC532-G (energy) couple. Figure 6.3 provides an illustration of how the values of α and β depend on the cell geometry and maximum allowable temperature. Note that, although the figure plots cell width, this is the same as cell length since the length-to-width ratio is kept constant at 3. From this analysis, the functional form of the expression was found to be:

$$\alpha = \alpha_1 L + \alpha_2 L^2 + \alpha_3 T_{max} \tag{6.3}$$

$$\beta = (\beta_1 L + \beta_2 T_{max} L + \beta_3 T_{max} + \beta_4 T_{max}^2) \frac{ASI_{105,50\%}}{12.5}$$
(6.4)

Equations 6.3 and 6.4 highlight that the slope (α) is not a function of chemistry dependent parameters and is mainly dictated by operation. However, the intercept (β) does have a dependency on the reference 10s ASI value at 50% SOC.

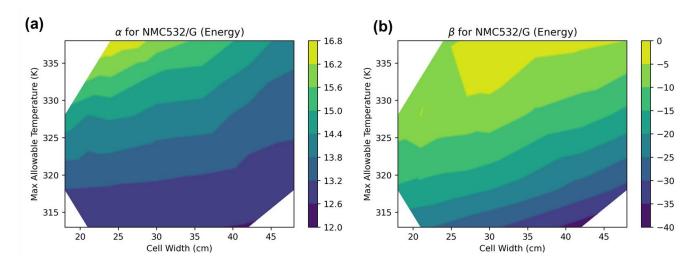


Figure 6.3. Parameters space for a) α and b) β as a function of cell geometry and maximum allowable temperature.

Once the functional form was determined, the constants of the expressions were optimized via the default parameters given in BatPaC. The constants, which are given in Table 6.1, were fit across all the BatPaC default chemistries. The ASI value in Eq. 6.4 was included during the optimization process to provide better agreement across all electrode couples.

Parameter	Value
α1	0.0151
α2	0.000255
α ₃	-0.0985
β_1	-2.36
β_2	0.00587
β_3	1.24
β_4	0.0000257

Table 6.1. Constants used in fast charging for equations 6.3 and 6.4

Figure 6.4 highlights the errors expected with this correlation. The figure compares the positive electrode thickness calculated with the correlation to the positive electrode thickness determined from the full charging simulation. The figure contains results for all default electrode couples in BatPaC v5.0, which are distinguished by their color in the figure. The line corresponds to a perfect correlation. Good agreement is observed across all simulations. Figure 6.4 suggests BatPaC may slightly overestimate the electrode thickness for situations that produce thinner electrodes (<30 μ m). Thinner electrodes typically correspond to shorter charge times. Further analysis of the results (data not shown) indicated that charge times less than eight minutes have an error of ±3 μ m, with the energy couples tending to have a slight over-prediction in the thickness.

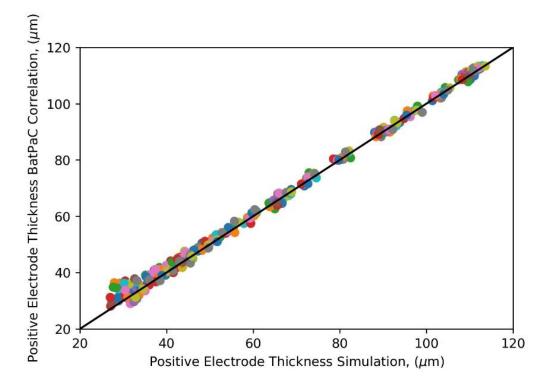


Figure 6.4. Correlation of predicted positive electrode thickness from Eq. 6.1 versus thickness obtained from fast charge simulations. Colors represent the different, default electrode couples in BatPaC v5.0.

6.4 Implementation in BatPaC

The above calculation is performed in BatPaC if electric vehicle fast charging is selected on 'Dashboard.' If selected, the calculation determines the maximum allowable thickness to achieve charging. The default maximum allowable temperature is 55 °C, but it can be overridden. All other constants (*i.e.*, coolant temperature, maximum C-rate, and plating potential limit) are fixed. BatPaC compares the electrode thickness from this correlation to the electrode thicknesses in Section 5.2 (*i.e.*, calculated thickness and maximum allowable thickness). If the electrode thickness from charging is thinner than the other thicknesses, the calculation is modified in the manner described in Section 5.2.4, whereby δ_{max} is replaced by the thickness calculated from the charging model.

7. BATTERY MANAGEMENT SYSTEM

Electrified vehicles require auxiliary systems for the battery to meaningfully interact with the vehicle. The main auxiliary system is the Battery Management System (BMS), which controls the electrical operation of the battery. There is also a thermal management system, which is discussed in the next section. This section describes the various components of the battery management system and explains how BatPaC estimates the cost, mass, and volume of the BMS.

7.1 Battery Management System Overview

The BMS in BatPaC integrates the modules and battery into the overall electric drive system. The BMS includes measurement and control features such as the following:

- Measurement of the battery pack current and voltage
- Balancing the module voltages (cell balancing is done within the module)
- Estimating the battery pack state-of-charge (SOC) and state-of-health (SOH)
- Estimating the module SOC and SOH
- Monitoring and signaling of the battery thermal management
- Toggling between charging and discharging modes using battery disconnects

The complexity, size, and cost of the BMS depends on many aspects of the pack and vehicle. The costs of the components depend on the maximum current and voltage observed by the cell to prevent a catastrophic thermal runaway. The assembly and structure of the BMS varies amongst manufacturers, each balancing the pros and cons of specific design decisions to suit their preferences. BatPaC aims to model a range of generic battery packs for various uses and sizes. Therefore, the BMS in BatPaC reflects a generic design. The number and size of the components in the BMS was estimated by looking at a series of teardown reports and estimating the number of components needed based on the type of battery, the number of cells, and the number of modules. From this, the cost, mass, and volume of an 'average' BMS is estimated for each battery design.

BatPaC organizes the full BMS into the following four segments, which are also shown schematically in Figure 7.1:

- 1. *Battery Management Unit (BMU)*: components used to provide cell-to-cell balancing and ensure that each cell is charged and discharged safely
- 2. *Battery Disconnect Unit (BDU) and Power Electronics*: components used for the safe interfacing with external power consumers and chargers
- 3. *Interfaces between electronic system*: the low and high voltage wiring and connectors between the various parts of the BMS (listed as "wiring to BMU" in figure)
- 4. *Module electronics*: the various sensors and fuses in the modules

The total cost, mass, and volume of the BMS is the sum of these four segments. The remainder of this section provides the detailed calculation for each segment.

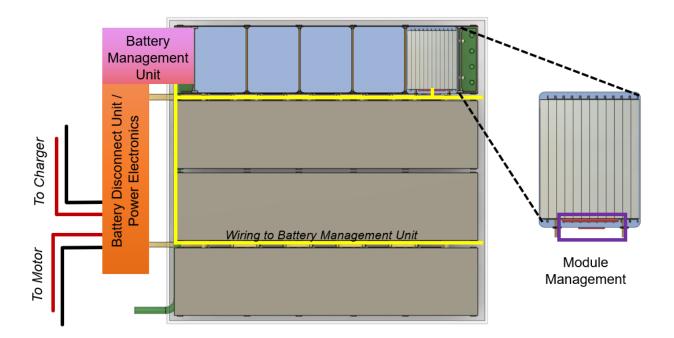


Figure 7.1. Top view of the battery pack with the jacket removed showing the general locations of the components in the battery management system.

7.2 Battery Management Unit

The battery managment unit (BMU) controls how each cell is charged and discharged to ensure the designed life of the battery. This includes balancing how much current goes to each cell to prevent a worse performing cell from overcharging or overdischarging, possibly causing a catostrophic result. Cell-to-cell balancing is done across cells in series. The number of equivalent cells in series in the pack is:

$$N_{series} = \frac{N_{cells/mod}N_{mod/pack}}{N_{cells,||}N_{mods,||}}$$
(7.1)

where the subscripts *cells/mod, mod/pack, cells,*//, and *mods,*// refer to the number of cells per module, the number of modules per pack, the number of cells in parallel, and the number of modules in parallel, respectively. BatPaC splits the control of the battery and the cell-to-cell balancing among many circuit boards, where each board controls several cells using an application specific integrated circuit (ASIC). The number of cells controlled by each ASIC is denotated as $N_{cells/ASIC}$ (default = 10). The number of ASICs needed is defined by the following equation:

$$N_{ASIC} = N_{series} / N_{cells/ASIC}$$
(7.2)

The number of BMU components, *i*, in the pack $(N_{i/pack})$ depend on N_{ASIC} as follows:

$$N_{i/pack} = M_{vehicle} \left[N_{fixed} + \left(N_{i/ASIC} N_{ASIC} - N_{offset} \right) \right]$$
(7.3)

where N_{fixed} is the fixed number of components needed for a given vehicle, and $N_{i/ASIC}$ is the number of each component, *i*, per ASIC. N_{offset} is an offset number used to adjust N_{ASIC} . This term is generally needed when boards are in a master/slave configuration with one or two of the boards controlling the others. The term in the parentheses is rounded up to the nearest whole number. Finally, $M_{vehicle}$ is a multiplier for a given vehicle type. $M_{vehicle}$ equals one for all components in the BMU. Its value will change for some BDU components (see next sub-section). Table 7.1 provides the values of each term for each component in the BMU.

Component	Cost, \$/unit (C _o)	Volume Basis for Cost (N_{θ})	p- Value	Fixed Number (N _{fixed})	# per ASIC (N _{i/ASIC})	Offset per ASCI (Noffset)	Vehicle Multiplier (M _{vehicle})
PCB	5.00	1,000	0.9	1	0	0	1
Connector-20 pin	1.58	5,000	0.9	1	0.5	0	1
Connector-16 pin	1.30	5,000	0.9	1	0	0	1
Conformal coating	0.50	1,000	0.9	2	0.166	0	1
Main micro	20.30	500	0.9	1	0	0	1
Piezoelectric crystal	0.11	10,000	0.9	1	1	0	1
Flash memory	0.37	25,000	0.9	1	0	0	1
V sense micro	3.95	2,000	0.9	0	1	0	1
V sense ASIC	2.95	1,000	0.9	0	1	0	1
CAN transceiver	0.52	12,500	0.9	4	0	0	1
Common mode choke	0.64	12,000	0.9	3	0	0	1
5V ref-main	0.78	5,000	0.9	0	1	0	1
5V reference - V _{sense}	1.89	500	0.9	1	0	0	1
Dual isolators	1.09	1,000	0.9	0	1	-2	1
Single optocouplers	1.58	3,000	0.9	0	0.5	0	1
Buffers	0.08	125,000	0.9	0	0.3333	0	1
Schottky diode	0.70	5,000	0.9	1	0	0	1
Diodes	0.04	75,000	0.9	26	26	0	1
Resistors-0603	0.01	50,000	0.9	51	45	0	1
Resistors-0805	0.01	50,000	0.9	51	45	0	1
Resistors-1206	0.32	1,000	0.9	8	20	0	1
Electrolytic capacitor	0.04	100,000	0.9	2	1	0	1
Capacitor-0603	0.002	15,000	0.9	26	31	0	1
Capacitor-0805	0.01	4,000	0.9	25	30	0	1
Capacitor-1206	0.04	4,000	0.9	12	2	0	1
Transistors	0.08	30,000	0.9	14	14	0	1
Resistor jumper	0.004	125,000	0.9	2	0	0	1
Contactor control	10.00	1	1	1	0	0	1
BMU enclosure	3.00	1	1	1	0	0	1

Table 7.1. Reference costs and amounts for components in the battery management unit (BMU).

Table 7.1 also provides reference values used to calculate the cost of each component. The table includes a reference cost (C_0) for a given reference manufacturing volume (N_0) and a scaling factor (p), which is used to adjust the cost for the volume of components used per year. The individual cost of each component is calculated using the following equation:

$$C_i = C_{i,0} \left(\frac{N_{i,0}}{N_{i/pack} N_{pack/year}} \right)^{1-p}$$
(7.4)

In Eq. 7.4, *N_{pack/year}* is the number of packs manufactured per year, which is set on 'Dashboard.' For a given BMU component in Table 7.1, its total cost within the pack is calculated by multiplying Eq. 7.3 and Eq. 7.4. The total BMU cost per pack is the sum of all component costs.

BatPaC does not set the mass and volume of each component in the BMU. Instead, the mass and volume are calculated based on a set value for each printed circuit board (PCB) plus an additional amount for each ASIC. This methodology ensures the mass and volume of the BMU increase with increasing complexity of the system. The PCB mass and volume have default values of 40 g and 0.16 L, respectively. The default additions per ASIC are 20 g and 0.08 L. An additional 10% of the total BMU mass/volume is included in the total BMS mass/volume to account for the enclosure around the BMU. Note that the calculation also increases the mass and volume of the PCB based on the number of main contactors in the system (see next sub-section). This is used as a proxy to increase the size of the BMU for larger, higher-voltage packs. For packs with one module or <50 V, the PCB mass/volume and the contactor control cost in Table 7.1 are not included in the BMU. These values are excluded to reflect the decrease in complexity of the BMU for smaller packs.

