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Cost Analysis of a Sodium-ion Battery Pack for Energy and Power Applications using Combined Multi-physics and Techno-Economic Modeling

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The renewable energy transition requires energy storage technologies for grid-balancing and transportation. Lithium-ion batteries have been widely adopted for these applications, but supply risks due to geopolitical tensions have motivated the search for alternative chemistries less dependent on critical raw materials. Sodium-ion batteries have garnered notable attention as promising post-lithium chemistry due to the relative abundance of sodium and its similar manufacturing process to lithium-ion batteries. This work estimated the cost of producing sodium-ion battery packs from cells optimized via multiphysics modeling for energy or power-based applications. This study replicated a multiphysics model of a pouch format sodium-ion battery from literature in COMSOL Multiphysics®. This model determined the optimal active material used in batteries under 0.1C to 10C discharge rates to maximize the energy density. The cost of battery packs produced from the optimized cells was then determined using the Battery Performance and Cost (BatPaC) model of Argonne National Laboratory, which considers material and manufacturing costs. The optimization results reveal that energy cells have thicker electrodes and lower porosities (217 μm thick 0.11 porosity anode, 237 μm thick 0.10 porosity cathode for 0.1C), which maximize the amount of active material per unit mass. Power cells have thinner electrodes and larger porosities to minimize electrical resistance (58 μm thick 0.32 porosity anode, 63 μm thick 0.31 porosity cathode for 10C), reducing energy losses at high currents. Moreover, we compared the calculated production cost for energy and power applications for sodium-ion batteries, highlighting essential parameters affecting the price. The model observed a 26.42% increase in total material cost per kWh when transitioning from energy to power cells. The model may also be refined by considering sodium-ion batteries with different cathode and anode chemistries in different formats and their applications in different use cases.

1. Introduction

Lithium-ion batteries (LIBs) have been the prevalent energy storage since their commercialization in the 1990s. The high energy capacity and technological maturity of LIBs have attracted various use cases, from mobile applications to grid-scale energy storage and transportation. Although a prominent candidate in energy storage, there have been growing concerns regarding the sustainability aspect of LIB components such as lithium sources and rare transition metals used as cathode material. Non-sustainable mining practices, limited availability, and accelerating energy storage demand increases the price of LIBs and components. These challenges of LIBs engage interests in studies to pioneer post-lithium energy storage that would meet the performance of existing LIB chemistries without sacrificing economics and sustainability. One perceptible prospect is the use of sodium in place of lithium. Sodium (Na) is a low-cost and highly abundant alternative to lithium. Furthermore, several studies theorize that Na-ion behaves similar to Li-ion in its rocking chair mechanism of intercalation and deintercalation. Na-ion batteries (NIBs) have a redox potential close to existing

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LIBs, appealing for applications where weight and volume are not of much concern, such as stationary energy storage, power tools, and light-duty electric vehicles. NIBs have taken the energy storage market at an accelerating pace where various market players have given tremendous research efforts and investments to develop ground-breaking NIB technologies (Chen et al., 2018).
The design of individual cells is typically performed via multiphysics modeling, which simulates the reactions and ion transport in an electrochemical system. The model can determine the distribution of continuum-scale parameters, such as concentration, potential, and temperature, in a battery (Li et al., 2015). More importantly, the model can determine the allocation of materials that optimizes the performance of a battery. For instance, Schneider et al. (2019) used a NIB multiphysics model to determine the electrode thicknesses and porosities that maximize the energy density at various C-rates. The authors investigated the environmental impact of Na-ion batteries through a life cycle assessment from the optimized material usage. Multiphysics modeling was also utilized to optimize LIBs (Hosseinzadeh et al., 2017), lead-acid, and vanadium redox flow batteries. A review of these studies can be found in (Castro et al., 2021). BatPaC is a bottom-up cost and battery pack design modeling tool developed by Argonne National Laboratory (Nelson et al., 2019). A unique advantage of BatPaC is that the battery electrochemical performance, such as power and energy metrics, can be bridged to analyze the cost to performance relationship of a battery design. The chemistry and design of the battery can be modified to compare and screen various materials and the impact of altering their properties, such as dimensions, pricing, and sizing. A study by Vaalma et al. (2018) compared the cost and performance of existing LIB technologies and exchanging materials to tailor-fit the NIB chemistry for stationary power applications. Their works concluded the price advantage of NIB technologies would overcome LIB when the supply of lithium and rare earth materials in LIB becomes an issue and the price point increases. Another study by Peters et al. (2019) examined the economic impact of a cylindrical cell geometry for LIBs and NIBs. The study notes that existing NIB technologies may have difficulty matching the price per kWh of $LiNiMnCoO_2$-graphite (NMC) in energy density but would have a competitive economic and performance advantage against $LiFePO_4$-graphite (LFP) for stationary applications providing enhanced safety, cycle life, and viable cost. Despite multiphysics and cost and performance modeling being powerful tools in breaking the laboratory barrier of battery chemistries to advance commercial applications, no study has been reported to merge these techniques to analyze NIBs. This study addresses the research gap by developing a multiphysics model for NIB and translating the optimized cells' relevant parameters to establish the economic comparison of manufacturing energy and power-type NIBs by providing detailed information on the cost contribution of cell components.

