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# Fraction of the theoretical specific energy achieved on pack level for hypothetical battery chemistries

Damla Eroglu [a, b, *], Seungbum Ha [a, b], Kevin G. Gallagher [a, b]

[a] Joint Center for Energy Storage Research, Argonne National Laboratory, Argonne, IL, USA
[b] Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, USA

## HIGHLIGHTS

- Fraction of the theoretical specific energy achieved on pack level is estimated.
- Fraction of the theoretical specific energy depends greatly on OCV, $\bar{E}_{theo}$ and ASI.
- Lower $\bar{E}_{theo}$ systems capture higher fraction of the theoretical specific energy.
- Pack-level properties are independent of $\bar{E}_{theo}$ in low OCV systems at moderate ASI.
- Reducing impedance in low OCV systems leads to higher pack-level specific energies.

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## ABSTRACT

In valuing new active materials chemistries for advanced batteries, the theoretical specific energy is commonly used to motivate research and development. A packaging factor is then used to relate the theoretical specific energy to the pack-level specific energy. As this factor is typically assumed constant, higher theoretical specific energies are judged to result in higher pack-level specific energies. To test this implicit assumption, we calculated the fraction of the theoretical specific energy achieved on the pack level for hypothetical cell chemistries with various open-circuit voltages and theoretical specific energies using a peer-review bottom-up battery design model. The pack-level specific energy shows significant dependence on the open-circuit voltage and electrochemical impedance due to changes in the quantity of inactive materials required. At low-valued average open-circuit voltages, systems with dramatically different theoretical specific energies may result in battery packs similar in mass and volume. The fraction of the theoretical specific energy achieved on the pack level is higher for the lower theoretical specific energy systems mainly because the active materials mass dominates the pack mass. Finally, low-valued area-specific impedance is shown to be critical for chemistries of high theoretical specific energy and low open-circuit voltage to achieve higher pack-level specific energies.



## 1. Introduction

New lithium-ion and beyond lithium-ion battery chemistries are being developed in the hopes of enabling cost-effective electric vehicles [1–17]. In the search for new candidates, the theoretical specific energy (i.e. W h $kg^{-1}$) is frequently used for the justification of research and development investment in particular chemistries. The theoretical specific energy, $\bar{E}_{theo}$, is calculated considering the mass of the active materials as shown in equation (1) [2–5,7]. However the pack-level specific energy, $\bar{E}_{pack}$, depends on the mass of the entire battery pack (i.e. active and inactive materials) [18]. The implicit assumption with the use of $\bar{E}_{theo}$ to value candidate materials is that the pack-level specific energy is a constant fraction of the theoretical value as shown in equation (2) [1,2,4,6,7]. Since these new chemistries are not yet commercialized, practical specific energies and energy densities are not available; system-level properties are predicted using the packaging factors for today's batteries. In the literature, values of 0.2–0.45 are commonly used for $f_m$ [1,2,4,6,7].

$$\bar{E}_{theo} = \frac{C \cdot U_{Batt}}{(m_{ne,act} + m_{pe,act})} \quad (1)$$

* Corresponding author. Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700 S Cass Avenue, Bldg. 200, Argonne, IL 60439-4854, USA. Tel.: +1 630 252 1974.
*E-mail addresses:* eroglud@anl.gov, damlaeroglu@gmail.com (D. Eroglu).

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$$\bar{E}_{pack} = \bar{E}_{theo} \cdot f_m \quad (2)$$

Here $C$ is the cell capacity, $U_{Batt}$ is the average battery open-circuit voltage (OCV), $m_{ne,act}$ and $m_{pe,act}$ are the mass of the active materials in the negative and positive electrode, respectively, and $f_m$ is the fraction of the theoretical specific energy achieved on pack level.

Although the fraction of the theoretical specific energy is commonly used for pack-level estimations, there are no studies in the literature to our knowledge that investigates $f_m$ as a function of the cell chemistry. The theoretical energy content of a material does not depend on the individual magnitude of the cell capacity or average voltage but rather the product of these two values, $C \cdot U_{Batt}$ (equation (1)). However, we will show that the resulting specific energy of the battery is more strongly dependent on the voltage when battery packs are designed at constant peak power efficiency. In this study, the peer reviewed, bottom-up Battery Performance and Cost (BatPaC) model [19,20] has been modified to systematically estimate the fraction of the theoretical specific energy and energy density achieved on pack level as a function of OCV and $\bar{E}_{theo}$. In other words, the objective of this work is to understand how the relative ratio of active to inactive materials changes within a battery pack as physicochemical properties of a material change, namely the voltage, specific capacity, and impedance. The need to remove energy from the battery at finite power levels directly affects the amount of inactive materials through changes in cell area and electrode thickness [18]. While comparison of the calculated values in this study with nonexistent commercially available battery packs is impossible, the trends that are demonstrated will hold true for the future chemistries that are currently under development in laboratories worldwide. Therefore, the value of this theoretical assessment is to highlight challenges that must be overcome through science and engineering advancements for materials that might initially appear to promise extremely high specific energy.

