Summary of Updates / Changes in BatPaC 4.0

Contents

BatPac v4.0 – Updates and Changelog

1 Dashboard

1.1 Purpose of 'Dashboard'

The addition of the "Dashboard" worksheet has been added to aid the user and give BatPac a better user interface. Dashboard allows the user to modify the most commonly altered parameters based on user feedback, summarizes the key outputs from a simulation and highlights errors is design choice.

1.2 Resetting the calculator

After changing the design parameters, it is common that the parameters will need to be re-converged and many of the output cells will show a #N/A error. To reset the calculator

If Macros are Enabled: CTRL + SHIFT + R
If Macros are NOT Enabled: Set D56 on 'Dashboard' Worksheet to 0, then change back to 1

If the calculation finds a converged solution, the key outputs will then show up. In addition, the user must have iterative calculations enabled on excel. [File>Options>Formulas: Check the "Enable iterative calculation" box]

1.3 Changing values on 'Dashboard'

DASHBOARD							
Automatic input (Change using Override)		Default input values (may be changed)		Required input by user		Optional override input	
INPUTS							
Chemistry	Current Selection	Choose / Override		**Costs**	Current Selection	Choose / Override	
Electrode Pair	NMC622-G	NMC622-G					
Positive Electrode				Positive Electrode, $/kg			
Positive Active Material Specific Capacity, mAh/g	180			Active material	$20.60		

There are multiple types of cell input on Dashboard, which have been colored for ease of use.

Applied Value Cells – These are the applied values that will be used for your simulation. These cells **should not be changed directly**; if needed, they can be changed elsewhere, depending on their functionality, such as in the tabs named 'Chem', 'Battery Design', 'Cost Input', etc.

Required by User – The users need to select from among the options in the dropdown menu. These include the chemistry, type of battery and battery configuration. For example, choosing between EV, PHEV, microHEV, HEV-HP (other values are not allowed).
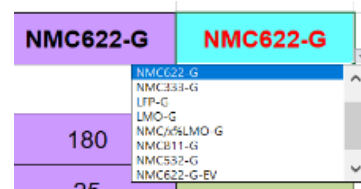
Optional Override Values – These cells allow the user to override a default value.

There are other values that can be changed depending on the user's needs, and this is preferably done with an understanding of the interactions of the many cells and worksheets in this file, along with the full user manual.

Default Inputs (may be changed) – These cells contain defaults that are generally applicable, but the user may alter directly in this cell. For example, 'Battery Design' Row-27, Row-32, etc.

INPUTS							
Chemistry	Current Selection	Choose / Override		**Costs**	Current Selection	Choose / Override	
Electrode Pair	NMC622-G	NMC622-G					
Positive Electrode				Positive Electrode, $/kg			
Positive Active Material Specific Capacity, mAh/g	180			Active material	$20.60		
Void Volume Fraction, %	25			Carbon	$6.60		
Positive Current Collector Thickness, μm	15			Binder	$9.50		
Maximum Cathode Thickness, μm	120			Solvent (NMP)	$3.10		
Negative Electrode				Negative electrode material, $/kg			
Negative Active Material Specific Capacity, mAh/g	360			Active Material	$12.50		
N/P Capacity Ratio after Formation	1.15			Carbon Black	$6.60		
Void Volume Fraction, %	25			Binder	$10.00		
Negative Current Collector Thickness, μm	10			Solvent (Water)	$0.00		
Separator Thickness, μm	15			Al Foil, $/m2	$0.30		
				Cu Foil, $/m2	$1.20		
Maximum charging current density, mA/cm^2	9.00			Separator, $/m^2	$1.10		
				Electrolyte, $/L	$15.00		

Figure 1: The Chemistry Input section on Dashboard. They show both the applied value used for calculations along with the corresponding override cells.

In the chemistry section, the most important selection that should be made is the selection of the chemistry couple. Choosing one of these will change the default values that are shown in the Chemistry section on 'Dashboard'. The default couples that we include in BatPaC 4.0 are the following.

