BatPaC Model Development

Project Name: Core BatPaC Development and Implementation

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Project ID: ES228

Overview

Timeline

- Start: 2012
- End: 2016

Barriers

Development of a PHEV and EV batteries that meet or exceed DOE/USABC goals

A. Cost

C. Performance

Budget

- FY14: 575K
- FY15: 575K

Collaboration/Interaction

- U.S. Environmental Protection Agency
- B&W MEGTEC, GM, LGChem, PPG
- 3M, Amprius, Envia

Relevance

- This modeling effort supports projects through the development and utilization of efficient simulation, analysis, and design tools for advanced lithium ion battery technologies.
- This project provides assessment of the technology developments through projections of cost and performance at the pack level
- The EPA uses BatPaC to predict the cost of battery technologies for their 2017-2025 rule making
    - Argonne updates BatPaC with cost inputs, modification of constraints, allow variable factory utilization, etc.
- BatPaC is the only peer-reviewed LIB design and cost model available in the public domain

Objectives and Approach

Objective: Develop and utilize efficient simulation and design tools for Li-ion batteries to predict:

- Precise overall and component mass and dimensions
- Cost and performance characteristics
- Battery pack values from bench-scale results

Approach: Design a battery based on power and energy requirements for a specific cell chemistry, feeding into a cost calculation that accounts for materials and processes required

- Optimized battery design to meet the specifications
- Cost based on a described manufacturing process

Approach: Reduce uncertainty in model predictions

- Update the default material and processing costs
- Develop higher fidelity models of the physical and electrochemical phenomenon, and manufacturing flow path (quantify energy needs)
- Validate results with OEMS, manufacturers, component developers

BatPaC designs the battery and calculates its mass, volume, materials, heat transfer needs, and cost

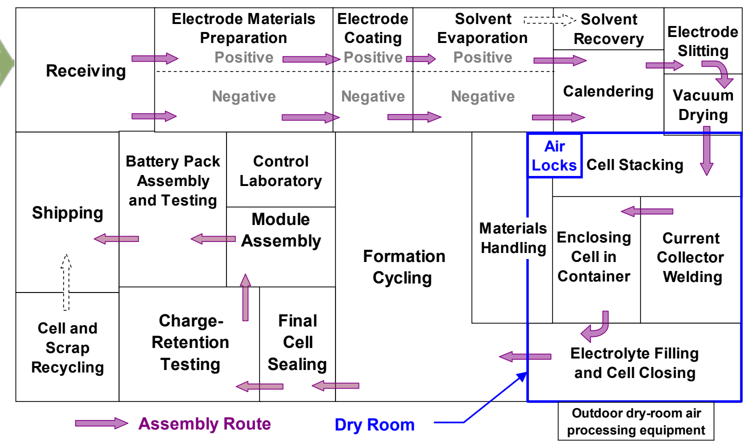
Iterate Over Governing Eqs. & Key Design Constraints

- Cell, module, & pack format
- Maximum electrode thickness
- Fraction of OCV at rated power

Battery Pack Components

- Volume
- Mass
- Materials
- Heat generation

$$Process\ cost = Baseline\ cost \cdot \left(\frac{Processing\ rate}{Baseline\ processing\ rate}\right)^p$$



- **Pack specifications**
  - Power and energy (range)
  - Number of cells
- **Cell Chemistry**
  - Area-specific impedance (ASI)
  - Reversible capacity C/3
  - OCV as function of SOC
  - Physical properties

Governing Equations

$$E = N \cdot C \cdot \left(U_E - \frac{C}{3} \frac{ASI_E}{A} \right)$$

$$L = \frac{C}{Q \cdot \rho \cdot \varepsilon \cdot A}$$

$$I = \frac{P}{A \cdot N \cdot U_P \left[\frac{V}{U}\right]}$$

$$A = \frac{ASI_P \cdot P}{N \cdot (U_P)^2 \left[\frac{V}{U}\right]\left(1 - \left[\frac{V}{U}\right]\right)}$$

$$ASI = \frac{\alpha + f(I)}{L} + \beta$$

Total Cost to OEM

- Materials & purchased items
- Individual process steps
- Overhead, depreciation, etc.
- Warranty

P.A. Nelson, K.G. Gallagher, I. Bloom, D.W. Dees, Modeling the Performance and Cost of Lithium-ion Batteries for Electric Vehicles, second ed., Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL USA, 2011. ANL-12/55.