## 2. Model description

The BatPaC model (a detailed model description is available elsewhere [19,20]) is a publically available bottom-up design and cost model developed through support by the U.S. Department of Energy Vehicle Technologies Office. BatPaC was peer reviewed sponsored by the U.S. Environmental Protection Agency (EPA) [21] and used to assist the 2017–2025 light duty vehicle rule for fuel economy and greenhouse gas emissions in the United States [22].

The design methodology used in BatPaC has been previously validated against cylindrical wound cell formats [23]. The calculated materials quantities agreed with the actual values within 3%. Moving to the prismatic format now used in BatPaC simplifies the current collection calculation while leaving the governing equations unchanged. The performance calculation has also been improved by including additional physics in the impedance calculation. This approach has been validated against experimental measurements with a graphite/$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ cell using electrodes up to 100 μm in thickness [24].

By bottom-up design model, we mean all necessary components required to produce DC electricity are sized and included in the pack-level values (e.g. current collectors, cell packaging, battery housing, and thermal management). Fig. 1 presents a schematic of the cell- and pack-level designs in the BatPaC model. The cell design is similar to those that exist in commercial products while the module and pack design reflect the expected improved packaging that will result from continued engineering improvements in product design. Thus the projected pack-level specific energy and energy density can be considered optimistic compared to values obtain in vehicles batteries used in model year 2013.

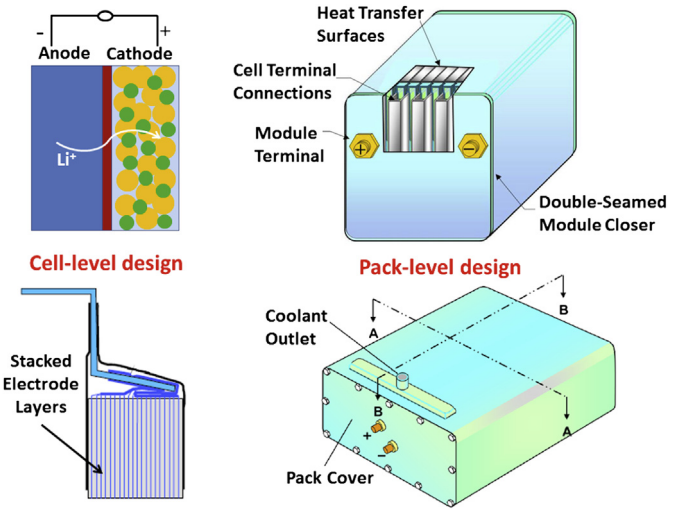


**Fig. 1.** Schematic of cell-level and pack-level designs in BatPaC.

The pack is designed for a 50 kW h, 100 kW and 360 V battery containing 50% excess lithium-metal (Li-metal) as the negative electrode. For the positive electrode, hypothetical OCVs and specific capacities required for batteries with $\bar{E}_{theo}$ of 500, 750, 1000, 1500 and 2000 W h $kg^{-1}$ are considered. The specific capacity of the positive electrode at a given $\bar{E}_{theo}$ is calculated as a function of OCV using equation (3) (derived from equation (1)) and then fed into the modified BatPaC model with the other design parameters as shown in Table 1. The change in the number of cells in a battery pack with the OCV to keep the pack voltage constant at 360 ± 10 V is also taken into account in the model as shown in equation (4). The pack voltage is set by the powertrain electronics architecture and should not be battery chemistry specific, to the first order of analysis.

$$c_{pe} = \frac{1}{\left(\frac{U_{OCV}}{\bar{E}_{theo}} - \frac{[N/P]}{c_{ne}}\right)} \quad (3)$$

$$U_{Batt} = U_{OCV} \cdot N_{cell} \quad (4)$$

Here, $c_{pe}$ is the specific capacity of the positive electrode and $N_{cell}$ is the number of cells in a battery pack. The definitions of the other variables are given in Table 1.

Pack-level specific energy, energy density and the fractions of the theoretical values on the pack level are calculated using the modified BatPaC model for these hypothetical $U_{OCV}$ and $\bar{E}_{theo}$ couples. For the material properties of the hypothetical cathodes, the experimentally measured properties of NMC441 ($Li_{1.05}(Ni_{4/9}Mn_{4/9}Co_{1/9})_{0.95}O_2$) in the BatPaC model is used [19,20,25]. The properties

**Table 1**
Parameters used in BatPaC for the pack design.

| Parameter | Symbol | Value |
|---|---|---|
| Energy (kW h) | $E$ | 50 |
| Rated power (kW) | $P$ | 100 |
| Average battery open-circuit voltage (V) | $U_{Batt}$ | 360 |
| Average cell open-circuit voltage (V) | $U_{OCV}$ | 1.5–4.5 |
| Negative electrode specific capacity (mA h $g^{-1}$) | $c_{ne}$ | 3860 |
| Negative to positive capacity ratio | $[N/P]$ | 1.5 |
| Theoretical specific energy (W h $kg^{-1}$) | $\bar{E}_{theo}$ | 500–2000 |
| Target voltage efficiency at rated power | $[V/U]$ | 0.8 |
| Maximum electrode thickness limitation (μm) | $L_{pos,max}$ | 100 |
| Area-specific impedance parameter (Ω $cm^2$) | $ASI_{const}$ | 33 |