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Water-based manufacturing of lithium ion battery for life cycle impact mitigation

Chris Yuan[a*], Huajun Cao[b], Kang Shen[a], Yelin Deng[c], Dan Zeng[b], Yan Dong[d], Michael Hauschild (1)[d]

[a] *Department of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland, OH, USA.*
[b] *School of Mechanical Engineering, Chongqing University, Chongqing, China.*
[c] *Department of Civil and Environmental Engineering, Soochow University, Soochow, China.*
[d] *Department of Technology, Management and Economics, Technical University of Denmark, Copenhagen, Denmark.*
** Corresponding author, Tel: 216-368-5191; Fax: 216-368-6445; email: chris.yuan@case.edu*

Abstract:

Water-based manufacturing processes are under development for greener manufacturing of lithium ion batteries but their environmental impacts are unclear with new introduced materials and a large consumption of deionized water. We report a life cycle assessment (LCA) study on the water-based manufacturing of the most popular NMC-graphite battery pack configured with 57 kWh capacity. A life cycle model has been developed based on experimental and mathematical studies of the water-based manufacturing processes. Per kg battery pack produced, the water-based manufacturing can reduce the manufacturing energy by 43% and lower the cradle-to-gate life cycle impacts by 0.6%~88% over conventional battery manufacturing.

Keywords: Life cycle; Analysis; Battery manufacturing.

1. Introduction

Lithium ion batteries are widely used nowadays for powering electric vehicles and portable electronics [1]. It has been reported that the global cumulative annual demand for the lithium ion batteries reached 526 GWh in 2020, and will reach 9,300 GWh by 2030 [2]. Among various types of lithium ion battery chemistries, the one using Lithium Nickel Manganese Cobalt Oxide (NMC) cathode and graphite anode is most popular due to its high energy density (150-220 Wh/kg), long cycle life (1,000-2,000 cycles), and good thermal stability (210 °C thermal runaway) [3].

However, current lithium ion battery manufacturing generates significant environmental impacts, mainly due to its high energy consumption and heavy use of toxic chemicals in the manufacturing processes. In current manufacturing of NMC-graphite lithium ion batteries, the processing of electrode materials requires the use of a toxic chemical solvent, N-methyl-2-pyrrolidone (NMP), to dissolve the Polyvinylidene fluoride (PVDF) binder to enable such manufacturing processes as mixing, coating, drying, calendaring, slitting and vacuum drying. It has been reported that in industrial manufacturing of NMC-graphite battery for electric vehicles (EV), approximately 3.1 kg of NMP solvent is required to produce 1 kWh of NMC-graphite battery [4]. Based on our previous study, manufacturing a 24 kWh battery pack for a mid-size EV requires 58.7 GJ of energy input, of which 38% is used to dry the electrodes and to evaporate and collect the NMP solvent [6]. The greenhouse gas emissions from cradle-to-gate battery production can be as high as 172 kg CO_{2eq}/kWh for the NMP-based manufacturing processes, of which 62% is reported being generated during battery production [4].

As such, a greener manufacturing of lithium ion battery is important in advancing the lithium ion battery technology to future broader applications [6]. Recently, water-based processes using deionized water to dissolve aqueous binders, e.g., PVDF Latex, are being developed to eliminate the use of the NMP solvent from the lithium ion battery manufacturing processes [7]. They also have the potential to reduce the drying time of the battery electrodes considerably, thereby reducing the manufacturing energy of the lithium ion battery [8,9]. The electrochemical performance of the lithium ion battery pouch cells produced with the water-based manufacturing

process is comparable to that of the lithium ion battery manufactured with the conventional NMP-based processes [7].

As the water-based manufacturing processes introduce new aqueous binder materials and require large quantities of deionized water, there are trade-offs on the life cycle environmental impacts of the battery manufacturing between the introduced impacts from the aqueous binder material and the deionized water and the reduced impacts from the shorter drying time and the eliminated NMP solvent. No life cycle assessment has yet been performed to study the water-based manufacturing processes for lithium ion batteries, and hence it is uncertain whether the water-based manufacturing is more environmentally friendly than conventional NMP-based manufacturing for lithium ion battery. In this paper, we report our collaborative efforts on development of an LCA model to assess the potential environmental impacts of the water-based lithium ion battery manufacturing processes from adoption of the aqueous binders over the conventional NMP-based manufacturing processes.