Technical Accomplishments and Progress
A new version (3B) of BatPaC has been released

Milestone: Release new BatPaC version, Q2-FY15.

- Status: Completed

- Added a table of results corresponding to USABC format
  - Updated thermal management calculations
  - Provided rapid gas discharge pathway from modules
  - Reconfigured to enable cell cost calculations
- Updated costs of LFP cathode, current collectors, separator, and electrolyte
- Expect to release a newer version later this year
  - Developing understanding of uncertainties
    - Electrode thickness limitation, cathode material cost, etc.

The results have been tabulated to USABC format

Data to Meet USABC Guidelines				
	Parameters in BatPaC			
	Number of cells per battery system	96		
	Number of modules per battery system	4		
	Number of packs per battery system	1		
	Battery system total energy storage, kWh	4.0		
	Battery power, kW	60		
	Nominal battery system voltage (OCV at 50% SOC),V	380		
	Battery capacity, Ah	10.6		
	Maximum current at full power, A	204		
	Cooling system power requirements, W	1094		
USABC Parameters			**Battery 1**	
Subsystem	**Contents**	**Mass, kg**	**Volume, l**	**Cost, $**
Cells		28.1	12.1	1,237.18
Additions at Module Level				
Module hardware	Housing, thermal conductors, terminals	2.8	1.9	154.96
CSC	Cell-to-cell balancing, sensors, and low-voltage wiring	0.8		250.18
Addition at Pack Level				
Pack hardware	Tray, compression structure, housing	4.5		122.74
Thermal management system	Heaters, coolant	4.1		140.00
High voltage wiring	Bussing between modules, and pack terminals	1.1		41.00
BMU & Disconnects	Battery management, module balancing, 2-way comm	4.0		395.00
Total Battery Pack(s)		45.2	30.7	2,341.06
Exterior Cooling System	Additions to AC for thermal management	7.0	2.8	120.00
Total Including Cooling System		52.2	33.5	2,461.06
Cell Fractions of Total Pack		0.62	0.40	0.53

Technical Accomplishment and Progress
Analysis of a flex plant enabled an understanding of the cost learning curve

- A flex plant produces multiple types of batteries either in parallel lines or by periodically reconfiguring the equipment
- Analysis showed that a uniform electrode size (length and width) can be used to assemble different types of batteries
  - Adjust electrode layer thickness, cell thickness, series/parallel, module size, …
- The power to energy ratio automatically determines the electrode thickness

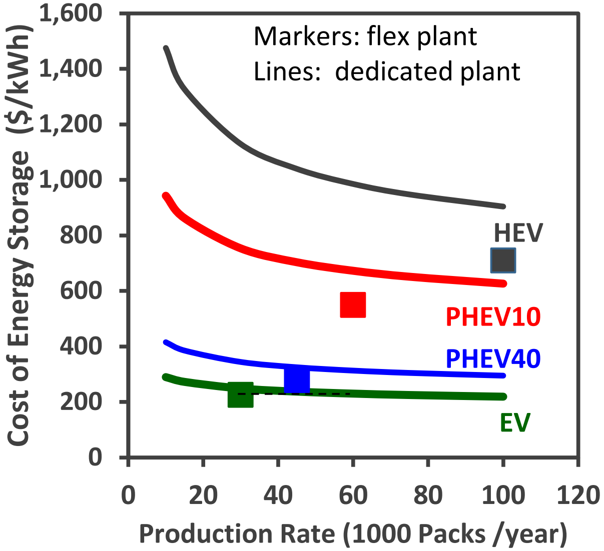
Vehicle type	HEV	PHEV10	PHEV40	EV
Vehicle range (miles)*	1.25	10	40	150
Target total energy (kWh_{Total})*	1.0	2.86	11.4	35.3
Useable battery energy (% of total)	25	70	70	85
Target power for 10 seconds (kW)	35	65	130	150
Annual production volume (packs/year)	100,000	60,000	45,000	30,000