2. Methodology

The methodology is divided into three parts, where the schematics are shown in Figure 1. First was the multiphysics modeling of the NIB varying performance of energy and power applications. Second, the generated multiphysics model's optimized parameters were translated to the cost model to demonstrate battery production economics. Lastly, the cost and performance correlation of the optimized energy and power NIBs were investigated.

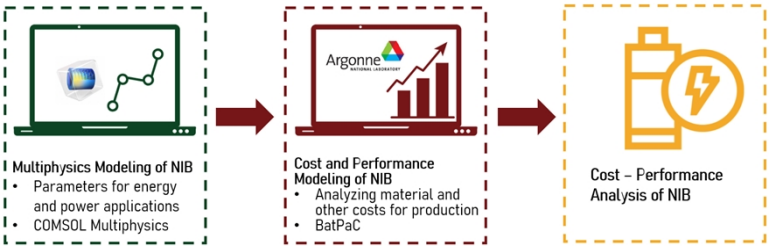

Figure 1: Schematic representation of methodology from multiphysics modeling to cost analysis and finally, cost-performance examination of NIBs.

2.1 Multiphysics modeling

The NIB considered in this work utilizes a hard carbon anode, $NaNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode, and $NaPF_6$ electrolyte and is described in Schneider et al. (2019). The battery is described by the pseudo-2D (P2D) model illustrated in Figure 2, which couples the 1D charge and mass transport of Na^+ ions across the battery (i.e., from the anode to cathode during discharge) and the 1D diffusion of Na^+ ions into the spherical electrode particles. Na^+ ion transport in the electrolyte is described by Newman's concentrated solution theory, which accounts for the interactions between ions in addition to diffusion, migration, and convection effects. The porous electrodes

are also modeled according to Newman's porous electrode theory, which averages their solid and liquid phase properties weighted according to their volume fractions. It is worth noting that the P2D model was pioneered by Doyle, Fuller, and Newman (1994) for LIBs and has been applied in the modeling of NIBs (Chayambuka et al., 2022). The mathematical formulation of the P2D model and the input model parameters are detailed in the work of Schneider et al. (2019). This work replicates the same model in COMSOL Multiphysics®.

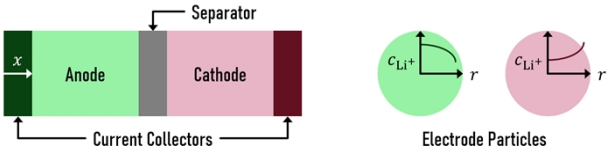

Figure 2: Schematic diagram of the P2D model. 1D mass and charge transport across the battery is coupled with 1D diffusion into the electrode particles.

After building the multiphysics model, the anode thickness, porosity, and cathode porosity are determined. The battery's energy density is maximized under various C-rates: C/10, C/4, 1C, 4C, and 10C discharge until a 1.8 V cut-off voltage. Low C-rates result in optimized cells for energy, while high C-rates yield batteries designed for power. Note that the cathode thickness is adjusted. Its coulombic capacity balances the anode's, as described by Schneider et al. (2019); hence it is not optimized like an independent variable.