7.3 Battery Disconnect Unit and Power Electronics

The battery disconnect unit (BDU) and power electronics are essential parts of any electrified vehicle. These units are responsible for transitioning between discharge and charge modes and cutting off power to/from the battery for repair or in emergencies. The specific components will change between different vehicle types.

The number and cost of the components are calculated in a similar manner to the BMU components (*i.e.*, equations 7.3 and 7.4). The major difference is that none of the BDU or power electronics components depend on the number of ASIC or include an offset – *i.e.*, $N_{i/ASIC}$ and N_{offset} equal zero in Eq. 7.3. Table 7.2 lists the BDU and power electronics components and provides the values for N_{fixed} and $M_{vehicle}$. $M_{vehicle}$ equals one for all components except the auxiliary contactor and the charger fuse. Their values are one for plug-in hybrid and full electric vehicles (PHEVs and EVs), which undergo charging from an external source, and zero for mild and high-power hybrid vehicles (mildHEV and HEV-HP).

Three of the BDU and power electronics components are also adjusted based on the size of the pack. The main contactors (Contactor – main), precharge contactors, and current sensors are excluded in the BMS for small packs – *i.e.*, packs with one module or <50 V. These components are either not needed or replaced with a significantly cheaper/smaller component that can be

neglected in the calculation. For packs between 50 and 100 V, one main contactor is included. Two main contactors are included in packs with >100 V.

Component	Base Cost, \$/unit (C ₀)	Volume Basis for Cost (N _o)	p- Value	N _{fixed}	Vehicle Multiplier (M _{vehicle})	Volume (L/unit)	Mass (g/Unit)
Contactor - Main	Table 7.3	200,000	0.95	2	1	0.3193	750
Contactor - Aux	10	100	1	2	0 or 1	0	180
Precharge contactor	10	10,000	0.9	1	1	0.125	90
Precharge resistor	4.44	1,000	0.9	1	1	0.08	185
Service disconnect	1	10,000	0.9	1	1	0.576	150
Service disconnect fuse	10	10,000	0.9	1	1	0.0884	80
Charger fuse	3	10,000	0.9	1	0 or 1	0.004	24
Current sensor	60.33	50	0.9	1	1	0.0365	55

Table 7.2. Reference costs and amounts for components in the battery disconnect unit and power electronics. Not shown are modifications to the main contactors, precharge contactors, and current sensors for smaller packs (see text for details).

The cost of the main contactor is a function of the current and voltage. If the voltage is less than 50V, the main contactor would be replaced by a significantly cheaper switch and its cost is neglected (see previous paragraph). At >50 V, the cost is assumed to scale linearly with peak pack current based on the values in Table 7.3.

Reference for Contactor-Main	Base Cost, $\$/unit (C_{\theta})$	Volume Basis for Cost (N_{θ})	p-Value
10A Contactor	10	200,000	0.95
600A Contactor	52.86	200,000	0.95

Table 7.3. Reference costs for determining base cost of the main contactor.

The mass and volume of the BDU and power electronics components are calculated by multiplying the number of each component by their per-unit value (*i.e.*, L/unit or g/unit) in Table 7.2.

7.4 Interfacing Electronics

The interfacing electronics include the low and high voltage wiring between the BMU, BDU, and module management system. Its cost will depend on the pack current and is calculated by linearly extrapolating between the two default scenarios in Table 7.4. These scenarios are estimations for a generic pack based on vehicle battery teardown reports. The entire cost is neglected for small packs (one module or < 50 V). BatPaC does not provide a mass for the interfacing electronics because its mass is small and assumed to be accounted for by the other BMS components. For instance, its mass is lumped into the default mass inputs for the BMU (Section 7.2) and module management system (Section 5.3.2). No volume is added to the BMS since the interface electronics are assumed to reside within the void spaces of the pack.

Table 7.4. Reference costs for the interface electronics.

Reference for Interface Electronics	Cost, \$/unit	Pack Current, A
Scenario 1	20	50
Scenario 2	60	500

7.5 Module Electronics

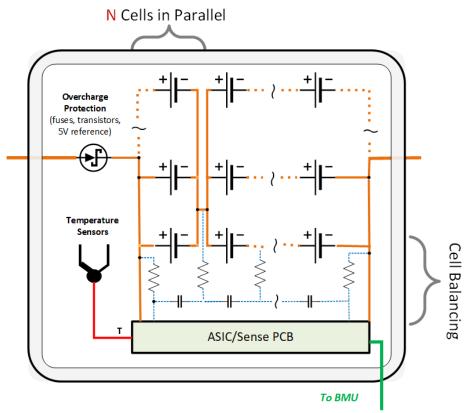


Figure 7.2 provides a schematic of the module management unit for a single module. The module management unit includes over-charge protection (*i.e.*, sense line fuses), temperature sensors, and a sense printed circuit board (PCB) to prevent abusive operation of the cells. The number of sense line fuses is calculated using the following equation:

$$N_{sense} = \left(\frac{N_{cells/mod}}{N_{cells,||}} + 1\right) N_{mod/pack}$$
(7.5)

which is rounded to the nearest whole number and corresponds to one fuse for every cell in series in a module plus an additional fuse per module. Two temperature sensors are included per module plus two additional at the pack level. One sense PCB is included for each module. The costs of the module electronics components are determined using Eq. 7.4 with the inputs from Table 7.5. The masses and volumes of these components are not directly calculated. They are included in the mass/volume of the module management system described in Section 5.3.2. The values for the module management system account for all these components plus equipment for interfacing the cells with the front and back plates, along with connectors from the inside to the outside of the module.

Module Electronic Component	Base Cost, $\$/unit (C_0)$	Volume Basisfor Cost (N_{θ})	p-Value
Sense line fuses	0.33	10,500	0.9
Temperature sensors	0.23	1,000	0.95
Sense PCB	0.50	1	1

 Table 7.5. Reference costs for the module electronics.

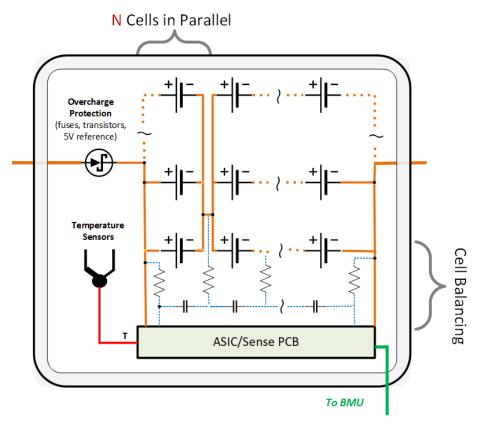


Figure 7.2 Schematic of module management unit for a single module

7.6 Total BMS Mass, Volume, and Cost

The total BMS mass and volume are calculated by adding the BDU, power electronics, and BMU values (including BMU enclosure) and multiplying by 1.3 to account for further enclosures. The masses for the interface electronics are assumed to be incorporated in the other BMS components. There is no volume addition for the interface electronics since they are assumed to reside within the void space of the pack. The mass/volume of the module electronics are also excluded from these totals because they are already included in the module design (see previous section and Section 5.3.2). The BMS is delocalized in BatPaC, and its mass and volume are added at the pack level. No distinction is made on the location of the components since a variety of options have

been observed in industry -e.g., different amounts of BMU components and module electronics inside and outside of the module and pack have been observed. The cost of the BMS is the sum of the costs of all the individual components.

The mass, volume, and cost of the BMS are included in all pack-specific metrics listed in BatPaC (*e.g.*, Wh/kg, Wh/L, L, kg, \$, \$/kWh, etc.). The module-specific metrics only include the mass, volume, and cost of the module management system. They do not include extra costs for the module electronics. In addition, the cell-specific metrics do not include any BMS mass, volume, or costs. Finally, BatPaC also provides battery system metrics, which include all packs (BatPaC allows for multiple packs) and thermal equipment. The BMS mass, volume, and cost described herein are included for each pack within the battery system.

8. THERMAL MANAGEMENT SYSTEM

The temperature can drastically impact the performance and degradation of lithium-ion batteries. Therefore, the temperature of the pack must be controlled. This involves removing excess heat generated during operation, maintaining cool temperatures during warm ambient conditions, and providing heat during start-up at cold ambient conditions. The thermal management system for the battery in BatPaC is designed in the 'Thermal' worksheet. This worksheet performs calculations which approximate the size and mass of the cooling and heating systems. It also conducts a check to determine if the cell geometry calculated in 'Battery Design' (see Section 5) can be adequately cooled during sustained operation. This worksheet also provides supporting results that may be of interest to the user, but do not directly affect the overall pack specifications. These supporting results include the temperature rise during the rated power pulse under adiabatic conditions, the adiabatic temperature rise during sustained operation, the power required to pump and compress the coolant, and the pressure drop in the coolant system.

8.1 Overview of Thermal Management System

The thermal management system in BatPaC contains four main parts: i) a coolant flow system within the pack, ii) coolant management equipment external to the pack, iii) battery pack heaters external to the pack, and iv) upgrades to the air conditioning unit. An overview of the thermal management system is shown in Figure 8.1. The coolant flow system in the pack was described in Sections 2.4, 2.5, 5.4, and 5.5 and will be revisited in Section 8.2. It contains the coolant along with the tubes and panels which facilitate the coolant flow within the pack. The coolant management equipment external to the pack pumps the coolant through the pack and manages the heat transfer between the coolant and a refrigerant connected to the AC unit. The heaters provide heat to the pack during cold starts. The AC upgrades are needed to handle the additional cooling requirements of the vehicle.

BatPaC v5.0 assumes all packs are cooled using a 50/50 solution (by weight) of ethylene-glycol and water (EG/W). Previous versions of BatPaC had an option to cool the pack with cabin air. This was facilitated with a modification to the module and pack design to force air directly across the cells. This feature has been removed in BatPaC v5.0 to simplify and speed-up the tool, as well as

to align with the trajectory of the EV industry. To elaborate, battery packs are continuously incorporating higher energy density materials that allow for increased range. Higher energy density materials increase safety and degradation risks which can be managed with improved thermal management. Coolant systems have superior cooling capabilities over air cooled. As a result, the BatPaC group has observed an increase in their use within EVs, especially in all electric and plug-in hybrid EVs. Therefore, only the liquid cooled option is provided in BatPaC v5.0.

BatPaC has chosen the EG/W system as a representative thermal management system for a battery pack. Some vehicles in industry may cool the pack with air, other dielectric liquids (*e.g.* transformer fluids), and/or phase change materials. The remainder of Section 8 should provide the user with sufficient detail to understand the baseline calculations. This knowledge can be employed by the user to modify the thermal management system for custom cooling strategies.

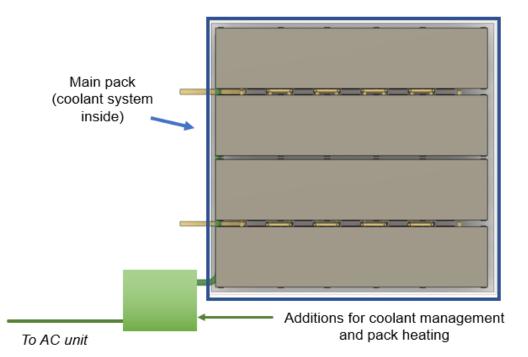


Figure 8.1. Schematic overview of thermal management components in battery pack: *i*) coolant system within the pack, *ii*) coolant management equipment (pumps, heat exchanger, and valving to the refrigerant line), *iii*) pack heater, and *iv*) additions to the AC unit. The schematic includes generic labels and places holders for *ii*), *iii*) and *iv*) since their exact locations in the vehicle are not specified by BatPaC.

8.2 Coolant Flow System

BatPaC v5.0 assumes all packs employ liquid cooling systems like the one shown in Figure 8.2. The coolant flows through stainless steel cooling panels which are located on the top and bottom of the module row racks. A separate set of cooling panels are used for each module row rack. An inlet coolant manifold at the front of the pack brings the coolant to the top cooling panels, which

are hydraulically connected in parallel. The coolant first flows over the top of the modules and then along the bottom, with the transition made by connecting tubes at the back of the pack. The bottom cooling panels are connected in parallel to a pack outlet manifold which returns the coolant to the heat exchanger external to the pack (not shown). The thickness of the cooling panel walls, thickness of the open coolant channel within the cooling panels, and diameters of the manifolds and connecting tubes are all default input parameters that can be modified in the 'Battery Design' worksheet (see Section 5.4 for their values). The length of each cooling panel is equal to the length of the module row rack, and the width is equal to the length of the aluminum thermal conductors within the modules (refer to Figure 5.7c and Figure 5.8b for detailed images of the thermal conductors and panel widths, respectively.).

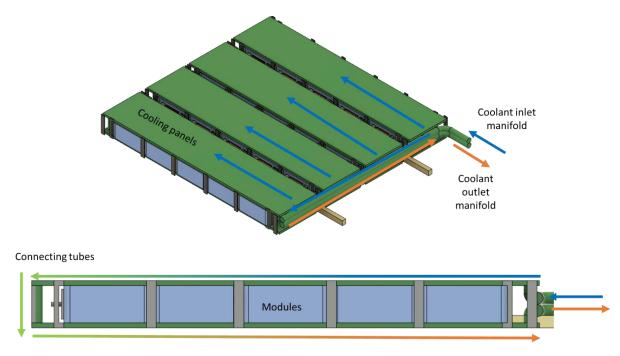


Figure 8.2 Coolant flow in BatPaC battery pack, with coolant flowing above and below the module row racks.