2. Method

An attributional LCA model has been developed combining experimental results and calculated data using mathematical modelling and, to study and understand the potential environmental impacts of the water-based manufacturing processes of a NMC-graphite lithium ion battery pack using aqueous binders, and then benchmark the impacts with those of the conventional NMP-based battery manufacturing processes to identify the trade-offs and the potential impact mitigation, aiming to improve the environmental sustainability of the lithium ion battery product in future [10,11]. In this study, the LCA boundary is set from cradle to gate, divided into five stages: raw material extraction, material processing, component manufacturing, battery cell manufacturing, and battery pack assembly, as shown in Figure 1. The functional unit is set to 1 kg of the NMC-graphite lithium ion battery pack manufactured. In the inventory analysis,

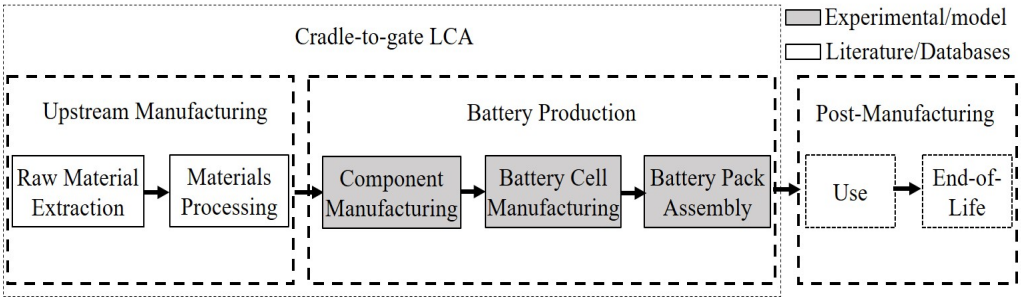

Figure 1 LCA scope and boundary for the lithium ion battery

the battery cell manufacturing is modelled based on our industrial partner's pouch cell manufacturing processes from our previous study [5]. The inventory analyses on raw material extraction and material processing are modelled with inventory data retrieved from the GaBi 10 professional database and Ecoinvent v3.6 database [12]. The ReCiPe method (version 1.08) is used to characterize the life cycle impacts of the battery pack. Finally, the life cycle impacts of the NMC-graphite battery pack produced from the water-based manufacturing processes are benchmarked against those of the battery produced with conventional NMP-based manufacturing processes.

2.1 Water-based manufacturing processes for lithium ion battery

The water-based manufacturing processes of the lithium ion battery pouch cell is show in Figure 2 below.

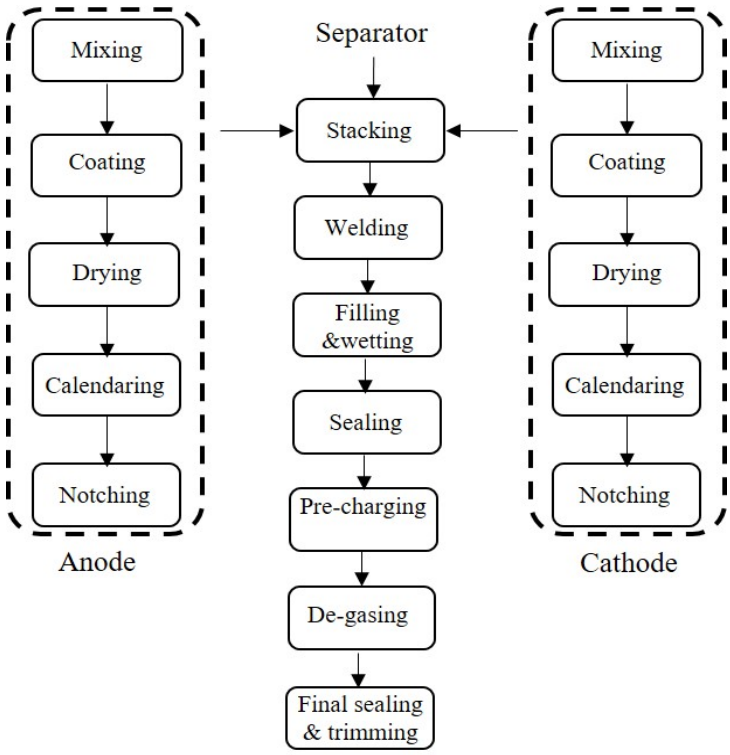

Figure 2 Manufacturing process flows of the battery pack produced from water-based manufacturing processes