2.2 Cost and performance modeling

The Battery Performance and Cost (BatPaC) 4.0 model was used to investigate the cost of NIBs geared towards energy and power applications (Nelson et al., 2019). The multiphysics model of NIBs allows the determination of integral parameters that impact the target application of the battery pack, whether for energy or power. These parameters were carried forward to the cost model to determine their influence on the battery expense. The optimized parameters for NIB energy and power cells used in the study are shown in Table 1. This study analyzed a 7 kW, 11.5 kWh prismatic battery pack consisting of 72 cells designed for stationary applications adapted from the works of Vaalma et al. The BatPaC model was modified to adhere to specific energy and power requirements used in this study (Vaalma et al., 2018). Since large-scale production of NIBs still lack commercial cost data, pack material costs of NIB cells were adapted from the works of Vaalma et al. (2018).The material costs for various NIB performances obtained in the model were compared with LIB chemistries such as LFP and $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$-graphite (NMC-333). Furthermore, the cost distribution of individual cell components and the material cost pack energy price of NIBs was analyzed and compared with LIBs.

Table 1: Optimized parameters from the multiphysics model translated to the BatPaC model

Parameter	Energy Cell		Power Cell		
C-rate where parameters were optimized	C/10	C/4	1C	4C	10C
Cathode active material capacity (mAh/g)	119.00	119.00	119.00	119.00	119.00
Cathode active material density (g/cm^3)	4.7500	4.7500	4.7500	4.7500	4.7500
Cathode electrolyte volume fraction	10.384	12.985	25.281	22.764	31.330
N/P ratio after formation	0.9989	0.9989	0.9989	0.9989	0.9989
Anode active material capacity (mAh/g)	329.00	329.00	329.00	329.00	329.00
Anode active material density (g/cm^3)	1.7000	1.7000	1.7000	1.7000	1.7000
Anode electrolyte volume fraction	10.635	16.832	23.546	15.058	31.601
Open circuit voltage at 20% SOC (V)	2.3916	2.4093	2.3863	2.3939	2.3424
Open circuit voltage at 50% SOC (V)	2.8048	2.8184	2.774	2.6889	2.5383

LIB chemistries parameters and material costs use default BatPaC 4.0 values.

3. Results and discussion

3.1 Multiphysics modeling

The optimized electrode thicknesses and porosities, and cell energy densities of energy and power cells are presented in Figure 3. It can be readily observed that energy cells have thick electrodes and low porosities, while power cells have thin electrodes and high porosities. The difference is because energy cells must have a higher coulombic content, utilizing larger and densely packed electrodes. In contrast, power cells are plagued with ohmic losses due to higher currents; hence, they need thinner electrodes and larger porosities to minimize electrical and ionic resistances. Ohmic losses in power cells also explain their lower energy density than energy

cells. It is worth noting that Schneider et al. (2019) and Hosseinzadeh et al. (2017) observed similar trends in electrode thicknesses and porosities during the optimization of NIBs and LIBs, respectively.

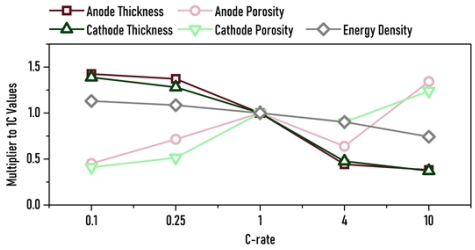

Figure 3: Optimized electrode thicknesses and porosities and the resulting cell energy densities at various C-rates relative to their values at a discharge C-rate of 1.