8.3 Additions for Coolant Management

BatPaC assumes additional components outside the pack are required to manage the coolant. These components include pumps to circulate the coolant, a heat exchanger (chiller) to transfer the thermal energy from the coolant to the refrigerant loop, and valving on the refrigerant line from the AC unit [19]. The mass, volume, and cost of these additional components are determined based on the cooling requirements within the pack. This sub-section describes the calculations used to determine the cooling requirements, the sizing and cost of the additional components, the pressure drop, and pumping power.

8.3.1 Cooling Requirements

The total cooling requirement for the pack is the sum of two values: the heat generation during sustained operation (q_s) and the rate of heat transfer from hot ambient conditions (q_{amb}).

8.3.1.1 Heat Generation During Operation

In BatPaC, the heat generation during sustained operation (q_s) is calculated as follows:

$$q_s = I_s^2 R_s \tag{8.1}$$

where I_S and R_S are the current (A) and resistance (Ω), respectively, during a sustained discharge. The resistance is calculated from the area specific impedance described in Section 5.2.2 as follows:

$$R_s = \frac{ASI_E N_{cell}}{A_{pos} N_{cell,||}^2 N_{mod,||}^2}$$
(8.2)

where ASI_E is the area specific impedance for energy, A_{pos} is the total positive electrode area in a cell, N_{cell} is the number of cells in the pack, $N_{cell,||}$ is the number of cells in parallel in a module, and $N_{mod,||}$ is the number of modules in parallel in the pack. The current is calculated from the average power during sustained operation as follows:

$$I_s = \frac{P_s}{V} \tag{8.3}$$

where P_s is the average sustained power, and V is the voltage. V is calculated with respect to the open circuit voltage of the pack (U_E) from the following equation:

$$V = \frac{U_E + \sqrt{U_E^2 - 4P_s R_s}}{2}$$
(8.4)

The power during steady-state operation (P_s) is calculated by comparing the power at a sustained speed with the power at a C/3 discharge and taking the larger value. The power at a sustained speed (P_{ss}) is calculated using the same method employed by the Autonomie model available from Argonne's Advanced Powertrain Research Facility [12]. The total power at a sustained speed is calculated as follows:

$$P_{ss} = \frac{1}{f_e} (P_a + P_f + P_d)$$
(8.5)

where P_a , P_f , and P_d are the accessory power, rolling friction power, and aerodynamic drag power, respectively. All values have units of Watts (W). f_e is a factor accounting for the efficiency from the battery to the wheels and accessories. It has a default value of 0.833 in BatPaC, which was determined from a simulation of a midsize plug-in hybrid-electric vehicle (similar to a first

generation Chevrolet Volt) using the Autonomie model [12]. This factor accounts for power losses in the power converter, the motor, and the gears. This vehicle efficiency factor is assumed to be sufficiently constant over the vehicle speeds of interest. The accessory power (P_a) has a default value of 0.5 kW. The rolling friction power is calculated as follows:

$$P_f = f_f S \tag{8.6}$$

where S is the sustained speed in mph and f_f is a friction power factor. f_f is assumed to be proportional to the energy requirement of the vehicle (\dot{E} , Wh/mile) and is calculated using Eq. 8.7.

$$f_f = f_{f,0} \left(\frac{\dot{E}}{250}\right) \tag{8.7}$$

In Eq. 8.7, $f_{f,0}$ is the friction factor for the midsize plug-in hybrid-electric vehicle in the Automomie simulation referenced above, which had an energy requirement of 250 Wh/mile. The default value of $f_{f,0}$ is 0.065 kW/mph. The aerodynamic drag power is calculated as follows:

$$P_d = f_d S^3 \tag{8.8}$$

where the factor for aerodynamic drag, f_d , is calculated using the following:

$$f_d = f_{d,0} \left(\frac{\dot{E}}{250}\right)^{0.7} \tag{8.9}$$

The power factor of 0.7 in Eq. 8.9 arises from the assumption that the friction factor is less than proportional to the vehicle mass and volume. $f_{d,0}$ has a default value of 0.00004 kW/mph³.

BatPaC assumes a different sustained vehicle speed (*S*) for each vehicle type. These values are provided in Table 8.1. BatPaC provides the option to override these values, as well as the value for \dot{E} (default = 250 Wh/mile).

Table 8.1. Default sustained speed assumed by BatPaC for thermal calculations

	mildHEV	HEV-HP	PHEV	EV
Sustained Speed (mph)	0	35	70	70

A comparison between these calculations and the full Autonomie model showed excellent agreement and is discussed in detail in the previous version of the manual [12]. The previous manual also showed that the battery power associated with a PHEV at a sustained speed of 70 mph is similar to the average power during a US06 drive cycle, which includes rapid acceleration and deceleration with sustained speed driving. This was used as justification for the sustained-speed model in BatPaC. The average power during the US06 cycle was assumed to be a reasonable proxy for the cooling targets since the thermal mass of the battery evens out temperature fluctuations from power bursts.

The rate of heat transfer from hot ambient conditions is calculated using the following equation:

$$q_{amb} = \frac{k_{insulation}A_{insulation}}{\delta_{insulation}} \left(T_{H,amb} - T\right)$$
(8.10)

where *k*, *A*, and δ are the thermal conductivity (default = 0.00027 W/cm/K), area, and thickness (default = 10 mm) of the pack jacket insulation, respectively. $T_{H,amb}$ is the hot ambient temperature (default = 50 °C), and *T* is the operating temperature. The area of the insulation in contact with the external environment is calculated from the pack jacket dimensions in Section 5.5.3.

8.3.2 Sizing of Cooling System

The cooling system is sized based on the total heat generation rate -i.e., the sum of q_s (Eq. 8.1) and q_{amb} (Eq. 8.10). BatPaC assumes four default systems whose properties are show in Table 8.2. BatPaC selects the smallest cooling system which can handle the total cooling requirements of the battery pack. The only exception occurs if EV charging is selected on the 'Dashboard' (see Section 6). If EV charging is selected, BatPaC automatically assumes the largest system with the 6-kW cooling capacity to handle the high heat generation during rapid charging.

System	Max Cooling Capacity (W)	Added Mass (kg/pack)	Added Volume (L/pack)	Performance Coefficient	Baseline Cost (\$/pack)
Refrig 1	500	2.0	0.8	2.5	30
Refrig 2	1000	3.0	1.2	2.5	80
Refrig 3	3000	5.0	2.0	2.5	120
Refrig 4	6000	7.0	2.8	2.5	200

Table 8.2. Parameters for cooling management systems

The masses and volumes of the refrigerant systems in Table 8.2 include the masses and volumes of all additional components (*i.e.*, pump, heat exchanger, and valving). These values are multiplied by the square root of the number of packs to account for added complexity associated with multiple packs. The performance coefficient is used to determine pressure drop in the heat exchanger (see Section 8.3.3). The baseline cost includes the cost of the coolant, pump, heat exchanger, valving, and additional refrigerant.

8.3.3 Pumping Power

BatPaC provides an estimate for the pumping power required to circulate the coolant through the pack and the heat exchanger. The total pumping power is calculated as follows:

$$P_{pump} = \frac{1}{f_P} \left(P_{clnt} + P_{exchg} \right) \tag{8.11}$$

where P_{clnt} and P_{exchg} are the pumping power required to move the coolant through the coolant flow system and heat exchanger, respectively. f_p is a pump efficiency factor with a default value of 0.5 The power required for the coolant system is calculated based on the pressure drop in a rectangular conduit under laminar flow, which yields the following:

$$P_{clnt} = \frac{Q_{clnt} 48\mu_{clnt} G_{clnt} L_{clnt}}{\rho_{clnt} D_h^2} \left(1 + f_{P,add}\right)$$
(8.12)

In Eq. 8.12, ρ_{clnt} and μ_{clnt} are the density (default = 1.07 g/cm³) and viscosity (default = 0.055 poise) of the coolant, respectively. D_h is the hydraulic diameter of the coolant channel. L_{clnt} is the path length traveled by the coolant within the cooling panels (twice the row rack length and height). G_{clnt} is the fluid mass flow rate (g/s/cm²) through a cooling panel. Q_{clnt} is the total flow rate of coolant (cm³/s), which is determined from the allowable temperature rise of the coolant from the inlet to the outlet of the pack. It is calculated using the following equation:

$$Q_{clnt} = \frac{q_s + q_{amb}}{C_{P,clnt}\rho_{clnt}\Delta T_{clnt}}$$
(8.13)

where $C_{P,clnt}$ and ΔT_{clnt} are the specific heat capacity (default = 3.264 J/g/K), and allowable temperature rise (default = 5 °C) of the coolant, respectively. In Eq. 8.12, $f_{P,add}$ is a factor accounting for additional pressure drop within the connections and around turns in the cooling panels (default value = 2).

The pumping power required through the heat exchanger is proportional to the required cooling rate and the performance coefficient (PC) in Table 8.2. It is calculated as follows:

$$P_{exchg} = \frac{q_s + q_{amb}}{PC} \tag{8.14}$$

8.4 Adequacy of Cooling

8.4.1 Adequacy of Cooling Grade

BatPaC includes a calculation which checks the adequacy of cooling by making sure the coolant input properties (*i.e.*, inlet temperature and allowable temperature rise) and cell geometry can maintain safe temperatures within the cell. BatPaC performs a heat transfer calculation during sustained operation and provides a rating based on the maximum temperature at the center of the cell. A rating of Excellent, Good, Fair, or Poor is given based on the difference between the maximum temperature at the center of a cell and the desired operating temperature set on 'Dashboard'. Table 8.3 provides the temperature ranges for these numbers. The grades for each battery design are included in the 'Thermal' worksheet and the *Calculation and Validation* section within 'Dashboard' (see Section 3.2.3.1).

Adequacy of Cooling	<i>T_{max}</i> - <i>T</i> During Sustained Discharge (°C)
Excellent	<5
Good	5 to 10
Fair	10 to 15
Poor	>15

Table 8.3. Temperature ranges for determining adequacy of cooling

A variety of changes can be made to the battery design to address inadequate cooling grades. This includes changes to the power, cell geometry, and cooling system. This paragraph discusses a few main factors. First, the cell geometry can be modified to improve heat transfer by adjusting the number of cells in the pack (which makes the cells smaller), the length-to-width aspect ratio ([L/W]), or the cell thickness. The grade can also be modified by reducing the inlet coolant temperature or the allowable coolant temperature rise in the coolant flow system. Neither of these will directly impact the pack design. Reducing the temperature rise will increase the required flow rate, which will increase the pumping power reported by BatPaC. Reducing the inlet coolant temperature will increase the demand on the air conditioning unit within the vehicle. This additional demand is not accounted for in BatPaC since it's outside the scope of the battery pack and depends on the vehicle design, ambient conditions, and vehicle use profile.

8.4.2 Cell Temperature Calculation

The maximum temperature at the center of the cell is approximated using the following equation:

$$T_{cell,max} = T_{clnt,in} + \Delta T_{clnt} + \Delta T_{c2w} + \Delta T_{w2f}$$
(8.15)

where $T_{clnt,in}$ is the inlet coolant temperature (default = 15 °C), ΔT_{c2w} is the temperature drop between the center of a cell and the coolant panel wall, and ΔT_{w2f} is the temperature drop between the coolant panel wall and the center of the coolant fluid. A detailed discussion on ΔT_{c2w} and ΔT_{w2f} can be found in the previous version of the manual [12]. In general, ΔT_{c2w} is calculated assuming heat leaves through the aluminum thermal conductors in contact to the edge and side face of the cell (see Figure 8.3). Heat transfer is assumed on all four large faces and not just the two shown in Figure 8.3. Heat transfer out of the tabs is neglected. The total temperature drop from the cell center to the cooling panel wall is calculated using the following equation:

$$\Delta T_{c2w} = \left(\frac{q_s + q_{amb}}{N_{cells}}\right) \left(\frac{1}{[q/\Delta T]_{cell,s} + [q/\Delta T]_{cell,e}}\right)$$
(8.16)

where the first set of parentheses corresponds to the heat rejection per cell and the second set divides this number by the total heat rejection per temperature difference between the cell center and cooling panel walls. $[q/\Delta T]$ has units of W/°C. The calculation assumes uniform temperatures in the thin metal components outside the cell (*i.e.*, aluminum conductors, module wall, and cooling panel wall). $[q/\Delta T]_{cell,s}$ and $[q/\Delta T]_{cell,e}$ are determined using empirical correlations. The correlations were developed from finite element simulations of the heat transfer in 70 representative cells. The previous version of the manual contains details on the methodology,

parametric ranges for the seventy cells, and validation data [12]. The correlations are given as follows:

$$[q/\Delta T]_{cell,s} = 1628L_{Al}k_y^{0.55}k_x^{0.58}\delta_{cell}^{0.21}W_{cell}^{-0.7}\delta_{metal}^{0.72}$$
(8.17)

$$[q/\Delta T]_{cell,e} = 3.917 L_{Al} k_y^{0.58} k_x^{-0.19} \delta_{cell}^{1.2} W_{cell}^{-0.75}$$
(8.18)

where δ_{cell} , W_{cell} , and L_{Al} are the thickness of the cell, width of the cell, and length of the aluminum thermal conductor, respectively. δ_{metal} is the thickness of the metal between the pouch cell and the coolant. It is comprised of the aluminum thermal conductor, steel module wall, and stainless-steel coolant panel wall. k_y and k_x are the thermal conductivities of the cell across the layers and parallel to the layers, respectively. The thermal conductivities are composite parameters calculated from default values for the aluminum foil, copper foil, positive coating, negative coating, separator, and folded edge. The default values can be adjusted in the 'Thermal' worksheet. The default conductivities yield values of 0.00934 and 0.20108 W/cm/K for k_y and k_x , respectively.