The water-based manufacturing processes of the lithium ion battery starts with the mixing of electrode materials to produce cathode and anode slurries. The cathode slurry is produced by mixing $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$ (NCM523), carbon black, Carboxymethyl cellulose (CMC), and PVDF Latex in a mass ratio of 90:5:1:4 [13], with a quantity of 1kg of mixed battery materials in 1.857 kg deionized water. The anode slurry is produced by mixing graphite, carbon black, CMC and Styrene-Butadiene Rubber (SBR) in a mass ratio of 92:2:2:4 [14], with a quantity of 1 kg of mixed anode materials in 1.857 kg deionized water. The water-based slurries for the anode and cathode are then coated onto copper foil and aluminium foil, respectively through doctor blade coating method. The coated anodes and cathodes are then heated to 100 °C for 2 hours to evaporate water from the coating layer. After drying, the anode and cathode are calendared to 34% and 36% of porosities, and at 6.5 mg/cm^2 and 12.5 mg/cm^2 of loading, respectively, then notched and stacked into pouch cells in a dry room with RH<0.1%. The separator stacked between the anode and cathode is the Celgard 2325 PP/PE/PP Trilayer membrane with 25 micron thickness. After stacking, the anode layer tabs are welded together using an ultrasonic welder as negative connector, and the cathode layer tabs are welded together as positive collector. In the dry room, the polymer-coated aluminum pouch with the stacked electrodes and separators inside is then filled with electrolyte, 1.2 M $LiPF_6$ in ethylene carbonate/diethyl carbonate (EC/DEC in 3/7wt). The electrolyte-filled pouch cell is sealed using a hot press sealer, to go through formation pre-charging, de-gassing, final sealing and trimming to finish the battery cell manufacturing.

2.2. Life cycle inventory analysis of the lithium ion battery pack

The manufactured pouch cell batteries from the water-based manufacturing processes are configured into a battery pack with 417 kg mass and 57 kWh capacity, using the BatPac, a battery design software from Argonne National Laboratory. In the configured battery pack, 384 pouch cell batteries are packed and integrated with a battery management system (BMS), a battery cooling system, supported and enclosed in battery packaging. The life cycle inventory analysis of the battery pack is conducted covering inputs of materials and energy as well as outputs of environmental emissions during its life cycle from cradle to gate.

The material composition of the 57 kWh battery pack produced from the water-based manufacturing processes is shown in Figure 3. In total, 330 kg of deionized water is used to process both the anode and cathode materials in the water-based manufacturing processes, with a ratio of 35% solid content to 65% deionized water in the prepared coating slurry based on actual lab experiments [15]. In comparison, conventional manufacturing processes requires

100.4 kg of NMP in the processing of the anode and cathode materials during the battery manufacturing for the same weight of 417 kg battery pack [16].

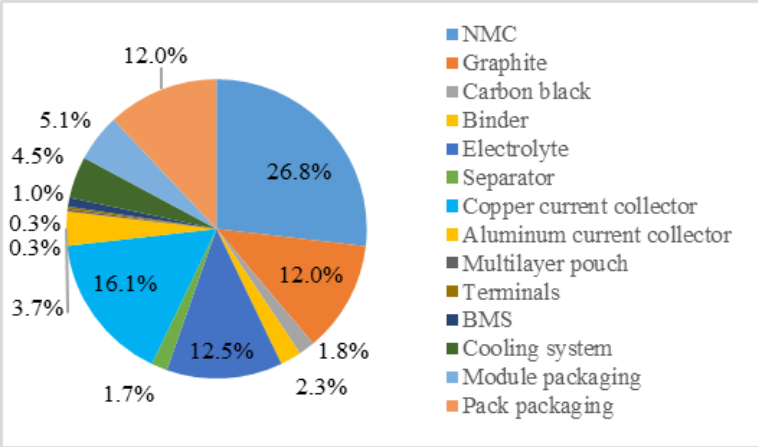

Figure 3 Material compositions of the battery pack produced from water-based manufacturing processes