3.2 Cost and performance modeling

Table 2: NIB pack material cost distribution generated from BatPaC

Cost per battery pack	Energy Cell		Power Cell		
C-rate where parameters were optimized	C/10	C/4	1C	4C	10C
Cathode ($/pack)	291.2802	289.9448	294.3518	303.1949	320.2595
Anode ($/pack)	219.5146	218.4143	221.4064	228.1189	240.4765
Carbon and binders ($/pack)	50.75068	50.50169	51.29572	52.92181	56.04062
Cathode current collector ($/pack)	30.63340	31.34421	36.87249	36.83832	43.54778
Anode current collector ($/pack)	32.19790	32.94491	38.67315	38.62207	45.60770
Separators ($/pack)	218.0745	223.2704	263.2035	262.8592	311.6324
Electrolyte ($/pack)	82.73342	102.9603	163.7348	137.0237	234.6476
Cell hardware ($/pack)	61.32324	61.67397	63.02704	62.76461	64.97423
Module hardware ($/pack)	250.1180	250.4179	253.0477	253.9965	259.8645
Battery jacket ($/pack)	257.8318	259.0939	283.4248	263.0981	312.1787
Total cost of materials ($/pack)	1494.460	1520.570	1669.040	1639.450	1889.230
Total battery pack energy price ($/kWh)	124.5400	126.7100	139.0900	136.6200	157.4400

The results of the cost of NIB pack on energy and power cells in terms of materials and total energy cost are summarized in Table 2, and an analogous figure is shown in Figure 4a.

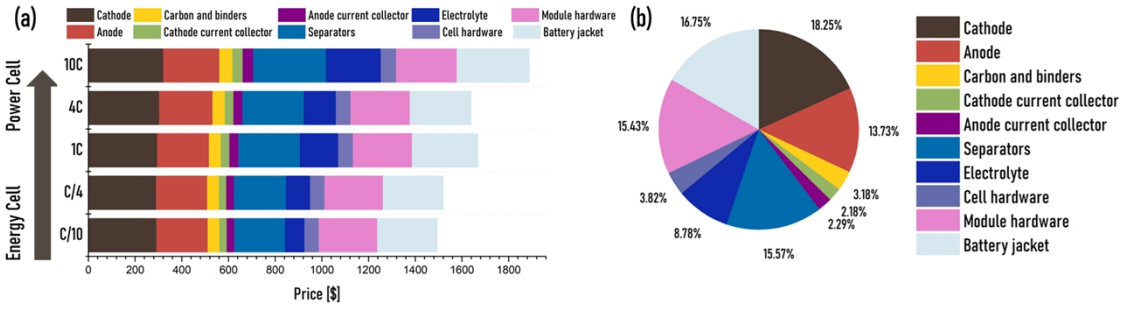

Figure 4: Material cost distribution of NIB pack (a) varying from energy and power applications and (b) in terms of average material contribution.

The NIB pack optimized for 10C operation intended for quick energy release and rapid response power applications exhibits the highest cost. The NIB pack optimized for C/10 operation intended for long-usage and long-cycling energy applications exhibits the lowest cost based on materials and energy price. A cost increase of 26% was observed comparing the C/10 energy cell and 10C power cell. The results show a general increasing total cost of material and pack energy price as the C-rate increases. This relationship denotes higher prices for NIB power cells compared to energy cells. Figure 4b illustrates the average individual cost distribution of NIB pack components. The cost distribution presents that the cathode price contributes the most to the overall

material cost (18.25%), followed by the battery jacket (16.75%) and the separator (15.57%). When neglecting the non-active component, such as the battery jacket, these results are analogous to Hirsh et al. Their study displayed the same cost trend for NIBs containing nickel, cobalt, or both (Hirsh et al., 2020). Despite the separator being the third most expensive component, for an energy NIB pack optimized for C/10, Table 2 exhibits that the anode cost is higher than that of the separator, indicating lesser separator materials are used for energy applications. This finding exposed a gap in current NIB studies focusing on lowering the cost of electrodes. An equally integral aspect of cost reduction is the separator which must also be prioritized and investigated. Furthermore, cost reduction on non-active material must be considered, such as the battery jacket. The energy price in terms of $/kWh was also examined for representative NIB cells and compared with commercially available LIBs shown in Figure 5a. Only the battery chemistry and respective cost of materials were substituted in the model to level the application towards 11.5 kWh stationary use cases. The model results exhibit that the NIB pack optimized for C/10 energy applications shows competitive price points against LFP and NMC-333. The NIB energy cell has a lower total material cost per energy than LFP, demonstrating a promising post-lithium alternative for energy storage in terms of economics and performance. The study of Roberts et al. emphasized how NIBs are more cost-efficient and provide higher safety and minimal maintenance than lead-acid batteries. This finding shows a promising outlook for NIBs in energy applications and would, in time, replace lead-acid batteries (Roberts and Kendrick, 2018). As NIBs are widely accepted as a drop-in technology from LIB, moving forward to NIB production would entail a more accessible entry to the market than competing energy storage technologies such as fuel cells.

