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Life cycle assessment of lithium sulfur battery for electric vehicles

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HIGHLIGHTS

- A hybrid LCA model is developed for lithium-sulfur battery for the first time.
- The inventory data are based on laboratory experiment and literature.
- The impacts are benchmarked with conventional lithium ion battery.
- Potential improvements to meet the USABC targets are identified.

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ABSTRACT

Lithium-sulfur (Li-S) battery is widely recognized as the most promising battery technology for future electric vehicles (EV). To understand the environmental sustainability performance of Li-S battery on future EVs, here a novel life cycle assessment (LCA) model is developed for comprehensive environmental impact assessment of a Li-S battery pack using a graphene sulfur composite cathode and a lithium metal anode protected by a lithium-ion conductive layer, for actual EV applications. The Li-S battery pack is configured with a 61.3 kWh capacity to power a mid-size EV for 320 km range. The life cycle inventory model is developed with a hybrid approach, based on our lab-scale synthesis of the graphene sulfur composite, our lab fabrication of Li-S battery cell, and our industrial partner's battery production processes. The impacts of the Li-S battery are assessed using the ReCiPe method and benchmarked with those of a conventional Nickle-Cobalt-Manganese (NCM)-Graphite battery pack under the same driving distance per charge. The environmental impact assessment results illustrate that Li-S battery is more environmentally friendly than conventional NCM-Graphite battery, with 9%–90% lower impact. Finally, the improvement pathways for the Li-S battery to meet the USABC (U.S. Advanced Battery Consortium) targets are presented with the corresponding environmental impact changes.

1. Introduction

The ground transportation sector generates approximately 27% of the total greenhouse gas (GHG) emissions in the U.S [1]. To address global warming concerns, the U.S. EPA has set a regulatory standard to reduce the average GHG emissions of the U.S. light passenger vehicles from 225 g $mile^{-1}$ in 2016 to 143 g $mile^{-1}$ in 2025 [2], mainly to be achieved through adoption of electric vehicles (EVs) [3–5]. Current EVs are all powered by lithium ion batteries (LIBs) due to their high energy density and higher power density relative to other battery technologies. However, with 80–150 Wh kg^{-1} energy density [6–8], current LIBs on board of EVs are not able to power the EVs for a comparable driving range with conventional vehicles. Meanwhile, current LIB technologies generate significant environmental impacts during their life cycle. For example, current LIBs consume 1141-1224 MJ-equivalent energy and generate 57–85 kg CO_2 equivalent emissions per kg battery during their life cycle [9,10]. Recent years have witnessed rapid progress on the research and development of next-generation battery technologies with higher energy density and better environmental performance.

Among various battery technologies under development, lithium-sulfur (Li-S) battery is widely recognized among the most promising battery technologies for next generation EVs [11–14]. Compared to the conventional Li-ion battery, Li-S battery offers a

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much higher energy density, i.e., sulfur with a specific capacity of 1672 mAh g^{-1} [14], corresponding to a high theoretical energy density of ~2600 Wh kg^{-1}. Besides, sulfur is abundantly available in nature and often considered as a more environmentally benign material than those heavy metals used in conventional lithium-ion batteries [15].

Li-S batteries have been facing some technical challenges, including rapid capacity fading due to the dissolution of sulfur active materials from the polysulfide shuttle effect, low ionic and electronic conductivity of the sulfur material, and low coulombic efficiency and dentrite growth of lithium metal anode, which all affect the battery life and cause safety hazard [12,14,16]. After recent years of intensive research and development, these technical challenges can now be effectively addressed. The dissolution of sulfur problem in Li-S batteries can be suppressed by confining the sulfur in thin film layered materials such as graphene [17–20]. Graphene including reduced graphene oxide has such functional groups as hydroxyl, carboxyl and ester groups which can effectively bind S_8 and polysulfide species, and hence to successfully trap polysulfide from dissolution [21]. It has been reported that the graphene-sulfur composite (GSC) with nitrogen-doping can achieve a stable cycling performance up to 1440 mAh g^{-1} with a decay rate as low as 0.028% over 2000 cycles [22]. Another study demonstrates that depositing nanosulfur on graphene layers can result in a low capacity fading of 0.039% per cycle over 1500 cycles in an ionic liquid electrolyte [23,24]. Recently, a water-based solution precipitation method has been developed for GSC production with a high yield rate, which eliminates the use of toxic solvents and is regarded as a low-cost and environmental-friendly process, with promising potential for future industrial-scale productions [20,22,25]. The low conductivity problem of sulfur can be resolved by adding such conductive additives as carbon black, carbon nanotubes, etc. in the active material [14].