The energy consumption in the inventory analysis is calculated for the embedded energy in the battery materials, the water-based manufacturing processes, and the battery pack assembly. The embedded energy in the battery materials are all modelled using the GaBi 10 software with Ecoinvent v3.6 database. The energy consumption in the water-based manufacturing processes is calculated using the unit energy analysis model we developed for lithium ion battery pack manufacturing [5]. The major difference is in the drying of water-based manufacturing processes which requires a different amount of energy for water evaporation [17], and eliminates the vacuum drying process from the conventional battery manufacturing [18]. Here, the water drying system for the battery electrodes is modelled using the following equation based on the 1st law of thermodynamics [19]:

$$\sum P + H_{A1} + \Phi_{J1} = H_{A2} + \Phi_{J2} + q_m \frac{u_f^2}{2000} + \sum \dot{E_{zl}} \qquad (1)$$

Where $\sum P$ is the total power of the drying system, kW; Φ_{J1} and Φ_{J2} are sensible heat of wet and dry electrodes, kW; H_{A1} and H_{A2} are the enthalpy of the fresh and waste air per unit time, respectively, kW; q_m is the exhaust air mass flow, kg/s; u_f is the exhaust air speed, m/s; $\sum \dot{E_{zl}}$ is the total power of pressure loss in the drying system, kW. The enthalpy of air is calculated by:

$$H_A = q_m[1.005t_a + d(2501 + 1.86t_a)] \qquad (2)$$

Where t_a is the temperature, °C; d is the air moisture content, kg (water vapor)/kg(dry air).

The sensible heat of the electrode is calculated by:

$$\Phi_J = ubt_j[\delta_j c_j \rho_j + \delta_t c_t \rho_t (1 + x\frac{c_w}{c_t})] \qquad (3)$$

Where u is the electrode transport speed, m/s; b is the width of the electrode, m; t_j is the temperature of the electrode, °C; δ_j and δ_t are the thickness of substrate and coated electrode, respectively, m; x is the moisture content of the coated electrode material, %; c_j, c_w and c_t are the specific heat capacity of substrate, water and coating solute, respectively, kJ/(kg·°C); ρ_j and ρ_t are the density of substrate and coated electrode, respectively, kg/m^3.

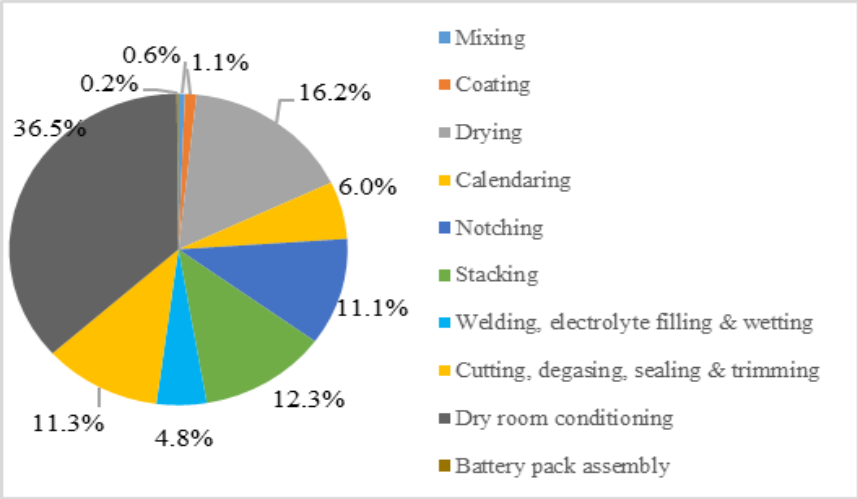

Figure 4 Manufacturing energy consumption in the water-based manufacturing processes of battery pack

As calculated, the specific energy consumption in the water-based manufacturing of the NMC-graphite battery is 19.2 kWh/kg battery pack manufactured. The proportion of energy use in each manufacturing process is shown in Figure 4. From the calculated results, drying process for the water evaporation accounts for 16.2% of the manufacturing energy consumption, while dry room conditioning overall takes 36.5% of total manufacturing energy. For comparison, the conventional NMP-based manufacturing processes need 33.9 kWh of energy per kg of battery pack manufactured. Employing the water-based manufacturing processes can reduce energy consumption in the battery production by 43.2%. The battery pack assembly is mainly done by manual operation and a specific energy consumption of 0.03 MJ/kg was estimated in our previous study [5].