- NCA-G
- NMC622-G
- NMC333-G
- LFP-G
- LMO-G
- NMC532/50%/LMO-G
- NMC811-G
- NMC532-G
- LMO-LTO

Directions for adding a new, user-defined chemistry couple are provided in section 2.3 of this document. Also, editing chemistry parameters other than those highlighted here can be done on the 'Chem' tab. For both the anode and cathode, the capacity (mAh/g), the volume void fraction, and the thickness of the current collector can be varied independently. In addition, the maximum allowable cathode thickness can be altered along with the N to P ratio after formation, separator thickness, and the max allowable current density. Finally, the costs of materials can be directly changed on 'Dashboard' as well. It should be noted that the values for the void fractions and negative specific area may change depending on the power/energy needs of the vehicles.

1.4 Battery Design Inputs

This worksheet is for selecting the type of battery and the key parameters and requirements for the pack.

Battery Design	Current Selection	Choose / Override			Available battery energy, % of total (EV)	85		Add Default # of Cells/Modules for given system
Vehicle type	EV	EV						
Coolant Type	EG-W	EG-W						
Calculate Fast Charging?	No	No						
Fast Chg for EV only								
	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7	
Target battery pack power, kW	180	220	260	300	120	400	360	
Number of cells per module	12	12	12	12	14	12	18	
Number of cells in parallel	1	1	1	1	1	1	2	
Number of modules in row	5	5	5	5	5	5	6	
Number of rows of modules per pack	4	4	4	4	2	4	4	
Number of modules in parallel	1	1	1	1	1	1	1	
Number of battery systems manufactured per year	100,000	100,000	100,000	100,000	100,000	100,000	100,000	
Energy requirement of vehicle on UDDS cycle, Wh/mile	250	250	250	250	200	250	350	
Select capacity, energy, or vehicle range, but only one.								
Pack capacity (Ah)								
Pack energy (kWh)								
Vehicle range (miles)	180	220	260	300	100	270	300	
EV Charging								
Time to Recharge from 15% to 75% SOC (ΔSOC=60%), min	10	15	20	25	30	35	40	
Optional Cathode Thickness Override								

Figure 2: Example section of the battery design input section on 'Dashboard'. The choice of vehicle type, and other key properties of the battery are chosen in this section. Also, this section contains a button to add a selection of default Cells/Modules for a given system.

Here we can change design parameters not related to the chemistry couple. Detailed definitions of these terms can be found in the full manual.

- **Vehicle Type:** EV, HEV-HP, microHEV, PHEV (this will change default values for many parameters, such as *Available Battery Energy, % of Total*)

- **Coolant Type:** EG-W (50%/50% Ethylene Glycol/water), CA (Cabin Air), CoolA (Cooled Air).

- **Calculate Fast Charging (Only available for EV batteries): CTRL + SHIFT + F** Toggling between Yes and No turns the fast charging calculations on/off. The toggle is available only for EV batteries. In addition, the Macro is only active when EV has been selected.

  Fast charging refers to charging rates greater than 1C, and therefore there must be values in the **Time to Recharge from 15% - 60%.** To toggle fast charge and to ensure that the values have converged if Macros are not enabled;

- Set D56 on the 'Dashboard' Worksheet to 0, then change back to 1
- Set E30 (fast charge cell) to "No", then switch to "Yes"

While other parameters will change, when "Yes" has been selected, the "Extra cost of meeting fast charge requirements" will now show a value instead of #N/A.

- **Available battery energy (% of total):** This cell is selected based on the vehicle type, (60% for HEV-HP, 70% for PHEV, 85% for EV and 25% for microHEV). However, these values can be overridden.
- **Add Default # of Cells/Modules for Given System (Macro Button):** This macro will, based on the selected battery type, fill out values that are acceptable for the default chemistries in this document. If the macro is activated in succession, the program will cycle through several configurations based on the vehicle type. The user can then make any modifications to the values that work best. An example of one such data set is shown for an EV battery.