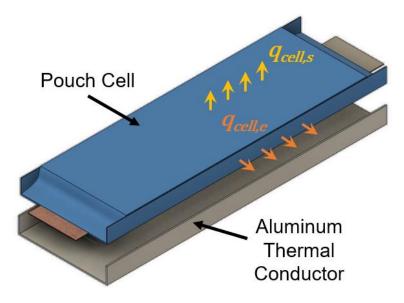


Figure 8.3. Schematic of pouch cell and aluminum thermal conductor showing two directions of heat transfer from the side $(q_{cell,s})$ and edge $(q_{cell,e})$ of the cell.

The temperature drop from the coolant panel wall to the bulk coolant fluid is calculated using the following equation:

$$\Delta T_{w2f} = hA_{w2f}q_{ss} \tag{8.19}$$

where A_{w2f} is the effective area between the wall and the coolant fluid. It is equivalent to the coolant panel area in contact with the modules at the top and bottom of the module row racks. *h* is the heat transfer coefficient (W/cm²/K) between the panel wall and the fluid. It is calculated as follows:

$$h = \frac{k_{clnt} N u}{D_h} \tag{8.20}$$

where k_{clnt} is the thermal conductivity of the EG/W (0.0043 W/cm²/K). Nu is the Nusselt number. It is determined from an empirical correlation that was developed by solving a set of numerical simulations involving heat transfer between a fluid and a plate. It is based off the correlation from Nickolay and Martin, which relates the Graetz number and the limiting solution, Nu_∞ = 5.385, to the mean Nusselt number [20]. It is given as follows:

$$Nu = \left[Nu_{\infty}^{n} + \left(C_{1}Gz^{1/3} \right)^{n} \right]^{1/n}$$
(8.21)

where the constants *n* and C_1 were found to have values of 3.592 and 2.255, respectively. G_z is the Graetz number, which is defined as:

$$Gz = 2\frac{D_H}{L_{clnt}}RePr$$
(8.22)

where *Re* and *Pr* are the Reynolds and Prandlt numbers, respectively. They are calculated as follows:

$$Re = \frac{\rho_{clnt} u D_H}{\mu_{clnt}} \tag{8.23}$$

$$Pr = \frac{\mathcal{C}_{P,clnt}\mu_{clnt}}{k_{clnt}} \tag{8.24}$$

where u is the average velocity and all other terms have been previously defined in this section. The simulations used to determine the Nu correlation assumed an incompressible, laminar fluid; negligible radiation; and steady state conditions.

8.4.3 Adiabatic Temperatures

BatPaC provides two calculations within the 'Thermal' worksheet which determine the temperature in the pack under adiabatic (zero heat transfer) operation. The calculations provide the temperature after an adiabatic sustained discharge and an adiabatic power pulse. The results do not impact any of the pack design. These calculations are included as an upper bound to inform the user of the worst-case scenario in their design. The temperature after a full adiabatic discharge at the sustained power is calculated as follows:

$$T_{ad,dch} = T + \frac{E_{pack} \left(1 - f_{e,dch}\right)}{C_{P,pack} m_{pack}}$$
(8.25)

where E_{pack} is the available pack energy (kWh), $C_{P,pack}$ is the estimated specific heat capacity of the whole pack (default = 0.85 J/g/K), and m_{pack} is the mass of the pack less 50% of the jacket mass. $f_{e,dch}$ is the efficiency during sustained discharge and is calculated as follows:

$$f_{e,dch} = \frac{P_s}{P_s + q_s} \tag{8.26}$$

The adiabatic temperature rise during the rated power pulse is calculated using the following:

$$T_{ad,pulse} = T + \frac{t_{pulse} l_{pulse}^2 R_{pulse}}{C_{P,pack} m_{pack}}$$
(8.27)

Where t_{pulse} is the duration of the power pulse, I_{pulse} is the pack current during the power pulse (see Eq. 5.4 and Section 5.2.1), and R_{pulse} is the pack resistance during the pulse. R_{pulse} is calculated using Eq. 8.2 but with ASI_P (the area specific impedance for power) instead of ASI_E .

8.5 Battery Heating

Some battery packs require heating elements to warm up the battery on cold days before starting the vehicle. BatPaC adds an additional mass to the pack to account for these heaters. The heaters are assumed to weigh 0.2 kg per kW of heater power. The heater power is included as an input with a default value of 1 kW. BatPaC assumes the cost of the heaters depends on the vehicle type (mildHEV, HEV-HP, PHEV or EV). Its value for each vehicle is provided in Section 9.2.3.

BatPaC includes a side calculation in the 'Thermal' worksheet to help the user determine a heater size which meets their heating requirements. The side calculation is given as follows:

$$t_{heat} = \frac{(T_{start} - T_{C,amb})C_{P,pack}m_{pack}}{P_{heat}}$$
(8.28)

where t_{heat} is the time required to heat the battery pack, P_{heat} is the heater power (default = 1 kW), T_{start} is the desired temperature to start the battery (default = 5 °C), and $T_{C,amb}$ is the cold ambient temperature prior to heating (default = -15 °C); This calculation lets the user tune P_{heat} to meet the desired heating time for a given set of ambient conditions. BatPaC provides no additional guidance on these numbers but anticipates significant variability amongst users depending on the use case and operational environment of their vehicle.

8.6 Distribution of Cost, Mass, and Volume within BatPaC

Table 8.4 provides an explanation for how the cost, mass, and volume of the four main components in the thermal management system are distributed in BatPaC. The cost, mass, and volume of the coolant system within the pack are included in all pack-specific metrics (\$, \$/kWh, L, kg, etc.). This includes the coolant within the system.

The cost of the additions for coolant management are also included at the pack-level. However, the mass and volume of this equipment are not incorporated in any pack-specific metrics. They only appear in the full battery system metrics. This distinction is made because the pack mass and volume in BatPaC reflect the mass and volume that require a single, designated location within the vehicle. The coolant management components are typically stand-alone devices that interface between the coolant system and the vehicle's refrigerant system. They do not have to be next to the pack; therefore, they do not impact the pack's mass and volume. In addition, their exact locations are not specified in BatPaC, as this will depend on the preferences of the vehicle manufacturer.

The cost and mass of the battery pack heaters are included in the total pack metrics since they must be in contact with the pack. Their volume addition to the pack is assumed negligible. Finally, cost upgrades for the AC unit to handle the extra cooling capacity are only incorporated on the system level. No mass or volume is assumed for these upgrades. Costs for the AC upgrades are discussed in Section 9.2.3

Table 8.4. Explanation of how the cost, mass, and volume of each component in the thermal management system is handled by BatPaC. The table lists the battery level whose metrics first include the thermal component.

Thermal Management Component	Cost	Mass	Volume
Coolant flow system	Pack	Pack	Pack
Additions for coolant management	Pack	System	System
Additions for pack heating	Pack	Pack	-
AC upgrades	System	-	-

9. MANUFACTURING COST

9.1 Approach

The manufactured cost of a battery pack is calculated with input from the design information generated in modeling the cell and pack performance (Sections 5 to 8). The design modeling determines the annual materials and purchased items requirements, which includes battery management and thermal management systems in the pack. The manufacturing cost is then added to these materials and systems costs to reach the unit cost of a single pack.

The manufacturing costs for the designed pack are scaled from a baseline plant. The baseline plant accounts for the size, speed, number of units, direct labor, and depreciation of the capital cost for each processing step. The process expenses are summed with the additional costs of operating the manufacturing facility. These costs include launch costs; working capital; variable overhead; general, sales, and administration (GSA); and research and development. The baseline plant produces 500,000 EV battery packs per year with 100-kWh rated energy and 300-kW rated power. The plant costs represent near-future estimates for materials, labor, capital, and plant area. The values were determined to provide reasonable estimates for manufacturing rates of 10-200% of the baseline rate.

BatPaC v5.0 includes additional features for calculating the manufacturing cost that were not available in previous versions. For instance, options are provided for modeling manufacturing costs in plants operating at less than 100% utilization/capacity. In addition, the user can control the method for manufacturing the pack: *i*) all manufacturing from cells to modules to packs is done in-house, *ii*) the cells are purchased from a 3rd party vendor and used to manufacture the modules and packs, and *iii*) the modules are purchased from a 3rd party vendor and used to manufacture the packs. Each scenario impacts the investment and materials costs incurred by the pack manufacturer with materials purchased from 3rd party vendors incurring price mark-ups for profit and warranty. Finally, the user can control whether the final pack cost includes profit and warranty. This section provides details of the cost calculation including further information on these new features.

9.2 Materials Costs, Purchased Items, and Pack Integration

This subsection provides the default costs, including rationale, for the materials, purchased items, and pack integration costs used in BatPaC v5.0. All costs assume a high-volume market. Modifications to costs can be made in the 'Dashboard,' 'Chem,' and 'Cost Input' worksheets.

9.2.1 Battery Specific Materials Costs

The default costs of the main battery materials are provided in Table 9.1. These values are included in the model upon selection of an electrode couple. Their values can be overridden in either the 'Dashboard' or 'Chem' worksheets.

BatPaC provides default values for several choices of positive and negative electrode materials. All positive electrode materials are either in a commercially viable state of development or are currently utilized in Li-ion batteries produced today. A notable absence from the list is lithium cobalt oxide (LCO), which is not considered a viable option for transportation applications due to safety and lifetime concerns. Most of the positive electrode material costs track with the price of the raw materials, with the prices of cobalt and, to a lesser extent, nickel controlling the cost. The one exception is NMC811, which, despite its low cobalt content, has a higher cost because it is manufactured with the more expensive LiOH, as opposed to Li_2CO_3 .

Material	Chemistry	Abbreviation	Unit	Cost
Positive Electrode			\$/kg	
Manganese spinel	Li _{1.06} Mn _{1.94-x} M' _x O ₄	LMO		9.00
Phospholivine	LiFePO ₄	LFP		10.00
Layered oxide	LiNi _{0.80} Co _{0.15} Al _{0.05} O ₂	NCA		26.00
	LiNi _{1/3} Mn _{1/3} Co _{1/3} O ₂	NMC333		25.50
	LiNi _{0.5} Mn _{0.3} Co _{0.2} O ₂	NMC532		24.00
	LiNi _{0.6} Mn _{0.2} Co _{0.2} O ₂	NMC622		25.00
	$LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$	NMC811		26.00
Negative Electrode			\$/kg	
Coated-natural graphite	C ₆	G		10.00
Lithium titanate spinel	Li ₄ Ti ₅ O ₁₂	LTO		15.00
Electrolyte	1.2 M LiPF ₆ in EC:EMC		\$/L	10.00
Separator	PP/PE/PP		\$/m ²	0.90
Current collector foil			\$/m ²	
Positive	Aluminum			1.20
Negative	Copper (Al for LTO)			0.20
Binders			\$/kg	
Positive	PVDF			15.00
Negative	Generic aqueous			10.00
Conductive additive	Carbon black		\$/kg	7.00
Slurry Solvents			\$/kg	
Positive	<i>N</i> -Methyl-2-pyrrolidone	NMP		2.70
Negative	Water			0.00

Table 9.1. Costs of major cell materials in BatPaC v5.0, released July 2022

Carbon-based materials are used as the negative electrode in most commercial cells. Many manufacturers use a proprietary blend of natural and artificial graphite and/or hard carbon. Significant differences in cost, capacity, lifetime, and rate-capability exist between artificial graphite, natural graphite, coated-natural graphite, and hard carbon. For simplicity, a coated-natural graphite is used as the default carbon-based material in BatPaC v5.0. Lithium titanate spinel is also included as a negative electrode, which may have advantages for high power and long-life applications.

The default separator and electrolyte are based on a single electrolyte-separator combination. The electrolyte is a lithium hexafluorophosphate salt, LiPF_6 , dissolved in a carbonate based solvent system. The carbonate solvent system is a blend of ethylene carbonate, EC, and a linear carbonate such as ethyl methyl carbonate, EMC, or dimethyl carbonate, DMC. The price listed in Table 9.1

is only for the base electrolyte (*i.e.*, no additional additives). The default separator is a porous polypropylene (PP) membrane with a polyethylene (PE) middle layer and a ceramic coating for structural integrity. PP and PE are inexpensive raw materials, but the separator has a relatively high cost due to the manufacturing process required to form the porous network. The middle PE layer is included as a shut-down feature, which will melt at high temperatures to prevent thermal runaway.