From the life cycle perspective, the total primary energy demand for the 417 kg battery pack comprising 384 pouch cells produced using the water-based manufacturing processes is 1.22 x 10^5 MJ throughout its cradle to gate life cycle. In comparison, the conventional NMP-based manufacturing processes gives the battery pack a primary energy demand of 1.67 x 10^5 MJ throughout its cradle to gate life cycle. A saving of 26.9% of primary energy can thus be obtained per battery pack by using the water-based manufacturing instead of the conventional NMP-based manufacturing.

2.3. Life cycle impacts of the lithium ion battery pack

The life cycle impacts of the lithium ion battery pack produced from the water-based manufacturing processes are calculated for the 13 impact categories in the ReCiPe method, including GWP (Global warming), FDP (Fossil depletion), FEP (Freshwater eutrophication), FETP (Freshwater ecotoxicity), HTP (Human toxicity), MEP (Marine eutrophication), METP (Marine ecotoxicity), MDP (Metal Depletion), ODP (Ozone depletion), PMFP (Particulate matter formation), POFP (Photochemical oxidant formation), TAP (Terrestrial acidification), and TETP (Terrestrial ecotoxicity). In order to understand the proportions of the impacts and identify the hotspots of the life cycle impacts, a contribution analysis of the life cycle impacts has been conducted on both the battery components and the battery life cycle stages. Figure 5 shows the contributions of each battery component (in colour bars) and contributions of each life cycle stage (in pattern bars) to the total life cycle impacts of the battery pack during its cradle to gate life cycle.

The covered life cycle stages are: raw material extraction, material processing, and battery production. The battery production, combing battery component manufacturing, pouch cell manufacturing and battery pack assembly, dominates the GWP impact category with 59% share, due to the heavy energy consumption in the battery pouch cell manufacturing. The raw material extraction stage dominates the FETP, FEP, HTP, METP, and MEP categories, with shares of 75%, 81%, 82%, 73%, and 62%, respectively. The material processing is the main contributor to the PMFP, MDP and TAP, contributing 71%, 60%, and 75%, respectively.

As to the contributions of each individual battery component, the pouch cell production accounts for 53% of GWP, and 54% of FDP, respectively, mainly because of the large energy consumption in battery manufacturing, particularly

during the process drying and dry room conditioning. The NMC cathode dominate the impacts of PMFP, MDP and TAP, contributing 68%, 52%, and 72%, respectively. The anode materials dominate the impacts of FETP, FEP, HTP, METP, and MEP, with 74%, 79%, 82%, 72% and 56%, respectively.

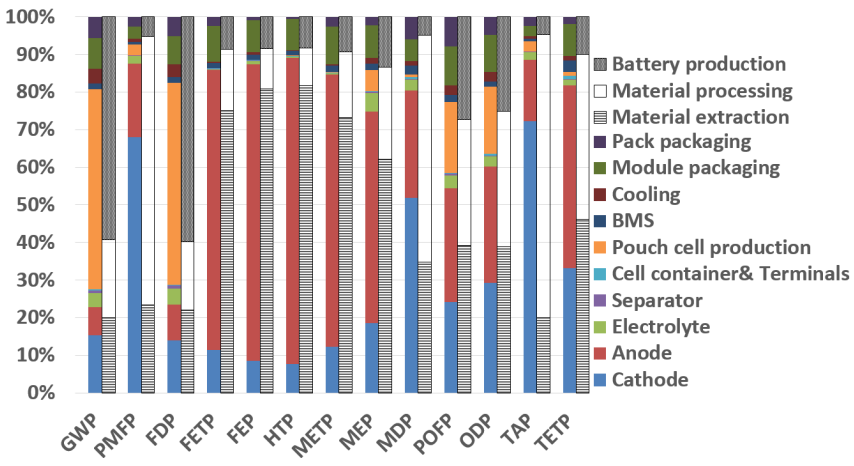

Figure 5 Cradle-to-gate life cycle impacts of the battery pack

2.4. Reference battery from conventional manufacturing process

The reference battery pack chosen for comparison is a NMC-graphite battery pack with the same weight of 417 kg, including 384 pouch cells produced with the conventional NMP-based manufacturing processes [16]. The battery pack is also configured with the BatPaC software from Argonne National Lab. Based on the actual specific capacity, the reference battery pack has 66 kWh capacity.