*based on 200 Wh/mile

J of Power Sources, Volume 283, 1 June 2015, Pages 506–516
http://dx.doi.org/10.1016/j.jpowsour.2015.02.142

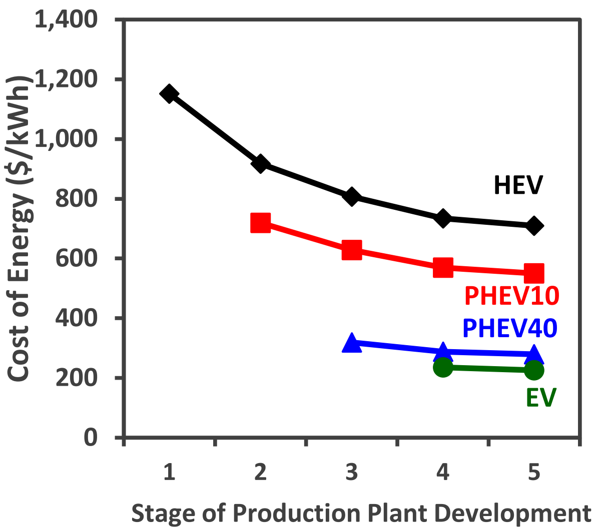
The flex plant lowers the cost of all batteries, with the most impact on the smaller HEV batteries

- Compared to a dedicated plant at a given production capacity, a flex plant can save
  - 9% for a EV battery, 21% for a HEV battery
- 30K EV batteries in a (235K) flex plant have the same unit cost as 60K EV batteries in a dedicated plant



- A flex plant can be designed to increase production rates matching market demands

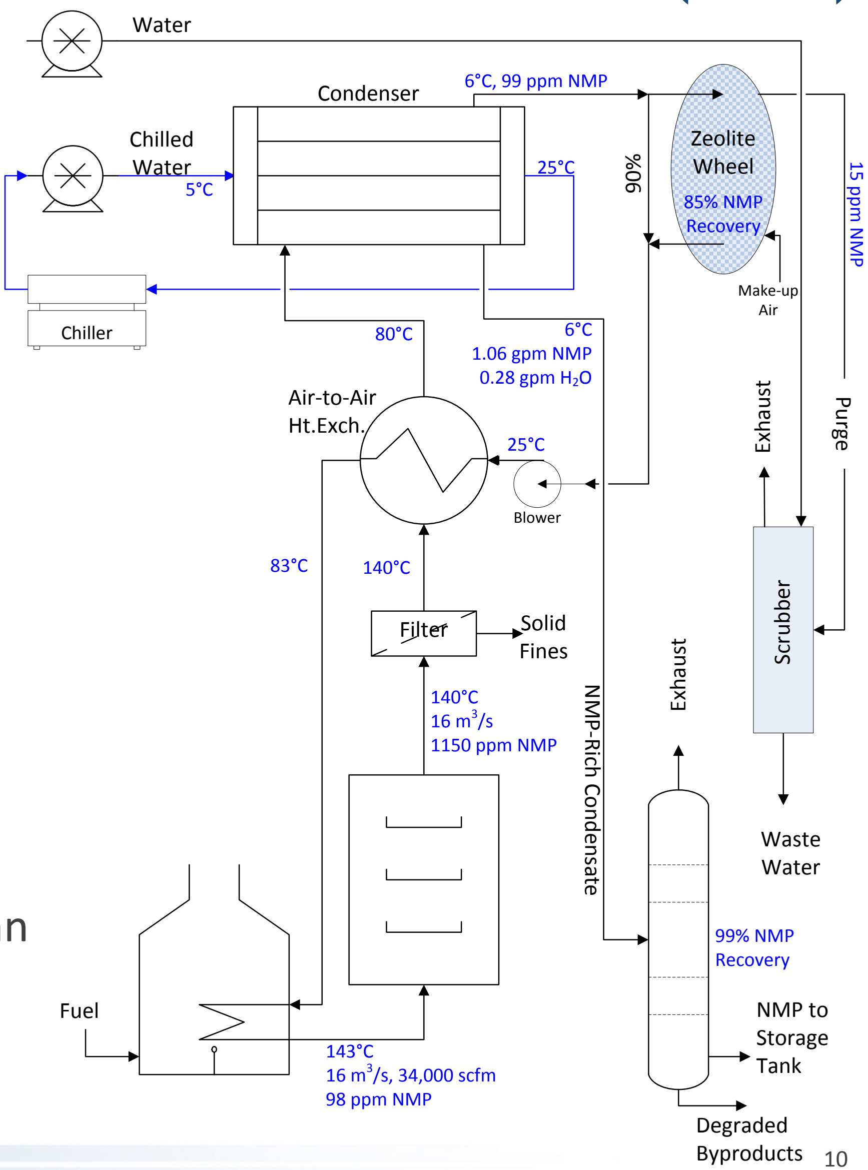
Stage of Development	Pack Production Volume (thousands per year)					Plant Utilization (%)
	HEV	PHEV10	PHEV40	EV	Flex Plant	
1	60				60	60
2	70	42			112	70
3	80	48	36		164	80
4	90	54	41	27	212	90
5	100	60	45	30	235	100