	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7
Target battery pack power, kW	180	220	260	300	120	400	360
Number of cells per module	12	12	12	12	14	12	18
Number of cells in parallel	1	1	1	1	1	1	2
Number of modules in row	5	5	5	5	5	5	6
Number of rows of modules per pack	4	4	4	4	2	4	4
Number of modules in parallel	1	1	1	1	1	1	1
Number of packs manufactured per year	100,000	100,000	100,000	100,000	100,000	100,000	100,000
Energy requirement for a UDDS cycle, Wh/mile	250	250	250	250	200	250	350
Select capacity, energy, or vehicle range, but only one.							
Pack capacity (Ah)							
Pack energy (kWh)							
Vehicle range (miles)	180	220	260	300	100	270	300

Figure 3: Example of battery configuration that can be set via the *Add Default # of Cells/Modules* macro.

1.5   Results

This section contains the reset cell for the iterative calculator. If the calculator could not find a converged value, the values in this section will show a N/A or NUM error. This may occur when one switches the vehicle type or chemistry couple. Thus, the calculation must be re-initiated and reset. This can be done with the following.

If Macros are Enabled: CTRL + SHIFT + R
If Macros are NOT Enabled: Set D56 on 'Dashboard' to 0, then change back to 1.

If errors persist after this, the current battery parameters can not be converged. This could be due to the choice of a parameter not allowing convergence in the given constraints. For example, if one were to say the capacity of the cathode to 2 mAh/g, no viable battery configuration will be achievable given the other constraints.

The following block provides importance notifications about parameter choice and performance. In many cases, the value may show that a specific requirement has not been meet, but will still calculate a cost.

Results							
Calculation and Validation							
Restart (0/1)	1	OR	**CTRL+ SHIFT + R if Macro Enabled to Reconverge Calculation**				
Setting 0 will initial the calculation, and setting back to 1 will allow the workbook to itterativly find the thickness of the cathode							
	Battery 1	**Battery 2**	**Battery 3**	**Battery 4**	**Battery 5**	**Battery 6**	**Battery 7**
Power-to-energy ratio	Acceptable	Acceptable	Acceptable	Acceptable	Acceptable	Acceptable	Acceptable
Adequacy of Cooling	Excellent	Excellent	Excellent	Excellent	Excellent	Excellent	Excellent
Cathode Thickness Limited By	Li Deposition	Li Deposition	Li Deposition	Li Deposition	Discharge	Discharge	Li Deposition
Capacity Requirements Met?	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Actual Capacity							
Chosen Time to Recharge Met? (Charging 60% SOC (15 to 75% SOC, 71% useable), min **----> only for EV**							
Actual Time to Recharge (min)							

Figure 4: Summary of validation table, which highlights convergence issues.

Each term means the following and will show the following values.

- **Power-to-Energy Ratio:** This cell will show a "Acceptable" if the computed cathode and anode thickness is between the coating limits. If the corresponding cell instead reads "Too High!", then the calculated required thickness of either electrode is below the coating limit/minimum electrode thickness.
- **Adequacy of Cooling:** Based on the maximum temperature at center of hottest cells, this cell will show either "Excellent", "Good", "Fair" and "Poor". A temperature of less than 35ºC will give an "Excellent" rating. Likewise, 35 – 40ºC is "Good", 40 – 45ºC is "Fair" and greater than 45ºC is "Poor".

- **Cathode Thickness Limited By:** The cathode thickness can be limited by either "Charger", "Discharge", or "Li deposition".
- **Capacity Requirements Met?:** Will show either Yes or No, based on whether the designed pack capacity is met based on design parameters. If not, the actual capacity will be shown in the cell below.
- **Chosen Time to Recharge Met?** Answers if the selected choice ('Dashboard' Row 46) for time to recharge from 15% to 75% SOC min, can be met. This row is only enabled if both EV has been selected as the vehicle type and if fast charging calculations are enabled.

The information at the bottom of this sheet summarizes some of the key results, as shown.