For a NIB pack power cell being used for stationary applications, the material cost per energy is higher than that of presented LIBs. NMC-333 and LFP are regarded to have similar power performance where this metric allows these technologies to be employed for electric vehicle (EV) applications (Ding et al., 2019). The results may indicate that using NIBs for power applications such as EVs may be more costly in the current market than existing LIB technologies. However, this study did not account for possible future market prices sensitivity. If the cost of lithium and other rare metals in the cathode material increases due to supply issues, a shift in overall costs is expected to move according to the market demand.

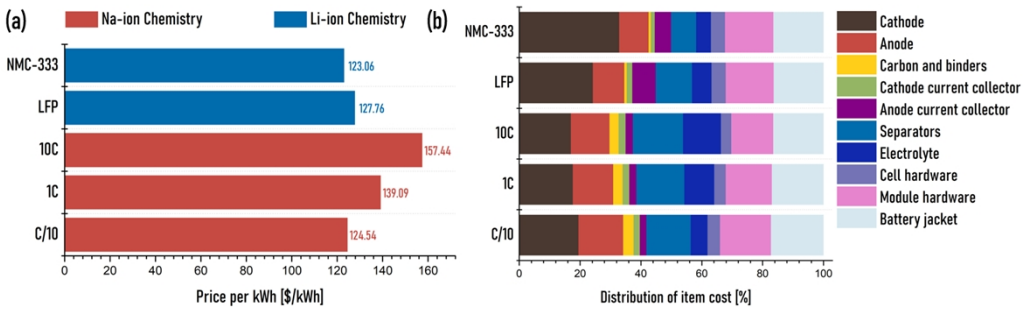

Figure 5: Cost comparison of LIBs and representative NIBs. (a) Price of energy for full cell LIBs labeled green and NIBs labeled in maroon. (b) Battery pack material component cost distribution of LIBs and NIBs.

The distribution of individual battery pack component costs of LIBs and NIBs examined are illustrated in Figure 5b. The results show an average of 13.00% decrease in cost contribution for both cathode and anode electrodes as the C-rate of application increases implying from energy application to power application. Although the cathode price increases as the use case shifts from energy to power, their cost contribution decreases, as shown in Figures 5a and Table 2. This is because thinner electrodes and larger porosities are required to lower electrical resistance for power applications. The cost contribution of the electrolyte provides the highest escalation from 5.54% for C/10 energy applications to 12.42% for 10C power applications, with an increase of 24.19% seen in Figure 4b. This finding recommends studies to heighten interest in advancing low-cost NIB electrolyte materials, notably for power applications. In contrast to LIB technologies, a general conclusion exists that NIBs have a lower cathode cost contribution than LIBs. This is mainly due to the cost of lithium and cobalt in NMC-333. Lithium alloys with aluminium at low potentials as such copper is employed as the LIB anode's current collecto which is not the case with NIBs as sodium does not alloy with aluminum at low potentials. Thus, aluminum as cathode and anode current collectors reduces the cost by substituting expensive copper. Results show that replacing the cathode and anode current collectorprovides the largest cost distribution reduction. For NMC-333 to C/10 NIB, a 40.64% cost distribution reduction was observed for cathode and 60.00% cost distribution reduction when replacing copper with aluminium as anode current collector.The combined cost and performance analysis provides insight into market viability and current use case preferential for NIBs.