Technical Accomplishments and Progress
Process for the recovery of the cathode solvent (NMP)

Ongoing discussions on using aqueous solvents or eliminating solvents in electrode coatings

- Understand and quantify the impact of these changes in the plant



Assumptions

- A large volume of air is needed to limit NMP concentrations to ~1200 ppmv, well below the lower explosive limit of ~1%
- 10% of the dryer air is purged to limit gas buildup
- 85% of the NMP and water are recovered in zeolite wheel
- 99% NMP recovered in the distillation column

The energy demand for the NMP drying and recovery process is quite significant

<u>Assumptions</u>

- Plant produces 100K packs of 4 kWh, 10.5 Ah PHEV batteries per year
- 10.1 million cells per year
- NMP required: 1.8 million kg/year
- 300 days per year, 6 year plant life

<u>Preliminary Results</u>

- 98.9% NMP is recovered
- 8.5 kWh/kg-NMP
- Cost calculations indicate
  - Installed capital cost = $2.6 M
  - Cost of NMP recovery
    - $1.40/kg$_{NMP}$
    - $24/pack

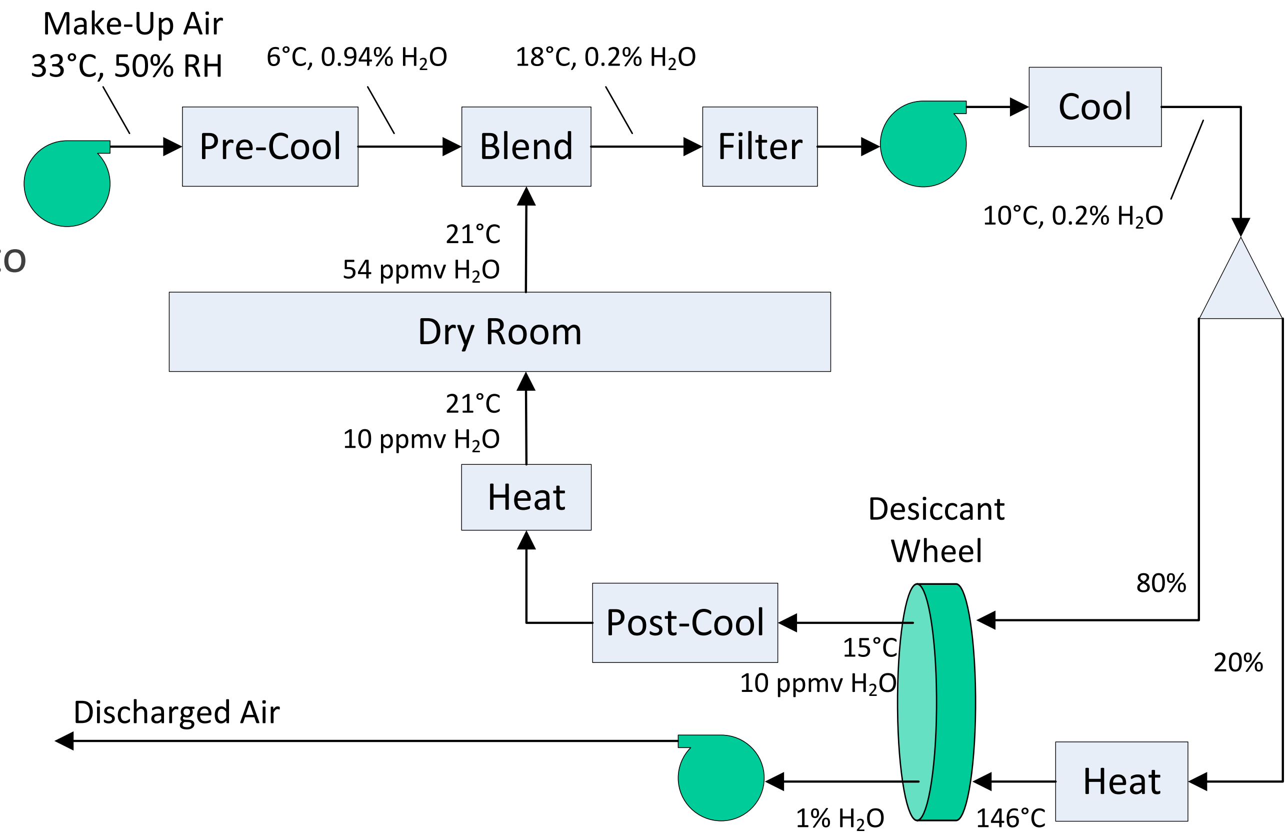