System	Table of Results and Graphable Data					Minimum Value Between batteries 1-7	
						Maximum Value Between Batteries 1-7	
System	EV Vehicle with NMC622-G Electrodes	Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6	Battery 7
1	Battery system total energy storage, kWh	52.94	64.71	76.47	88.24	23.53	79.41	124
2	Required battery system power, kW	180	220	260	300	120	400	360
3	Pack power to energy ratio	3.40	3.40	3.40	3.40	5.10	5.04	2.91
4	Pack charging time for 80% ΔSOC, min	56.00	56.00	56.00	56.00	56.00	56.00	56.00
5	Cell capacity inadequate if X							
6	Positive electrode thickness, μm	120	120	120	120	120	120	120
7	Positive electrode areal capacity, mAh/cm²	7.08	7.08	7.08	7.08	7.08	7.08	7.08
8	Negative electrode areal capacity, mAh/cm²	7.98	7.98	7.98	7.98	7.98	7.98	7.98
9	Cell capacity, Ah	59.49	72.72	85.96	99.19	45.31	89.26	77.12
10	Module mass, kg	9.78	11.80	13.82	15.83	8.87	14.38	18.77
11	Number of cells per pack	240	240	240	240	140	240	432
12	Nominal battery system voltage (OCV at 50% SOC), V	900	900	900	900	525	900	810
13	Cost of pack to OEM, $	$7,269	$8,156	$9,075	$9,931	$4,129	$9,350	$13,253
14	Pack total mass, kg	255	299	343	386	125	356	554
15	Pack volume, L	149	171	191	211	77.77	196	304
16	Total cost of cells, $/kWh	$95	$90	$87	$84	$112	$86	$83
17	Cost of cells, $/kWhUse	$112	$106	$102	$99	$131	$101	$97
18	Extra cost of meeting fast charging requirements, $	NA	NA	NA	NA	NA	NA	NA
19	Production volume, packs per year	100,000	100,000	100,000	100,000	100,000	100,000	100,000
20	Pack to cell cost ratio	1.44	1.40	1.36	1.34	1.57	1.37	1.30
21	Cell specific energy, Wh/kg	292	295	296	298	289	297	295
22	Cell energy density, Wh/L	718	730	738	745	702	740	733

Figure 5: Example summary of results table. These can be plotted against each other as shown in the following figure

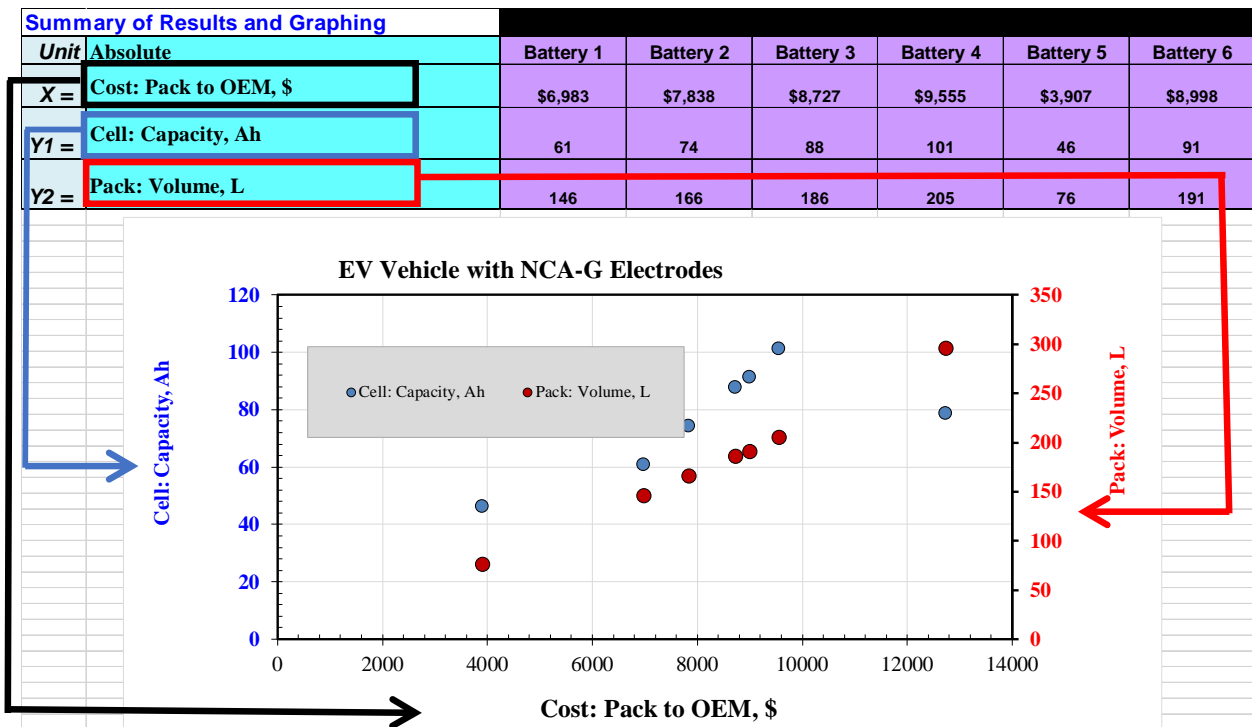| Summary of Results and Graphing							
Unit	Absolute		Battery 1	Battery 2	Battery 3	Battery 4	Battery 5	Battery 6
X =	Cost: Pack to OEM, $		$6,983	$7,838	$8,727	$9,555	$3,907	$8,998
Y1 =	Cell: Capacity, Ah		61	74	88	101	46	91
Y2 =	Pack: Volume, L		146	166	186	205	76	191