The current collector foils are based on copper metal for the negative electrode and aluminum for the positive electrode. The one exception is LTO, where aluminum is used at the negative electrode due to the high voltage of LTO relative to lithium. The price of these foils is based on raw materials and manufacturing costs. The aluminum foil is produced by rolling thicker stock foils into thinner sheets. Copper foil is mainly produced through an electrodeposition process. The foils used in batteries have additional requirements beyond the cheapest product available. Surface treatments are often necessary to promote adhesion of the composite electrode to the foil surface. In addition, alloying of the foil may be necessary to achieve the required material properties for long life. Due to these factors, the current metal ingot price is only a small fraction of the end foil price.

The binder and conductive additive in the positive and negative electrodes add a small but real cost to the battery. The positive binder is PVDF and the positive slurry solvent is *N*-Methyl-2-pyrrolidone (NMP). The cost of the NMP assumes the solvent is recovered after evaporation, distilled to a moderately high purity, and returned to the manufacturer for further purification into battery-grade NMP (99.99%). The price reflects a discounted rate (with respect to the market price of 99.99% NMP) negotiated between the battery and NMP manufacturers. The negative binder is a generic blend of water-soluble polymers. No cost is assumed for the water used in making the negative slurry. The price of the conductive additive represents a high purity and moderate surface area carbon black material.

As mentioned in Section 3.4.2, BatPaC 5.0 makes it possible to include additives in the positive electrode, negative electrode, and electrolyte. All default chemistry couples assume zero additives. The weight percentage, lithium percentage, and cost in \$/kg is required when including an additive. No guidance on additive type or cost is provided by BatPaC. See Section 3.4.2 for further details.

9.2.2 Purchased Items Costs

To simplify the cost calculations, it is assumed that all hardware items for the cells, modules, and packs are purchased from a third-party vendor. The costs for these items are estimated from a fixed value plus an additional value proportional to the mass of the item. The cost per mass is based on the ingot price of the raw material plus a form factor. All purchased items costs can be found in the 'Cost Input' worksheet. Details on the per mass costs are available in the 'Lists' worksheet.

Table 9.2 lists the purchased items for the cell, module, and pack. m_i in the equations refers to the mass of the component. C_{mod} is the module capacity. A_{ins} is area of insulation, which depends on the pack dimensions. The last column lists the per unit basis for the equation. For instance, the cost equation for the positive terminal refers to the cost per cell while the cost equation for the module management system refers to the cost per parallel cell group. The cell negative terminal and cell

interconnects are both made from nickel plated copper sheets. The costs shown for the terminals include an allotment for isolation tape that is necessary to protect the electrical connection.

There are several "Cost per unit" values in Table 9.2 that require further explanation. They are described in this paragraph. For the module, there is one interconnect per cell plus additional interconnects for cells in parallel and tabs to terminals. There are two interconnect panels and two terminals per module. For the pack, there is one module interconnect per module and per row of modules. There are two cooling panels per row of modules and two terminals per pack. The bus bar is a fixed cost and is only charged if bus bars exist within the pack (see Section 5.5.1).

Component, <i>i</i>	Material	Cost Equation, \$/unit	Cost per unit
<u>Cell-level</u>			
Positive terminal	Aluminum	$0.08 + 2.41m_i$	Cell
Negative terminal	Copper	$0.08 + 8.64m_i$	Cell
Container	PET-Al-PP	$0.20 + 3.00m_i$	Cell
Heat conductor	Aluminum	$0.15 + 2.41m_i$	Cell
Module-level			
Module management system	-	$2.00 + 6.00C_{mod}$	Parallel cell group
Cell interconnect	Copper	$0.04 + 8.72m_i$	Interconnect
Interconnect panel	Polypropylene	$0.20 + 2.30m_i$	Panel
Terminals	Copper	$0.35 + 8.64m_i$	Terminal
Enclosure materials	Steel	$0.50 + 2.40m_i$	Module
Provision for gas release	-	0.50	Module
Pack-level			
Row rack	Aluminum	$1.00 + 1.33m_i$	Pack
Pads between modules	Elastomer	$0.20 + 1.00m_i$	Module rows
Module interconnects	Copper	$0.40 + 8.84m_i$	Interconnect
Bus bar	Copper	$0.60 + 8.68m_i$	Pack
Cooling panels	Steel	$0.50 + 2.80m_i$	Panel
Coolant manifolds	Stainless Steel	$1.00 + 8.00m_i$	Pack
Terminals	Copper	$0.75 + 8.88m_i$	Terminal
Steel in jacket	Steel	$3.00 + 1.40m_i$	Pack
Aluminum in jacket	Aluminum	$3.00 + 2.81m_i$	Pack
Jacket insulation	-	$3.00A_{ins}$	Pack

 Table 9.2. Cost equations for purchased items

9.2.3 Pack Integration Cost

Various additional components are necessary to integrate the battery into the electric drive system. This includes additions for the battery management system, thermal management system, and system upgrades. Table 9.3 provides an overview of the additional costs added at the pack and battery system levels.

Additions for the battery management system are handled in detail in Section 7. Additions to the structure of the pack for thermal management -i.e., coolant plates, manifolds, tubing, etc. - are

discussed in detail in Section 8 and their costs are incorporated into the purchased items in Table 9.2. Additional systems are required to connect the thermal components to the vehicle. The baseline thermal system cost depends on the cooling requirements of the pack and is discussed in Section 8.3. It includes pumps to circulate the coolant, a heat exchanger (chiller) to transfer the thermal energy from the coolant to the refrigerant loop, and valving on the refrigerant line from the AC unit [19].

	Units	MildHEV	HEV-HP	PHEV & EV
Battery management system	\$/pack	see Section 7		
Thermal management system				
Baseline thermal system	\$/pack	see Table 8.2		
Heating system	\$/pack	0	20	20
Additions to AC system	\$/battery system	20	40	40
Additions for extra pack	\$/additional pack	50	100	150

Table 9.3. Pack integration costs

The heating system is assumed to either be a positive thermal coefficient (PTC) heater or a flexible mat heater. The PTC heater would directly raise the temperature of the heat transfer fluid in a reservoir while the mat heater would be placed between the battery jacket insulation and the internal metallic jacket sheet. Note that any pack costs listed in BatPaC include the battery management system, baseline thermal system, and heating system.

Pack integration also involves upgrades to the air-conditioning (AC) system in the vehicle to accommodate extra heat removal. This cost is added to the whole battery system and remains constant whether the vehicle is designed with 1 or multiple packs (see Battery System Parameters section in 'Battery Design' worksheet to adjust number of packs per vehicle). An extra cost is also included for each additional pack to account for additional complexity in the battery and thermal management systems. The additions for AC and extra packs are included on the battery system costs in BatPaC.

9.3 Baseline Manufacturing Plant

The model's baseline plant is designed for EV battery packs of NMC811-G chemistry for a sedan of moderate power and range at a manufacturing rate of 500,000 battery packs per year. These packs have 400 cells with 68 Ah capacities, providing a rated power of 300 kW and total energy of 100 kWh. The battery will provide 340 miles of vehicle travel with 85% of the pack energy for a vehicle requiring energy of 250 Wh/mile. The default pack can be modeled in BatPaC 5.0 using the default inputs for an EV with a NMC811-G (Energy) chemistry. The only required modification is setting the positive electrode thickness override to 70 μ m.

The schematic diagram of the plant (Figure 9.1) is designed to illustrate the flow of materials through the plant. The annual rate of 500,000 battery packs per year (50 GWh/year) is achieved by operating for three shifts at the equivalent of 320 days per year of full production. The exceptions to three-shift operation are for shipping and receiving which are active for only two shifts per day. The plant size was chosen to reflect near-future plant capacities.

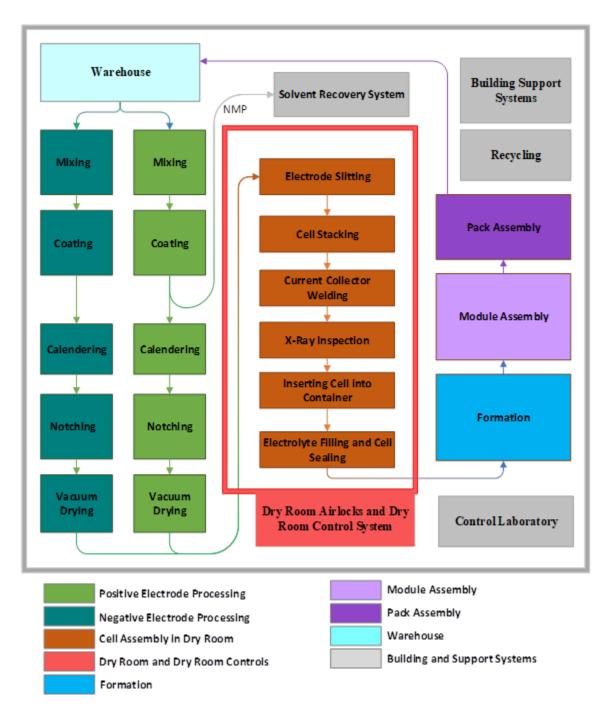


Figure 9.1. Schematic diagram of baseline lithium-ion battery manufacturing plant. Manufacturing rate: 500,000 NMC811-G battery packs per year, 100-kWh pack energy, 300-kW power, 68-Ah capacity, 400 cells. Operating year: 320 days per year with three 8-hr shifts.

The pertinent manufacturing rates for the baseline plant are provided in Table 9.4. The rates assume a 95% cell yield – *i.e.*, 95% of fabricated cells pass inspection. The rates also assume yields at each processing step which are provided in Table 9.5. The labor, capital equipment cost, and plant area for each processing step are provided in Table 9.6. The equipment costs include

installation. All this information can also be found in the 'Cost Input' worksheet. The cost factors for the individual processing steps are discussed in detail in the sections that follow. Overall, the plant requires ~500 workers per shift, \$4.2B worth of capital equipment, and 306,000 m² of plant area.

Table 9.4. Manufacturing rates in baseline plant. Values are shown to three significant figures	•
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Rate	Unit	Amount
Operational days	days/yr	320
Total pack energy	kWh/yr	50,000,000
Number of packs	packs/yr	500,000
Number of row racks	racks/yr	2,000,000
Number of modules	modules/yr	10,000,000
Number of cell interconnects	interconnects/yr	270,000,000
Number of accepted cells	accepted cells/yr	200,000,000
Total number of cells (adjusted for yield)	total cells/yr	211,000,000
Positive electrode area	m²/yr	303,000,000
Negative electrode area	m²/yr	315,000,000
Positive active material	kg/yr	72,500,000
Negative active material	kg/yr	49,100,000
Positive binder solvent evaporated	kg/yr	24,200,000
Negative binder solvent evaporated	kg/yr	40,100,000

Table 9.5. Material yields during electrode and cell fabrication.

Material	Material Mixing	Coating	Electrode Slitting	Cell Stacking	Electrolyte Filling	Total
Positive Electrode	99	95	99	99	Thing	92.2
Negative Electrode	99	95	99	99		92.2
Positive Current Coll.		95	92	99		86.5
Negative Current Coll.		95	92	99		86.5
Separator				98		98.0
Electrolyte					99	99.0
NMP solvent recovery						99.5

Process	Labor (hr/yr)	Capital Equipment (\$M)*	Plant Area (m ²)
Materials preparation/mixing	•		
Positive	200,000	200	8,000
Negative	270,000	280	8,800
Electrode coating			
Positive	59,000	90	16,000
Negative	59,000	78	16,000
Calendaring			
Positive	61,000	25	2,100
Negative	69,000	25	2,100
Notching	,		
Positive	250,000	29	3,200
Negative	250,000	29	3,200
Electrode vacuum drying	,		
Positive	41,000	14	2,000
Negative	35,000	11	1,600
Cell assembly in dry room			
Electrode slitting [†]	260,000	30	-
Cell stacking	700,000	170	-
Current collector welding	190,000	190	-
X-ray inspection	190,000	14	-
Inserting cell in container	49,000	11	-
Electrolyte filling & cell sealing	132,000	25	-
Dry room	8,000	7.3	61,000
Formation cycling, testing, and sealing	560,000	830	110,000
Module assembly	170,000	94	27,000
Pack assembly and testing	150,000	94	27,000
Warehouse	31,000	200	10,000
Building and supporting systems	, , , , , , , , , , , , , , , , , , ,		· · · · · ·
Building	-	1,700	-
Solvent recovery	17,000	36	1,100
Rejected cell and scrap recycle	38,000	9.3	3,300
Control laboratory	46,000	16	1,300
Total	3,876,000	4,222	305,700

Table 9.6. Labor, capital equipment, and plant area for each process step in the baseline plant. Values are approximated to two significant figures.

[†]both electrodes

*cost includes installation

9.3.1 Electrode Processing

9.3.1.1 Materials Preparation and Mixing

The electrode materials, which consist of active material, carbon, binder, and binder solvent, are mixed in small batches with planetary dispersing mixing machines. At the design production rate in the baseline plant, the positive electrode materials require eighteen, 2,300 L machines and the negative electrode materials require twenty-four, 2,700 L machines. These numbers assume solvent to binder ratios ($g_{solvent}/g_{binder}$) of 16 and 40 for the positive and negative materials, respectively. A 30% head space is assumed for all machines. The labor is calculated assuming 1.5 operators per machine per shift. The capital equipment costs and plant area for this step also factor in hoppers for materials handling, side mixers for the solvent-binder mixtures, storage vessels for transportation to the coater, and filtration systems for de-ionized water.