	Capacity	Heat Load, kW
Scrubber		
Filter		
Zeolite	2-h cycle	49 kW
Air Heating Furnace	1,300 kW	1,300 kW
NMP Storage Tank	350 m^3	
Condenser	2,600 m^2	1,795 kW
Distillation Column		173 kW
Air-to-Air Heat Exchanger	3,900 m^2	1,170 kW
Chiller	170 tons	598 kW
Blower	19 m^3/s	
Dryer	56 kW	56 kW
Annual Energy Required		**15 GWh/yr**

*20April2015

Technical Accomplishment and Progress
The Dry Room energy demand

<u>Assumptions</u>

- 4000-m^2 x 5-m high
- Air Turnover: 6 per hr
- Combination of cooling to 6°C and a desiccant to remove moisture
- Dry room exit moisture content < 100 ppmv
- 20% air discharged
- Moisture entry into Dry Room via
  - Personnel
  - Negative electrode
  - Air lock doors



Maintaining the Dry Room is an energy intensive step in the battery manufacturing plant

Assumptions

- Plant produces 100K packs of 4 kWh, 10.5 Ah PHEV batteries
- 300 days per year, 6 year plant life
- 30 people working 24 hours in the room each day
- Doors opened 120 times per day
- Negative electrodes contain 0.05% H_2O