Figure 6: Plotting across the seven batteries and toggling the axis with the X, Y1, and Y2. These are gathered from the summary of results table, as highlighted in Figure 4

2 Updated 'Chem' Worksheet

2.1 Overview of changes to 'Chem'

Many changes were made to the 'Chem' from the previous version. This tab contains parameters that are dependent on the chemistry couple that was chosen, but also houses a data base of all the provided chemistry couples that are available along with the user. The user may also add a couple in this database.

Selecting a new chemistry is done by toggling 'Dashboard'!E9. With the selection of a couple, the values in columns C:D on 'Chem' will populate. This can be seen below.

	B	C	D	E	F
Selected Chemistry - Choose a Chemistry in Dashboard					
System ID		NMC622-G	ID #	25	
Description					
Property		Applied Value	BatPaC Default	Override	Notes
Couple Name		Li1.05(Ni0.6Mn0.2Co0.2)0.95O2 / Graphite			
Positive electrode active material		NMC622	NMC622		
Positive electrode active material molecular weight		94.4	94.39		
Positive electrode active material capacity, mAh/g:		180.0	180.00		
Positive electrode composition, Weight %					
Positive electrode active material weight %		96.0	96.0		
Positive electrode carbon addtive weight %		2.0	2.0		
Positive electrode binder weight %		2.0	2.0		
Binder solvent for positive electrode		NMP	NMP		
Void, vol% of positive electrode		25.0	25.00		
Material Density, g/cm³					
Positive electrode active material density, g/cm³		4.65	4.65		
Positive electrode carbon additive density, g/cm³		1.83	1.83		
Positive electrode binder density, g/cm³		1.77	1.77		
Maximum thickness limit for positive electrode, mm		120	120		
Minimum thickness limit for positive electrode, mm		15.0	15		
Positive electrode specific particle area "a", cm²/cm³		80,000	80,000		
Positive foil material		Aluminum	Aluminum		
Positive foil thickness, μm		15	15		
Add 5% silicon to negative electrode?		No	No		
Negative electrode active		G	G		
N/P capacity ratio after formation		1.15	1.15		
Negative electrode active material capacity, mAh/g:		360	360		
Negative electrode composition, Weight %					
Negative electrode active weight %		98.0	98.0		
Negative electrode carbon addtive weight %		0.0	0.0		
Negative electrode binder weight %		2.0	2.0		

Figure 7: The selected chemistry section on 'Chem'.

2.2 Adding silicon (5wt%) to graphite electrode.

Toggling D28 on 'Chem' will allow the user to add 5% silicon to a couple where the anode is graphite (denoted as G). This cell will ignore any other user anodes if not graphite. This will change the anode capacity, electrode ASI, open circuit voltages and the anode material cost.

2.3 Adding a user-defined chemistry couple

The addition of a new chemistry couple is rather simple. One can override a couple that is already supplied in the document. However, if the user copies an existing chemistry couple (4 columns) in the 'Chem' tab and then copies them over to the right (number of columns in between does not matter), then this new chemistry couple will appear and be selectable from dashboard by uniquely renaming the new couple. The user may edit any entries in this couple.

Figure 8: Example of how to copy an existing electrode chemistry couple to create a user-defined couple.