3. Life cycle impact benchmarking of lithium ion battery pack

The cradle-to-gate life cycle impacts of the NMC-graphite battery pack produced from the water-based manufacturing processes are benchmarked with those of the reference battery pack across the 13 impact categories as characterized by ReCiPe method on the same functional unit of 1kg battery pack produced. The benchmarking results of the two battery packs from the water-based and NMP-based manufacturing processes are shown in Figure 6 below, presented with their life cycle stage contributions to each battery's cradle-to-gate life cycle impacts.

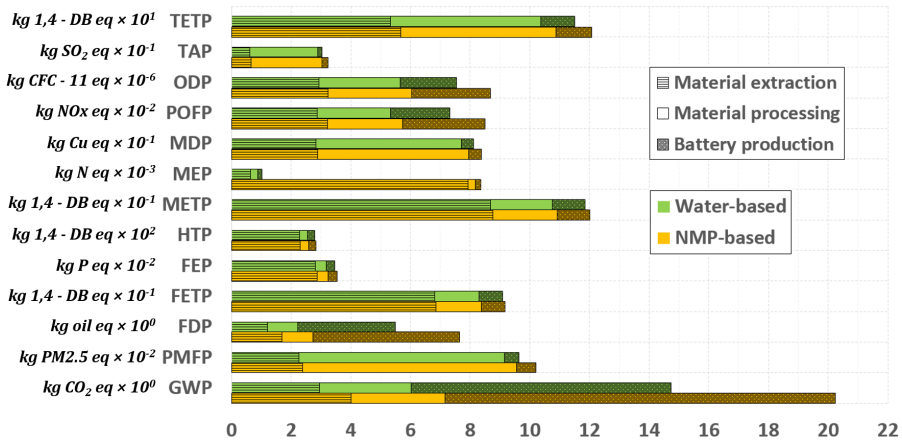

Figure 6 Benchmarking of cradle-to-gate life cycle impacts between water-based battery pack and NMP-based battery pack

From Figure 6, the battery pack produced from the water-based manufacturing processes has lower environmental impacts than the battery pack produced from conventional NMP-based manufacturing processes, for all the 13 impact categories as characterized using ReCiPe. A large difference is found for global warming where the impact potential of the water-based battery pack is 14.7 kg CO_{2eq}/kg battery, compared to 20.2 kg CO_{2eq}/kg battery for the conventional NMP-based battery – hence 27% lower. The difference is mainly due to the significantly reduced energy consumption in the battery manufacturing processes, with the reduced process heating energy much more than the introduced embedded energy in the added deionized water. The largest reduction in the life cycle impact is observed for the MEP where use of the water-based manufacturing processes can reduce the impacts of the battery pack by 88% from the conventional NMP-based manufacturing processes. But the water-based processes will consume more water. As an estimate, the global water footprint of the water-based battery manufacturing could be 7.84×10^{14} kg of water annually if all EVs employ the water-based battery pack in future, per the IEA (International Energy Agency) estimates of global EV fleet to increase from 7.6 million in 2019 to 245 million in 2030 [20].

It should be noted that the production of NMC-graphite pouch cells with water-based manufacturing processes is still operated at lab-scale and hence yet not up-scaled to commercial production and still with some uncertainties. There is potential for reducing the quantity of deionized water that is used to process the battery materials, and this will further reduce the drying energy and the life cycle impacts from the embedded energy in the deionized water. Furthermore, with the development of new binders to use with the water-based manufacturing process, the electrochemical performance of the battery cells can be further improved which will allow reducing the material use for the battery cells and thereby further lower their embedded energies and associated environmental impacts.

4. Conclusions

Water-based manufacturing of lithium ion battery is developed as an alternative to the conventional NMP-based manufacturing processes and in this study, a novel life cycle study is conducted to determine the cradle-to-gate impacts of a 57 kWh lithium ion battery pack containing 384 NMC-graphite pouch cells produced from water-based manufacturing processes. The specific energy consumption in the water-based manufacturing of the NMC-graphite battery is found at 19kWh/kg battery pack manufactured, 43% lower than that of the conventional NMP-based manufacturing processes. The cradle-to-gate impacts of the battery pack produced with the water-based processes are also considerably lower with a saving of 27% global warming potential, and 88% marine eutrophication as the extremes. Considering the remaining potential of optimization, the study shows the water-based manufacturing processes as a promising development path for a more environmentally sustainable lithium ion battery manufacturing.

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