9.3.1.2 Electrode Coating

The positive and negative electrodes are coated to the current collector foils using double-sided, slot-die coaters with a maximum coating width of 1.0-meter and a coating speed of 80 m/min. The double-sided coating is achieved with a two-level coating system. The first side is coated on the top-level followed by the second side on the bottom level. The coaters can produce two stripes per width, which allows for coating of four baseline cell-heights at once (see Figure 9.2). ~82% of the foil is coated, with three uncoated regions left in the middle and on either side of the stripes. Of the ~18% uncoated foil, ~10% is used for tabs. The other ~8% is lost during electrode slitting. The coaters include oven sections that can dry ~100-µm thick coatings at 80 m/min. At present, no changes are made to the capital cost or area of the oven sections for different electrode thicknesses. The capital cost assumes the coater has a precision pumping system, alignment inspection, in-line viscosity control, a surface defect detector, an insulation coating unit (ceramic and/or polyamideimide), and an auto splitting unit. The auto splitting unit is used to split the two stripes into two separate rolls to be fed into the calendering machine (next section). Automated guided vehicles for handling the rolls are also included in the cost. The baseline rates for both electrodes can be accommodated with five coaters each, even though the negative area is slightly larger than the positive. The costs associated with the positive electrode are higher than the negative in Table 9.6 due to the use of NMP in the positive, which must be condensed and recycled (see Section 9.3.7.2). It is assumed that 0.5% of the NMP is lost during coating. The labor rates assume 1.5 operators per coater per shift.

9.3.1.3 Calendering

After coating, the electrodes move to the calendering machines, where they are compressed by rolling to meet the specified void volume fraction. The baseline rates for the positive and negative electrodes can be accommodated with eight and nine calenders, respectively. Each calender operates at 100 m/min. The calenders require a larger m/min throughput than the coaters because of the increase in total roll length when the rolls were split after coating. All calenders include laser automatic thickness gauges. The per-piece size and cost of the positive calenders are larger than the negatives in Table 9.6 because the positive calenders require pre-heating and induction

heating annealing to perform the calendering at elevated temperatures. The negative calenders operate at room temperature. The labor rates in Table 9.6 correspond to one operator per calender per shift.

9.3.1.4 Notching

Notching machines slit the coated and calendered electrode foils into two electrode strips using a die cutter. Simultaneously, current collector tabs are cut using precision lasers on the uncoated portion of the foil. Figure 9.2 highlights the regions which are cut during this process. The estimated scrap loss of foil for this process is ~8%. The baseline rates can be accommodated with 34 machines each for the positive and negative materials (68 total) operating at 24 m/min. The labor rate is calculated assuming one operator per notching machine per shift.

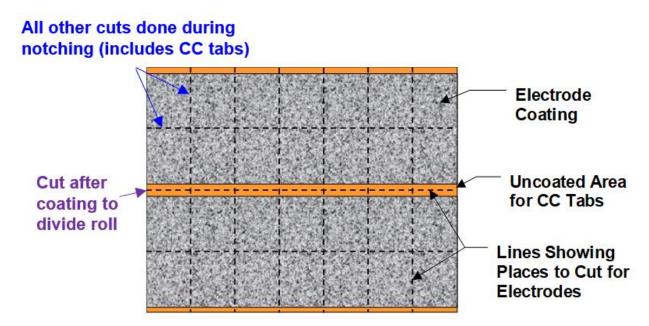


Figure 9.2. Schematic of electrodes coated on current collector foil showing regions that are cut after coating and during notching.

9.3.1.5 Vacuum Drying of Electrodes

Moisture from the electrodes must be removed prior to cell assembly to prevent harmful reactions between the electrolyte and water. The reels of notched electrodes are dried at elevated temperatures in vacuum drying ovens. Five and four vacuum dryers are required for the positive and negative electrodes, respectively. Each positive reel contains ~30% more coated area than its negative counterpart due to thinner electrodes. This corresponds to less total cathode reels that need processed (460 vs. 600 reels per day for the positive and negative, respectively). However, the drying time of the positive is 50% longer than the negative (3 vs. 2 hours) due to differences in the thicknesses of the electrodes. The combination of these two factors increases the total number of dryers for the positive electrode reels (5 vs. 4). The per-piece area and cost of all dryers is 400 m² and ~\$2.8M, respectively. The labor rate assumes one operator per dryer per shift.

9.3.2 Cell Assembly in Dry Room

This section describes the cell assembly steps which occur in a dry room to prevent water contamination. These steps include electrode slitting, cell stacking, current collector welding, X-ray inspection, insertion of cell into a container, and electrolyte filling. BatPaC v5.0 provides labor and capital equipment costs for all these steps. The area is provided as a lump sum for all steps in the dry room.

9.3.2.1 Electrode Slitting

Upon entering the dry room, the electrode foils are first slit into individual electrodes. The values in Table 9.6 were generated assuming 34 total slitters (17 for each electrode) with one operator per slitter per shift.

9.3.2.2 Cell Stacking

Cell stacking is accomplished by inserting the electrodes into a folded separator sheet. The positive-electrode tabs protrude on one side and the negative-electrode tabs on the other. The baseline rate can be met with 183 cell stackers operating at 2.5 cells per minute. The labor rate assumes 0.5 operators per stacker per shift.

9.3.2.3 Current Collector Welding

The current collector tabs for the negative and positive electrodes in the stacks are welded to their respective terminals by ultrasonic welding. The baseline rate is achieved with 25 welders operating at 18 cells per minute. One operator per welder per shift is assumed.

9.3.2.4 X-ray Inspection

After welding, the alignment of each electrode stack is inspected using an X-ray inspection machine. The machine can process 18 cell stacks per minute and includes an auto-reject feature to reject stacks with mismatched electrode alignments. The numbers in Table 9.6 assume 25 inspection machines and one operator per welder per shift.

9.3.2.5 Inserting Cell in Container

The welded electrode stacks are inserted into cell containers by thirteen machines operating at 36 cells per minute. The containers consist of two stiff, pre-shaped pouch halves, which are assumed to be purchased as finished parts. Each cell is enclosed in these containers, which are then partially sealed prior to injecting electrolyte. The machines include systems for visually inspecting the tabs and checking for shorts. The machines also include an ink-jet printer to mark the pouch cell containers. The machines are assumed to require 0.5 operators per machine per shift.

9.3.2.6 Electrolyte Filling and Cell Sealing

At this station, the cells are evacuated, filled with electrolyte, and temporarily sealed. The seal is temporary because the cells undergo a de-gassing step in the formation process discussed below. The filling and sealing are accomplished in the baseline plant using 25 machines operating at 18 cells per minute with 2/3 of an operator per machine. The electrolyte filling machines contain an auto rejection system based on the electrolyte and cell weights. The cells are automatically inserted into formation trays after filling.

9.3.2.7 Dry Room Airlocks and Dry Room Control System

The entire cell assembly process is conducted in a dry room with a maximum dew point temperature of -40 °C. 61,000 m² of plant area is required for all these processes. This includes a small addition for personnel air locks at the entry ways. The capital equipment expenses in Table 9.6 include the costs of the air locks and a dedicated control system for the dry room. Costs for insulative walls to prevent water vapor diffusion, a humidity management system, and equipment for purification and circulation of the dry air are included in the building support systems (Section 9.3.7.1). The labor is calculated assuming one control system operator per shift.

9.3.3 Formation Cycling

After filling and sealing, the cells leave the dry-room and enter a formation protocol. Formation is an expensive process because it takes considerable time. It is the largest, most expensive, and most labor-intensive process in the manufacturing plant. Formation protocols are proprietary with variability between manufacturers. As such, the labor, capital, and area listed in Table 9.6 are for the entire formation process with no breakdown for individual steps. It is assumed the formation process will likely contain the following steps:

- 1) Room temperature aging for 1-2 days
- 2) Pre-formation involving pressure, heat, and pre-cycling
- 3) Good/no good selection based on pre-formation performance
- 4) Rolling and degassing to remove gas from pre-formation
- 5) Final sealing
- 6) Formation cycling and aging over a 1- to 2-week period under temperature-controlled conditions
- 7) Electrochemical testing and grading
- 8) Final inspection

The equipment required to complete this process includes aging racks, hot-press machines, good/no good selector machines, rolling and degassing machines – which include final sealing, and charge/discharge cyclers. A conveyor system and stacker cranes are also employed for automated transfer of cells. Grading machines determine the electrochemical quality of the cells based on voltage, resistance, and capacity. Final inspection machines check the overall dimensions and weights. The entire process is tied together with an information measurement system that allows for real-time monitoring of the equipment and cells. The labor listed in Table 9.6 corresponds to 73 people per shift for the entire process.

9.3.4 Module Assembly

The accepted cells which do not fail the formation grading or final inspection are assembled into modules. This includes placing an aluminum heat conductor around each cell (see Figure 2.4) and connecting them through the interconnects. The module management system, terminals, enclosure, and provision for gas release are all included at this time (see Section 2.3). The modules in the baseline plant are assembled in eleven, automated lines operating at two modules per minute each. Two operators per shift per line are assumed.

9.3.5 Pack Assembly

The finished modules are assembled into battery packs with the aid of automated stations. There are twenty modules per pack in the baseline plant. The modules are placed into row racks with pads in between and connected using module interconnects and bus bars. The packs also include cooling panels, coolant manifolds, terminals, and enclosures/jackets (see Sections 2.4 and 2.5). The values in Table 9.6 assume five stations are used, each assembling packs at a rate of five minutes per pack with four operators per shift per station.

9.3.6 Warehouse

Warehouse space is required throughout the plant to support operations. This includes area for receiving, storage of raw materials, storage of materials between processes (to ensure continuous operation), storage of packs/finished goods, and shipping. The area, capital cost, and labor listed in Table 9.6 include all warehouse processes. The area is listed as one lump sum, but it is distributed throughout the plant. The area assumes efficient use of the vertical space within the plant to reduce the footprint. The capital cost includes the cost of stacking cranes and conveyor belts for automated handling of goods within the receiving, shipping, and storage areas. It also includes equipment for transportation of materials between process steps (electrode roll handling, cell trays, etc.). The labor values reflect a highly automated warehouse system. They include one person per shift in receiving, two people per shift in shipping, and two people per shift for other storage locations. Receiving and shipping assume two shifts per day. Other storage facilities assume three shifts per day.

9.3.7 Building and Supporting Systems

There are several building and supporting systems required to facilitate operations in the baseline plant. The labor, area, and costs of these systems are segmented into building support systems, solvent recovery, recycling, and control laboratory.

9.3.7.1 Building Support Systems

The building support systems are the largest capital expenditures. They include all modifications to the building required to support operation. The capital equipment cost in Table 9.6 includes piping, floors, walls, ceilings, and everything related to heating, venting, and air conditioning (HVAC). The HVAC systems include duct work, cooling towers, chillers, and boilers. The capital cost also includes a separate boiler and heat flow system for maintaining hot oil for the coaters.

Building modifications for the dry room are also included in the costs – *i.e.*, insulative walls to prevent water vapor diffusion, a humidity management system, and equipment for purification and circulation of the dry air. Finally, the cost includes the manufacturing execution system (MES), which controls the entire automated manufacturing process, and the air-conditioning automatic control system. There is no labor associated with these systems since plant maintenance is included in variable overhead (Section 9.6.1). There is also no area associated with these systems because they are incorporated within the existing structure of the building.

9.3.7.2 Binder Solvent (NMP) Recovery

A solvent recovery system is required to capture the solvent released from the drying ovens in the positive electrode coaters. It is necessary because the positive solvent, *N*-Methyl-2-pyrrolidone, is toxic and expensive. It is collected, distilled to a moderate purity, and returned to the supplier for further refinement. The capital equipment cost in Table 9.6 is associated with the collection and distillation systems. The labor reflects two people per shift for the entire system.

9.3.7.3 Rejected Cell and Scrap Recycle

Scrap is generated from preparation of the electrodes and from rejected cells after formation. The yields of materials in the various processing steps are shown in Table 9.5. The cost, labor, and area required to collect and process the scrap are included in the baseline plant. The scrap is gathered, sorted, and either packaged for shipment to a recycling center or disposed of as waste. In the BatPaC model, no credit is taken for the value of the scrap nor are costs charged for shipping the scrap or disposal of waste. The values in Table 9.6 are only for collecting and sorting the scrap. The labor corresponds to five people per shift for the entire scrap handling process.

9.3.7.4 Control Laboratory

The purpose of the control laboratory is to ensure that the raw materials and the electrodes being fabricated meet specifications. Laboratory personnel collect or supervise collection of samples and carry out analyses. The capital costs are for equipment used in the collection, characterization, and analysis of samples. The labor assumes six people per shift to run quality control for the whole plant.

9.4 Adjustment of Costs for Varying Production Volumes

9.4.1 Adjustment of Processing Steps

The labor, capital costs, and area for the processing steps in Table 9.6 were calculated to meet the baseline production rates in Table 9.4. Changes in the production volume (packs per year) or design of the pack will alter the production rates; thereby, altering the labor, capital, and area requirements at each processing step. Changes in production volume will cause all processing steps to change uniformly. Changes to the pack design may change processing steps non-uniformly. For example, some steps depend on the total amount of material (*e.g.*, mixing) while others depend on

the total electrode area being processed (e.g., coating and calendering). Some design changes may only increase the total area without impacting the amount of material (e.g., increasing the pack power while maintaining the same energy). This would cause the mixing cost to remain the same while increasing the coating and calendering.