Preliminary Results

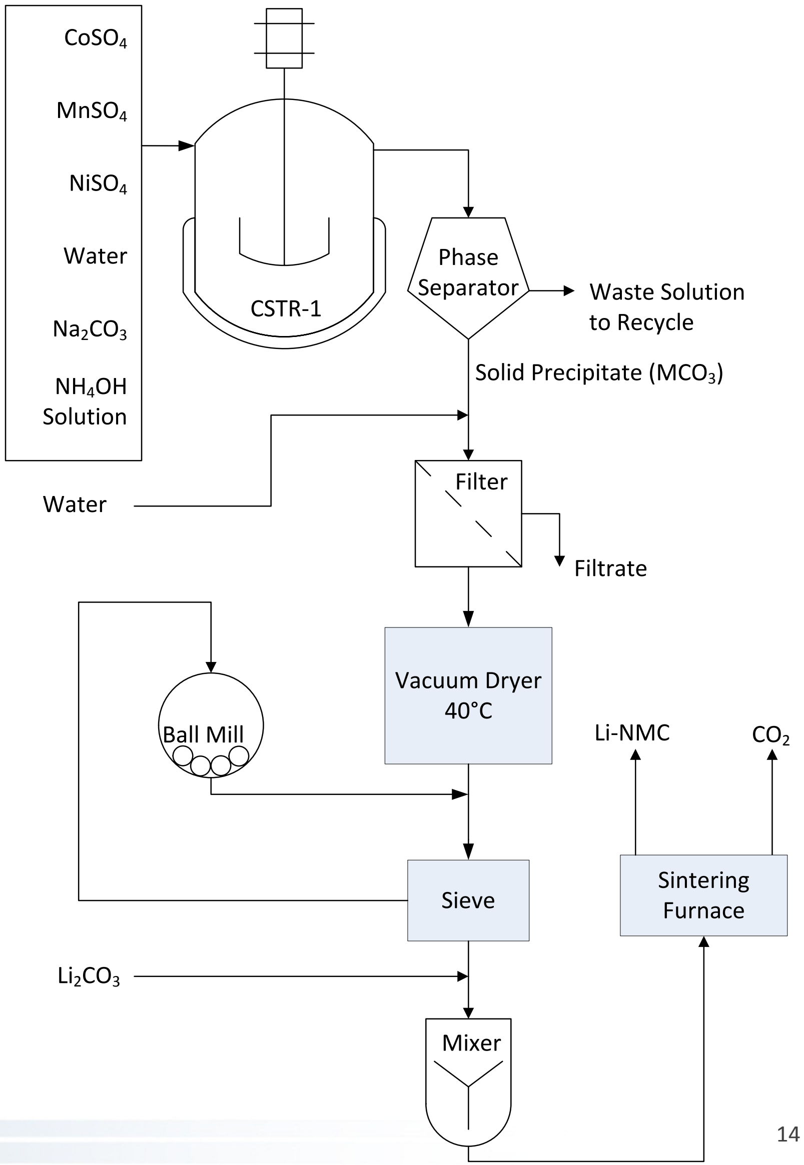
- Dry room exit gas contains 54 ppm H_2O
- Cost calculations indicate
  - Installed capital cost = $2.5 M
  - Cost of Dry Room adds $27/pack

Pre-Cool to 6°C, kW	505
Cool to 10°C, kW	976
Heat to Dry Room T (21°C), kW	234
Desiccant Regen Heat, kW	1372
Annual Energy Required , GWh/yr	**17.8**
Blower Power, kW	7
Total Refrigeration Power, kW	423
Cost of Electricity (8¢/kWh), $/year	$301K
Total Thermal (NG) Energy, kW	1,606
Cost of Natural Gas (2¢/kWh), $/year	$281K

Technical Accomplishment and Progress
Process for production of NMCxxx by coprecipitation