4. Conclusions

NIB technologies are receiving their comeback in interest for energy storage applications due to being a promising post-lithium alternative due to its drop-in capabilities in existing LIB plants. This study combines multiphysics modeling of NIBs for energy and power applications. It transposes the optimized parameters into a cost and performance modeling tool to investigate the impact of varying use cases on the overall cost. The multiphysics model revealed an average of 73.34% reduction in electrode thickness from energy to power cells. Energy cells tend to have thicker electrodes and lower porosities, increasing the coulombic content. In comparison, thinner electrodes and larger porosities characterize power cells to minimize ohmic losses incurred from high currents. The multiphysics model parameters were used to investigate the economics of a battery pack for stationary applications. The model demonstrates a 26.42% increase in total material cost per kWh when shifting from energy to power NIB pack. The cathode and separator provided the highest cost contribution for the active battery material. These findings suggest a research movement in engineering low-cost separators for NIBs aside from the current trend-focused solely on the electrodes. Energy cells have been found to have lower electrode cost contributions than power cells, as thinner electrodes are needed for rapid energy release in power applications. Also, NIBs designed for energy use have shown superior cost competency over existing LIB technologies being 2.59% cheaper than LFP in cost per kWh. Furthermore, cost reduction from LIB to NIB is mostly situated with the cathode price and replacing the copper current collector with aluminum. This study provides grounding on studies claiming NIBs to have a massive cost reduction with existing LIBs. Although NIBs can be a valued competitor to post-lithium chemistries, this study demonstrates that electrochemical performance must be improved to spearhead potential to market. This study provides a powerful birds-eye view of the NIB cost to performance relationship; however, it is limited to current market performance. A sensitivity analysis can be further conducted to capture future resource supply and demand outlook.

Acknowledgments

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References

Castro, M. T., Anne, J., Rosario, D. Del, Nan, M., Chuang, P. A., Lee, J., Ocon, J. D., 2021, Multiphysics modeling of lithium-ion , lead-acid , and vanadium redox flow batteries. Journal of Energy Storage, 42, 102982.

Chayambuka, K., Mulder, G., Danilov, D. L., Notten, P. H. L., 2022, Physics-based modeling of sodium-ion batteries part II. Model and validation. Electrochimica Acta, 404, 139764.

Chen, L., Fiore, M., Wang, J. E., Ruffo, R., Kim, D. K., Longoni, G., 2018, Readiness Level of Sodium-Ion Battery Technology: A Materials Review. Advanced Sustainable Systems, 2(3), 1700153.

Ding, Y., Cano, Z. P., Yu, A., Lu, J., Chen, Z., 2019, Automotive Li-Ion Batteries: Current Status and Future Perspectives. Electrochemical Energy Reviews, 2(1), 1–28.

Doyle, M., Fuller, T. F., Newman, J., 1994, The importance of the lithium ion transference number in lithium/polymer cells. Electrochimica Acta, 39(13), 2073–2081.

Hirsh, H. S., Li, Y., Tan, D. H. S., Zhang, M., Zhao, E., Meng, Y. S., 2020, Sodium-Ion Batteries Paving the Way for Grid Energy Storage. Advanced Energy Materials, 10(32), 2001274.

Hosseinzadeh, E., Marco, J., Jennings, P., 2017, Electrochemical-thermal modelling and optimisation of lithium-ion battery design parameters using analysis of variance. Energies, 10(9).

Li, J., Cheng, Y., Ai, L., Jia, M., Du, S., Yin, B., Woo, S., Zhang, H., 2015, 3D simulation on the internal distributed properties of lithium-ion battery with planar tabbed configuration. Journal of Power Sources, 293, 993–1005.

Nelson, P. A., Ahmed, S., Gallagher, K. G., Dees, D. W., 2019, Modeling the Performance and Cost of Lithium-Ion Batteries for Electric-Drive Vehicles, Third Edition.

Peters, J. F., Cruz, A. P., Weil, M., 2019, Exploring the Economic Potential of Sodium-Ion Batteries. Batteries, 5(1), 10.

Roberts, S., Kendrick, E., 2018, The re-emergence of sodium ion batteries: testing, processing, and manufacturability. Nanotechnology, Science and Applications, 11, 23–33.

Schneider, S. F., Bauer, C., Novák, P., Berg, E. J., 2019, A modeling framework to assess specific energy, costs and environmental impacts of Li-ion and Na-ion batteries. Sustainable Energy and Fuels, 3(11), 3061–3070.

Vaalma, C., Buchholz, D., Weil, M., Passerini, S., 2018, A cost and resource analysis of sodium-ion batteries. Nature Reviews Materials, 3(4), 1–11.