BatPaC uses a generic approach to estimate the change in cost, labor, and area of each processing step due to changes in production rates. This is accomplished by multiplying the known value (labor, cost, or area) by the ratio of processing rates raised to a power [21]. This is shown as follows:

$$C = C_0 \left(\frac{R}{R_0}\right)^p \tag{9.1}$$

where, C_0 is the known value (labor, cost, or area) in Table 9.6, R_0 is the known production rate from Table 9.4, R is the new production rate, and p is a power factor. A value of 1.0 for p implies that the C values are directly proportional to the processing rate and the value per unit of production is independent of the processing rate. However, p values are typically less than 1.0 due to increases in efficiency with increasing production volume. This causes the value per unit of production to decrease as the production rate increases. The relationships between unit value and processing rate for two-fold and three-fold rate changes are illustrated in Table 9.7. The unit value is determined by dividing the total value (C) by the production rate (R). Thus, for p = 0.7, the total value for twice the baseline rate is 1.62 times the baseline value, but the value per unit is lowered to 1.624/2 or 0.812 times the baseline value per unit.

	Total Process Ratio $C/C_o = (R/R_o)^p$		Prod	lue per Unit uced $(R/R_0)^{p-1}$
Scale Factor, p	$R/R_{\rm o}=2$	$R/R_{\rm o}=3$	$R/R_{\rm o}=2$	$R/R_{\rm o}=3$
0.25	1.19	1.32	0.596	0.439
0.3	1.23	1.39	0.616	0.463
0.4	1.32	1.55	0.660	0.517
0.5	1.41	1.73	0.707	0.577
0.6	1.52	1.93	0.758	0.644
0.7	1.62	2.16	0.812	0.719
0.8	1.74	2.41	0.871	0.803
0.9	1.87	2.69	0.933	0.896
1.0	2.00	3.00	1.000	1.000

Table 9.7. The effect of processing rate (R) on scaled values for various p-factors

The pertinent rates and p factors used in scaling the labor, capital equipment cost, and area for all steps in the manufacturing are provided in Table 9.8. The values were determined from a detailed analysis of each step for plants with 5, 25, and 50 GWh per year capacities. All plants assumed the same baseline pack described in Section 9.3. The p-factors generally range from 0.7 to 0.9 for

labor and 0.9 to 0.95 for capital equipment and plant area. These reflect a maturing industry where changes in production levels are matched by increasing or decreasing the number of identical pieces of equipment purchased, as opposed to procuring larger machines [12]. The *p*-factors imply all plants are employing highly automated, state-of-the-art machines which approach the practical limits of size and efficiency. The *p*-factors for labor are slightly lower than cost and area because relatively smaller additions to the labor crew permit operation of more equipment by overlapping crew responsibilities. No *p*-factor is used for the dry room labor since all dry rooms will require one operator regardless of plant size. Labor *p*-factors are 0.9 for the steps which require more dedicated operators per equipment. Labor *p*-factors are 0.5 for the warehouse and solvent recovery, which account for slight overlaps in responsibilities as plant size decreases. The value of *p* is unlikely to reach 1.0 because the equipment cost includes installation, for which there is some savings even in installing multiple units of the same processing capacity.

Process Step(s)	Pertinent Rate(s)	Labor (hr/yr)	Capital Equipment (\$M)	Plant Area (m ²)
Electrode processing/mixing	active material/yr	0.90	0.90	0.95
Electrode coating	electrode m ² /yr	0.70	0.90	0.95
	solvent kg/m ² /yr	-	0.20	-
Calendering, notching, & vacuum drying	electrode m ² /yr	0.70	0.90	0.95
Electrode slitting	total m ² /yr	0.70	0.90	0.90
Cell stacking	cells/yr	0.90	0.90	0.90
	cell capacity	0.95	0.95	-
Cell stacking, current collector welding, x-ray	cells/yr	0.90	0.90	0.90
inspection, inserting cell in container, electrolyte filling & cell sealing				
Dry room	total m ² /yr or cells/yr	-	0.90	0.90
Formation cycling, testing, and sealing	cells/yr	0.70	0.95	0.95
	cell capacity	0.30	0.30	0.30
Module assembly	modules/yr	0.70	0.95	0.95
Pack assembly and testing	packs/yr	0.70	0.95	0.95
	modules per pack	0.30	0.30	-
Warehouse	total pack energy/yr	0.50	0.95	0.95
Building	total pack energy/yr	-	0.95	-
Solvent recovery	NMP solvent/yr	0.50	0.95	0.95
Rejected cell and scrap recycle	cells/yr	0.70	0.90	0.95
Control laboratory	total pack energy/yr	0.70	0.95	0.95

Table 9.8. Pertinent rates and p-factors used to scale the labor, capital equipment cost, and area at each step in the manufacturing process.

The manufacturing process steps depend on one or two pertinent rates. For instance, electrode processing/mixing depends on the mass of active material processed per year for each electrode (positive or negative). Electrode coating, calendering, notching, and vacuum drying depend on the specific (positive or negative) electrode area processed per year. The cost of the electrode coater has a second dependence on the amount of solvent dried per year to account for necessary changes in the drier design. Electrode slitting depends on the total electrode area (positive and negative).

All other processes in the dry room (*i.e.*, cell stacking, welding, inspection, containing, and filling), formation, and recycling depend on the total cells processed per year (adjusted for yield). The labor and cost of stacking and formation have a second dependence on cell capacity to account for process changes with changing cell size. The formation capital cost is only increased if the cell capacity is greater than 80 Ah to account for higher current cyclers. The formation area also changes with cell size because all formation processes are assumed to maximize the vertical height in the building. Therefore, increases/decreases in cell size must be accommodated with increases/decreases in plant area. The dry room area depends on either the total electrode area or number of cells, whichever produces the largest labor, equipment cost, and area. Module and pack assembly depend on the modules and packs assembled per year, respectively. The labor and cost of pack assembly have a second dependence on the modules. The solvent recovery depends on the amount of NMP solvent evaporated per year. The warehouse, building systems, and control laboratory depend on the total pack energy per year (GWh/yr).

9.4.2 Adjustment for Materials and Purchased Items

The prices of materials and purchased items are also adjusted using the same scaling approach applied to the processing steps (see Section 9.4.1). *P*-factors can be adjusted on the 'Cost Input' worksheet. The raw materials in Table 9.1 (electrodes, solvents, electrolyte, current collectors, etc.) have default *p*-factors of 1.0. All plant sizes are assumed to benefit from the economies of scale of the fully developed raw-materials market. For the purchased items, the cost per mass is also invariant since the material price is tied to the whole market. However, the additional cost per unit (see Table 9.2) has a default *p*-factor of 0.85. Each purchased item is assumed to have a unique design for each pack. Therefore, the manufacturing cost of the item will depend on the demand of the item within a given plant. The cost of each purchased item is scaled based on the amount of that item purchased per year at the plant. For example, the module terminals are scaled based on the number of modules built per year, and the aluminum thermal conductors are scaled based on the number of accepted cells per year. The scaling calculations for all items are provided under the Direct Materials Costs section in the 'Manufacturing Costs' worksheet.

9.5 Plant Investment Costs

9.5.1 Base Case

In this model, the calculated investment costs are defined as those directly related with building and operating the plant (Table 9.9). Other costs that may require investment, such as research and development, are added separately to the unit cost of the battery (see next section). The largest investment cost is for the installed capital equipment. Each cost item for the battery under design is adjusted from the estimate of the baseline plant. The plant cost is calculated assuming \$3,000 per square meter of plant area (\$280/sq. ft), which includes the cost of land and utility hook-ups. These are generic building-related costs (foundation, exterior walls, roof, transformers, wiring, etc.). Building costs unique to a battery plant are included in the building support systems (Section 9.3.7.1). Launch costs include plant start-up, employee training and materials that are spent or recycled in early stages of production, beyond the normal amounts. Launch costs are estimated to be 5% of annual materials costs plus 10% of annual direct labor and variable overhead (see next section). Working capital is needed to cover the costs of payroll, receivables, and the inventories of raw materials, work in progress and finished product. The working capital is estimated to be 15% of the annual variable costs.

Investment Costs	Description	Method of Calculation
Capital Equipment	Equipment costs including installation	Estimates of costs for each processing step at baseline rates adjusted for actual rates.
Building and Land	Building, land, and utility hook-up costs	Multiplier on the area estimates for each processing step at baseline rates adjusted for actual rates.
Launch Costs	Plant start-up, training, out-of-spec product	5% of annual materials cost, 10% of direct labor plus variable overhead.
Working Capital	Cash to meet payroll, receivables, inventories of raw materials and of unfinished and finished product, minus payables	15% of annual variable costs.

Table 9.9. Battery pack manufacturing investment costs.

9.5.2 Modifications for Plant Utilization

The 'Dashboard' worksheet provides the option to modify the plant investment cost by adjusting the plant utilization. Changes in plant utilization can be used to determine the present-day penalty associated with over-build of the plant to target future production volumes. See Figure 3.8 and discussion in Section 3.2.2.3 for information on how to modify the utilization inputs. There are three options for plant utilization. The first, default option assumes 100% utilization of the plant. In this case, the plant investment costs are calculated as described in the previous section. The second option assumes that the entire building is constructed, but equipment is only purchased for the desired production rate. In this case, the capital equipment is scaled based on the desired production rate. However, the area used to calculate the building and land costs is based on the area for the plant operating at 100% utilization. The battery-plant-specific building systems (see Section 9.3.7) are not taken at 100% utilization and are scaled at the production rate for this option. The third option assumes the entire building is constructed and all the equipment are purchased assuming 100% utilization. In this case, both the capital equipment costs and building and land costs are calculated at 100% utilization. The Battery Assembly Costs section in the 'Manufacturing Costs' worksheet is designed to show how the calculation is modified when the utilization option is changed (see Figure 9.3).

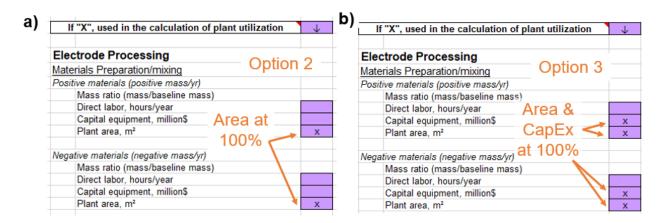


Figure 9.3. Screenshot of section in 'Manufacturing Cost' worksheet showing where to keep track of utilization factors. a) When option 2 is selected, x's indicate the area is calculated at 100% utilization while labor and capital equipment are calculated at the production rate. b) When option 3 is selected, both capital and area are taken at 100% utilization. Under option 1 (not shown), everything scales with production rate (no utilization). Options can be selected in 'Dashboard' and should <u>not</u> be modified in 'Manufacturing Cost' worksheet (note description of purple cells in Section 3.2.1 indicates they should not be modified).

9.6 Unit Costs for Battery Pack

The unit costs of the battery pack are calculated as summarized in Table 9.10. The total cost is the combination of variable costs, fixed expenses, profits, and warranty. Default assumptions for these calculations can be found and modified in the Cost Rates for Manufacturing and Cost Breakdowns section within the 'Cost Inputs' tab.

9.6.1 Variable Costs

The variable costs include the costs of materials, purchased items, direct labor, and variable overhead. The costs of the materials and purchased items are based on the costs discussed in Section 9.2. The costs of the raw materials in the pack are adjusted for the yields of materials and cells in the manufacturing process (see Table 9.5). The costs of the purchased items reported in Section 9.2.2 are adjusted based on production rate as discussed in Section 9.4.2. The entire calculation can be found in the Direct Materials Costs section of the 'Manufacturing Costs' worksheet.

The direct labor is the sum of the labor cost for each step in the process, which are calculated for the baseline plant and adjusted for the rate associated with each process step (see Section 9.4.1). The default labor rate in the 'Cost Input' worksheet is \$25 per hour. Variable overhead is the cost of indirect materials and labor, utilities, and plant maintenance. It is estimated to cost 40% of direct labor costs and 20% of total depreciation.

9.6.2 Fixed Expenses

Fixed expenses include General, Sales, and Administration (GSA), research and development (R&D), and depreciation. The cost of GSA includes the plant office, taxes on income and property, cost of sales, and insurance. It is estimated by the model as 25% of direct overhead and depreciation. The BatPaC model assumes ongoing R&D to continue cost- and performance-competitive battery production. R&D costs are set at 40% of the depreciation expense because the R&D costs should scale with investment in the plant and its equipment. Depreciation expenses provide funding for future investment in this plant, such as the replacement of equipment. The equipment and plant are depreciated at straight-line rates for 10-year life (10% per year) and 20-year life (5% per year), respectively.