- NMC333 production = 4,000 kg/day
- 320 days operation per year

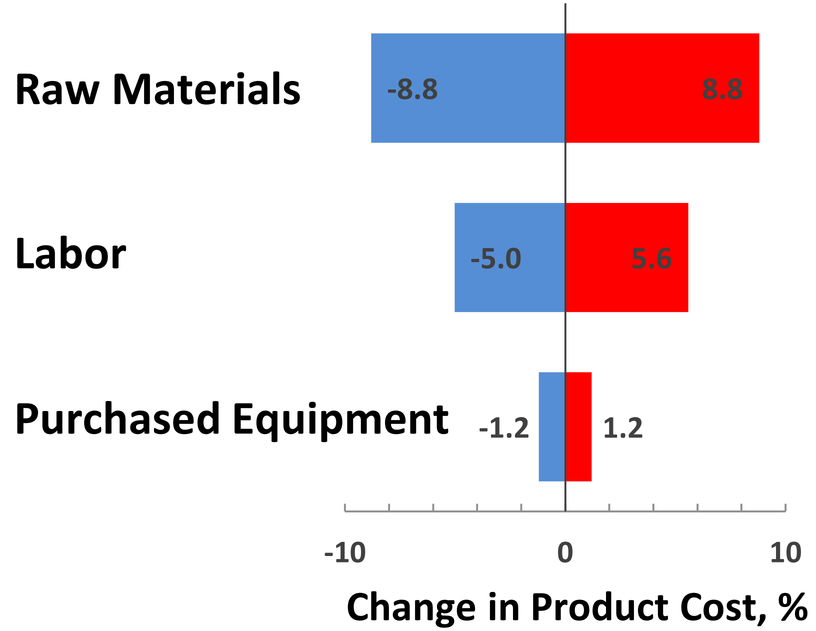
$MSO_4 + Na_2CO_3 = MCO_3\downarrow + Na_2SO_4$ M = Ni, Mn, Co	
T, P	95°C, 1 atm
MSO_4 Conversion	95-99%
Reactant Feed Rate	35,800 Liter/day
Residence Time	10 hours
Reactor Volume	18 m^3
Heat Load (Cooling)	43 kW



The product cost is most sensitive to the cost of raw materials.

	Heat Load
Sintering Furnace, kW	345
Water Heater, kW	129
Vacuum Dryer, kW	50
Reactor Cooling, kW	43
Energy Demand, GWh/yr	**4.0**
	Cost
Purchased Equipment, K$	$910
Total Capital Investment, K$	$3,319
Metal Sulfate, K$/day	$21-36
Lithium Carbonate, K$/day	$14
Total Raw Materials, K$/day	$35-50
Product Cost, $/kg$_{NMC}$	**$27-38**

Effect of 10% Change in Variable Cost on Product Cost



Collaboration

- Support EPA in using BatPaC for regulatory analysis
  - Updated the model in response to peer review and state-of-the-art in battery manufacturing and pack design
  - EPA has adopted BatPaC for determining cost of LIB in hybrid and electric vehicle applications
  - Share incremental improvements in BatPaC capabilities
- Project impact of improved components from DOE funded developers (3M, Amprius, Envia)
- Validate model results with GM model/experience
- Develop and validate NMP recovery process: B&W MEGTEC

Proposed Future Work

- Study upstream processes and steps in the battery plant to bring greater fidelity in energy and cost estimates
  - Update optimum electrode thickness calculation
  - Complete the cost calculations for the NMP recovery, dry room, and cathode development
  - Update BatPaC cost estimates based on supporting models
  - Include cathode material production processes
  - Explore the energy demands of other steps in the manufacturing process, e.g., electrode coating, formation cycling, etc.
- Support EPA calculations
- Include volume expansion mitigation designs (foam or springs, etc.)
- Incorporate use of a blended cathode in the model
- Evaluate fast charging of EV batteries

Summary

- The BatPaC spreadsheet model is a resource for DOE, EPA, and technology developers
  - Projection to the pack level performance helps understand the impact of component technology
- A flex plant provides economy of scale and lowers the cost of batteries
- Modeling the various processes in the battery manufacturing plant helps R&D decisions for cost reduction
  - Drying of NMP and Dry Room operations are very energy intensive
  - For the NMC cathode, the raw materials represent the largest cost

Summary Accomplishments

- A new version of BatPaC has been released (Slide s7-8)
  - Another update due in 2015.
- Completed analysis of the benefits of a flex plant (Slides 9-10)
- Continuing to support EPA calculations
- 3 process models have been set up to support BatPaC
  - NMP Drying and Recovery (Slides 11-12)
  - Dry Room (Slides 13-14)
  - Cathode material production (Slides 15-16)

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