3 New Features

3.1 'Dashboard'

- A 'Dashboard' worksheet has been added, where some of the more common input parameters can be reviewed (and changed if needed) by the user. Key results are also displayed and their sensitivity to another parameter can be plotted. The items seen in 'Dashboard' Rows 127 and below were selected from the sheet 'Summary of Results'. These results are also visible in a floating table in 'Battery Design' and 'Dashboard'.

3.2 'Summary of Results'

- The 'Summary of Results' sheet contains a collection of calculated values. Any of the items in this sheet can be displayed in 'Dashboard' by placing a number in Column A. The number sequence determines their order in 'Dashboard'. This table will plot up to 100 user-selected values, all of which can be plotted on the summary graph on 'Dashboard'.
- The bottom section of 'Summary or Results' includes a Summary of Input/Output, where the listed parameters are selecting by placing an "X" in the column A of the sheets ('Chem', 'Battery Design', 'EV Charging', 'USABC Data', 'Manufacturing Cost Calculations', 'Prices of Cells and Modules', 'Cost Breakdown', 'Recycle', 'Thermal', 'BMU'). This can also summarize single value constants, such as those on the 'Chem', though these can not be plotted (as they are a single value).

3.3 'Lists'

This worksheet has been added as a repository of lookup tables that are needed based on the chemistry, battery design and the vehicle type. The average user does not need to go through this sheet, as this is just to keep other sheets cleaner.

- List of constants that are found in the workbook, along with a Macro that can be used to add more values.
- A summary of the chemistry couples that are found within the document (automatically updates when the user adds or changes a couple).
- Location where the molecular weight calculations are performed.
- Location for the toggles for Vehicle type, coolant type, Fast Charge? And Available Battery Energy.
- The location of the cells where the camera view is taken for the movable table.
- The series of tables containing the default values for the battery design section in 'Dashboard' (these are used by the Macro on 'Dashboard').

3.4 Updates to other sheets

- Simplified the ability to add user-defined chemistry couples by updating how they are called.
- Added the 'BMU' tab to calculate the mass, volume and cost of the Battery Management Unit.
- Removed the constraint for sustained discharge in calculating the area (thickness) of the electrodes in 'Battery Design'.
- The fast charging constraint, in determining the electrode area and thickness, is considered only for the design of EVs.
- Many of the values in 'Chem' have been updated to reflect recent practice observed in commercial cells.
- Changed the mole fraction of all NMC type materials to have a mole fraction of 1.05 in the material.
- The values for 'Battery Design' Rows 84-85 are now drawn from 'Chem'56 and 'Chem'64, respectively.
- The density of all polymers, except for PET, are assumed to be 0.9, close to the value for both PE and PP. Depending on the exact polydispersity index (PDI) of the polymer used, the exact value of the density changes.
- The addition of named ranges for constants, such as material densities, have been added. This is to provide definitions of the constants that are being used in the cells.
- The 'EV Charging' sheet has been updated.
- A new 'Recycle' sheet has been added to report the inventory of recyclable materials in the pack.
- Units and qualifying statements have been added to many line items in column B across all tabs to help guide the user.
- Selecting the *Vehicle range* is no longer allowable for microHEV and HEV-HP type vehicles.
- Material properties have been added or updated in 'Chem'.
- The electrode thickness calculations in 'Battery Design' (Rows 97-112) have been updated and includes the limitations imposed due to fast charging for EV batteries. This includes a Yes/No toggle on the 'Dashboard' page.
- Added cell level costs in 'Battery Design' Rows 223-225.
- Cathode active material demand and Plant capacity are added in 'Summary of Results' Rows 111-112.
- The fast charging time constraints for each design are reported in 'USABC Data' Rows 13-14.
- The diagram in 'Plant Schematic' has been updated.
- Hourly worker wage has been updated from 18$/hour to 25$/hour ('Cost Input' K39), based on both trends in the last 4 years of chemical operator data and the 2024 jobs forecast from the Bureau of Labor Statistics.
- A movable results table is now available in 'Dashboard' and 'Battery Design', to monitor the effect of parameters on key results (this table can be copied and pasted to other sheets if needed).