	Description	Method of Calculation		
Variable Costs				
Materials and	All materials and purchased	Based on prices of materials, cost		
Purchased Items	items in finished product and	equations for purchased items, and		
	lost in processing	yields		
Direct Labor	Labor costs for operations and	Estimates of costs for each		
	immediate supervision	processing step at baseline rates		
		adjusted for actual rates		
Variable Overhead	Indirect materials, labor, utilities,	40% of direct labor cost plus 20% of		
	plant maintenance	depreciation		
Fixed Expenses				
General, Sales, and	Plant office, taxes on income and	25% of direct labor and variable		
Administration	property, cost of sales and	overhead plus 25% of depreciation		
(GSA)	insurance expenses			
Research and	On-going research needed to	40% of depreciation		
Development	upgrade product and maintain			
	competitive position.			
Depreciation	Provides funds for new	10% of capital equipment cost plus		
	investments to replace those in	5% of plant floor space cost		
	current equipment and plant			
Profit	Return on invested capital after	5% of total investment costs		
	taxes			
Warranty	Funds set aside for reimbursing	5.6% added to price based on		
	customers for battery pack	present worth of projected payments		
	failures			

Table 9.10. Unit cost of battery pack.

9.6.3 **Profits and Warranty**

The profit goal for this type of venture varies with the financial structure of the company, especially regarding long-term debt. For the model, the profit is set to provide a 5% return on the total investment, which is an approximate average for mature manufacturing. In general, the

chosen cost structure and the resulting margin are similar to a Tier 1 supplier in the automotive industry.

A warranty of 5.6% is added to the total cost of the pack. This 5.6% is calculated with respect to the total variable costs, total fixed expenses, and profit. The default value of 5.6% was determined assuming a 10-year warranty with full replacement in the first five years and shared cost of replacement for the last five years. The pack consumer (either vehicle owner or auto manufacturer) would pay an increasing share of the cost from 0% at 5 years to 100% at 10 or more years. The warranty was determined by calculating the present worth of future battery failures assuming a failure rate of 1.0% per year and an 8% discount rate. The warranty only applies to the cost of the pack and would not include any additional services that may be required to replace the pack in the vehicle. It is assumed these would be covered by the automobile manufacturer.

The user has the option to calculate the pack cost with and without profit and warranty using a pull-down menu on the 'Dashboard' worksheet (see Section 3.2.2.3). The default option is to include both profit and warranty. This is listed as the "Cost to Consumer" since it is the price a consumer (either vehicle owner or auto manufacturer) would have to pay to obtain the battery pack from the plant. The other option is listed as the "Cost to Build" since this is the cost the manufacturer must pay to build the pack before marking it up with profits and warranty.

9.6.4 Modifications for Pack Manufacturing Method

BatPaC v5.0 allows the user to select how much of the manufacturing process is done in the plant (see 'Dashboard' worksheet to change). Table 9.11 describes how inputs into the pack unit cost calculation change with each method. The default option (method 1) assumes all components, from cells to modules to packs, are assembled at the manufacturing plant. With this option, the pack cost is calculated using the baseline plant and the method presented above.

The second option (method 2) assumes the cells are purchased from a third party with the modules and packs manufactured in the plant. The materials and purchased items for this method include the module purchased items, the pack purchased items, and the full cost of the manufactured cells. The cell cost includes a markup for profit and warranty from the third party. The cell cost is determined by modifying the unit cost calculation described in Table 9.10. The calculation is modified by excluding the module and pack purchased items from the variable cost and using the multipliers for the "cell only" plant in Table 9.12 to determine the cell manufacturing cost. Table 9.12 provides the multipliers used to convert the baseline plant into a "cell only" or "cell to module" plant. The conversion is done by multiplying the labor, capital, and area for each process step in the baseline plant by its corresponding multiplier. The "cell only" plant includes labor, capital, and area from all cell-building processes, 1/3 of the warehouse values, and all building and support systems except the building-only systems. The capital of the building-only systems in the "cell only" plant is the total cost of the building-only systems in the baseline plant (Section 9.3.7.1) multiplied by the ratio of "cell only" plant area to baseline plant area. Returning to the pack calculation in Table 9.11, for method 2, the direct labor, capital, and plant area are modified to exclude the values in the "cell only" plant.

	<u>Method 1</u> : All In-House	<u>Method 2</u> : Cells from 3 rd Party	<u>Method 3</u> : Modules from 3 rd Party
Materials and Purchased Items	Same as Table 9.10	 Module and pack purchased items Cell costs calculated with method in Table 9.10 using "cell only" plant in Table 9.12 (w/ profits and warranty) 	 Pack purchased items Module costs calculated with method in Table 9.10 using "cell and module" plant in Table 9.12 (w/ profits and warranty)
Direct Labor	Total from Table 9.6	Total excluding labor from "cell only" plant in Table 9.12	Total excluding labor from "cell and module" plant in Table 9.12
Capital Investment	Total from Table 9.6	Total excluding capital from "cell only" plant in Table 9.12	Total excluding capital from "cell and module" plant in Table 9.12
Plant Area	Total from Table 9.6	Total excluding area from "cell only" plant in Table 9.12	Total excluding area from "cell and module" plant in Table 9.12

Table 9.11. Inputs for pack unite cost for each manufacturing method

Table 9.12. Multipliers used to convert baseline plant into a "cell only" or "cell and module" plant.% Area is the ratio of "cell only" or "cell and module" plant area to baseline plant area.

	Cell Only Plant			Cell and Module Plant		
Process	Labor	Capital	Area	Labor	Capital	Area
Mixing, coating, calendaring, notching, vacuum drying, cell assembly, formation	1	1	1	1	1	1
Module assembly	-	-	-	1	1	1
Pack assembly and testing	-	-	-	-	-	-
Warehouse	1/3	1/3	1/3	2/3	2/3	2/3
Building and supporting systems						
Building	-	%Area	-	-	%Area	-
Solvent recovery	1	1	1	1	1	1
Rejected cell and scrap recycle	1	1	1	1	1	1
Control laboratory	1	1	1	1	1	1

The third option (method 3) assumes the cells and modules are purchased from a third party with the packs manufactured in the plant. The materials and purchased items for this method include the pack purchased items and the full cost of the manufactured modules. The module cost includes a markup for profit and warranty from the third party. The module cost is determined by modifying the unit cost calculation described in Table 9.10 using the multipliers for the "cell and module" plant in Table 9.12. The pack purchased items are excluded in the variable costs for this calculation. The "cell and module" plant includes labor, capital, and area from all cell- and module-building processes and 2/3 of the warehouse values. The capital for the building and support

systems is modified using the same method described for the "cell only" plant. The direct labor, capital, and plant area in method 3 are modified to exclude the values in the "cell and module" plant.

9.7 Uncertainties in Price Estimates

In BatPaC, the error bars for the 95% confidence intervals for the price charged to an OEM for the battery pack are automatically calculated at the bottom of the 'Manufacturing Costs' worksheet. The two major categories of uncertainty in the default calculation of battery price are:

- Input costs of materials and capital equipment are estimated to produce a total error of $\pm 10\%$
- Errors associated with the limit on the thicknesses of the electrode coatings and the capacity limit on cells are estimated to cause an additional \pm 5%.

9.8 Cost Breakdown Worksheets

BatPaC assists in showing the relative importance of cost items by providing cost breakdowns from several perspectives as detailed in the 'Cost Breakdown' and 'Detailed Cost Breakdown' worksheets. The worksheets distribute the cost in several ways with 'Detailed Cost Breakdown' providing a more granular view, including percentage of pack breakdowns. The 'Cost Breakdown' worksheet contains default graphs for Battery 1 and Battery 7. The modeler may change the battery selection on the chart by selecting the pie image on the chart and then changing the Excel column for the cost values. Cost distributions are provided in both worksheets for the materials, purchased items, and manufacturing processes. The selected method of manufacturing (Section 9.6.4) will impact how the costs are distributed. For example, method 1 (all manufacturing in house) yields cost distributions for the cell manufacturing steps (*e.g.*, mixing, coating, etc.). If method 2 (cells purchased by third party) is selected, the cell manufacturing costs are included in the purchase items costs, and the cost for these cell manufacturing steps are set to zero in the worksheet.

Both worksheets provide cost breakdowns with the overhead items distributed to basic cost factors. The costs are distributed to the basic cost factors of (1) materials and purchased items, (2) labor, (3) capital equipment, and (4) building and land (calculated from plant area) by means of the factors in Table 9.13. These values are also provided in the 'Cost Input' worksheet. The multipliers are calculated from the percentages used to determine the overhead terms in Table 9.9 and Table 9.10. For example, the full impact of the materials and purchased items on the pack cost is calculated by multiplying the materials and purchased items by the multiplier in Table 9.13. The multiplier accounts for the percentage of the materials and purchased items used to calculate the launch costs (5%), working capital (15%), profits (5%), and warranty (5.6%).

Basic Cost Factor	Multiplier		
Materials and Purchased Items	1.06656		
Direct Labor	1.86648		
Capital Equipment	0.25370		
Building and Land	0.15325		

Table 9.13. Table for converting overhead costs back to their origins

10. RECOVERABLE MATERIALS

The 'Recycle' worksheet calculates the amounts of recoverable materials in the pack at the end of life. It also keeps track of recoverable materials that are rejected from the plant and includes both scrap materials (*i.e.*, from electrode slitting, coating, etc.) and from rejected cells that did not pass quality control tests.

At the top of the worksheet, there are four drop-down menus for selecting the elements to track in the electrodes (see Figure 10.1). Lithium is automatically tracked and is not an option in the dropdown menus. BatPaC uses several tables within the 'Lists' worksheet to determine the amounts of selected elements in the electrodes. The tables provide the molecular weights and elemental composition for all the default electrodes listed in Table 9.1. Additional electrodes can be added to the tables. Interested users should trace the formulas on the 'Recycle' worksheet to determine which tables should be updated. Knowledge of the MATCH, INDEX, and OFFSET functions in Excel is recommended to ensure all tables have been updated properly.

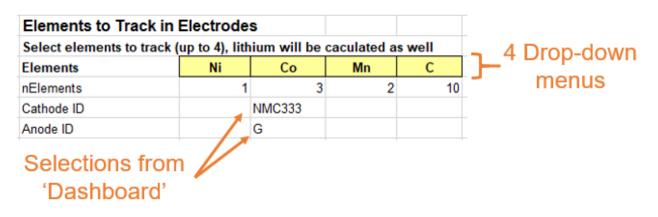


Figure 10.1. Drop-down menus in the 'Recycle' worksheet for selecting which elements to track in the electrodes and electrolyte.

The first set of calculations in the worksheet determine the recoverable materials at the end of pack life (in g/cell, kg/pack and/or kg/kWh) by performing an elemental composition analysis of the main components in the pack. The "Elemental Analysis of Electrodes and Electrolyte" sub-section performs mass balances on the electrode elements selected above. It also calculates the mass of lithium in the electrode, electrolyte, and additives. No other elements from the electrolyte or additives are tracked. Note that selecting carbon, "C," only tracks the carbon in the active materials. It does not include the carbon black conductive additive.

The "Elemental Analysis of Additional Components" sub-section calculates the recoverable mass for the aluminum and copper in the current collectors, terminals, thermal conductors, interconnects, bus bars, and pack jackets. The worksheet distinguishes between aluminum and copper current collectors and cell terminals using the foil properties for the negative and positive electrodes listed in the 'Chem' worksheet. The complete, correct spelling (*i.e.*, aluminum and copper) of the elements in 'Chem' is required for the elemental analysis to work correctly. The aluminum foil in the multilayer cell container is not included in the recoverable mass due to perceived difficulties in recovering it economically. The aluminum in this section also does not include aluminum in the electrode materials (*e.g.*, NCA). The aluminum in the electrodes can be tracked using the drop-down menus in Figure 10.1. The mass in the electrode will appear in the "Elemental Analysis of the Electrodes and Electrolyte" sub-section. The user must add this electrode mass to the other component mass in the "Elemental Analysis of Additional Components" sub-section to get the total amount of aluminum in the pack. The "Elemental Analysis of Additional Components" sub-section also reports the mass of steel and stainless steel in the structural and cooling components in the pack. The mass of the coolant, BMS electronics, polymer pads, pack insulation, pack heaters, and other less valuable materials are not included in this worksheet. The per pack mass of these components can be found separately in the 'Battery Design' worksheet.

The next section of the 'Recycle' worksheet calculates the recoverable materials rejected from the plant floor (in kg/yr) by performing an elemental composition analysis at various stages of the manufacturing process. The section starts with a calculation of the recoverable materials from the scrap expelled during the manufacturing process. The recoverable mass of the electrodes, current collectors, separator, and electrolyte are calculated based on yields from the mixing, coating, slitting, stacking, and filling steps during cell manufacturing in Table 9.5. An elemental breakdown from these components is then conducted for lithium, copper, aluminum, and the four electrode elements selected in Figure 10.1. The aluminum and copper are calculated from the current collectors. To calculate aluminum in the electrode, select "Al" in one of the drop-down menus in Figure 10.1.

A similar analysis is conducted for the materials in the cells that are rejected after testing. These are cells that did not pass quality control and would be recycled instead of shipped to customers. The same component analysis done for the manufacturing scrap is done for these cells. In addition, this analysis includes the recoverable masses of the cell terminals and containers. An elemental analysis is also conducted on the lithium, copper, aluminum, and four electrode elements in these components. The aluminum and copper analysis includes the current collectors and cell terminals. The aluminum in the cell container is excluded from the results, in continuity with the analysis of the recoverable materials at the end of pack life.

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Chemical Sciences and Engineering Division

Argonne National Laboratory 9700 South Cass Avenue, Bldg. #200 Lemont, IL 60439

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