The low coulumbic efficiency and safety concerns of using a lithium metal anode in the Li-S battery can be addressed by the formation of a passivation layer on the lithium metal surface to isolate the anode from undesired side reactions to suppress dendrite growth and improving coulumbic efficiency [16,26–28]. The passivation layer in nature is a lithium ion conducting ceramic membrane [29] that can be artificially produced by treating the lithium metal surface with such chemicals as tetraethoxysilane (TEOS) [30], chlorosilane [31], nitrogen [32], etc. In another way, a thin layer of materials including interconnected hollow carbon spheres [28], polymer nanofibres [33] and metal oxides [34] can also be coated onto the lithium metal surface prior to cell manufacturing to obtain the protective effect. Recently, the atomic layer deposition (ALD) technology has been applied for lithium metal anode protection through depositing a thin layer of Al_2O_3 [34]. In addition, $LiNO_3$ can be added into the lithium bistrifluoromethanesulfonimidate (LiTFSI) electrolyte in the dimethyl glycol (DME) and Dioxolane (DOL) solution to enhance the formation of the protective layer by reacting with the polysulfide species and lithium metal material [16,35]. It is also reported that adding $LiNO_3$ into the LiTFSI electrolyte can greatly improve the safety performance of the lithium metal anode in Li-S batteries [23] and also can substantially reduce the self-discharging of Li-S batteries from over 10% per day to less than 2% per month [36–38]. All these technical advances have prepared the Li-S battery as a promising alternative to the conventional Li-ion battery for next generation EV applications.

Li-S batteries are ready to enter commercial production for next generation EV applications [39–41]. The European Union has launched an Advanced Lithium Sulfur battery for EV (ALISE) project to promote the applications of Li-S battery on EVs in future. Current industrial prototypes of Li-S battery have already achieved 300 Wh kg^{-1} at the cell level and 200 Wh kg^{-1} at the battery pack level, almost twice of conventional LIBs on EVs [40]. While Li-S battery is promising for next generation EV applications, the life cycle environmental impacts of Li-S batteries have never been studied and understood. The Li-S battery uses a wide variety of toxic chemicals in the electrode/electrolyte material synthesis and manufacturing processes, including hydrogen fluoride, sulfuric acid, hydrogen chloride, etc. Besides, the Li-S battery requires energy-intensive processes for the electrode materials and cell manufacturing. For instance, the synthesis of the GSC involves 1–2 h of sonication of the GSC solution with an energy input of 140–300 kW per cubic meter [42,43]; battery cell manufacturing requires a 100–150 °C process heating to evaporate off the NMP solvent through around 8 h of continuous operation [44], as well as dry room facility to maintain a moisture level less than 100 ppm. As the Li-S battery is rapidly moving toward commercial-scale production, it is important to perform a comprehensive life cycle assessment (LCA) of Li-S battery technology to quantify and understand its potential environmental impacts.

In this paper, we developed a hybrid LCA model for an Li-S battery pack for EV application, using a graphene-sulfur cathode, a lithium metal anode, and LiTFSI electrolyte. The graphene-sulfur synthesis is modelled from our lab-scale fabrication process, and the battery cell manufacturing processes are modelled with actual data collected from our industrial partner's pilot scale production facilities. The life cycle environmental impacts are assessed by the ReCiPe method [45]. To understand the relative significance of the impacts, the life cycle environmental impacts of the Li-S battery are benchmarked with those of a conventional LIB pack using a Lithium-Nickel-Cobalt-Manganese oxide cathode and a graphite anode (NCM-Graphite). The LCA results can be useful in sustainable design and manufacturing of Li-S battery packs for future EV applications.

2. Method

2.1. Li-S battery pack configuration for a mid-size EV

The Li-S battery pack in this study is configured to power a mid-size EV for a 320 km driving distance (D) per charge with 120 kW power (Fig. 1, Section 1 and calculations supplied in the electronic supporting information (ESI) for details) [46]. For the battery system configuration, first, the battery energy for traction at wheel ($E_{traction,\ i}$) is calculated for the EV at various speeds under both highway and local driving conditions, respectively, using the EPA Urban Dynamometer Driving Schedule (UDDS) and Highway Fuel Economy Test (HWFET) patterns (Section 1.1 in the ESI) [47]. The amount of energy discharged ($E_{discharged,\ i}$) from the Li-S battery pack is the sum of traction energy divided by the product of motor efficiency (η_{motor}) and the EV transmission efficiency ($\eta_{transmission}$), plus the energy consumed by the auxiliary system (P_{aux}). The specific energy consumption is the ratio of the discharged energy ($E_{discharged,\ i}$) over the distance of the driving schedule (s_i). Afterwards, the composite discharged energy ($E_{discharged}$) is the weighted-sum of specific energy consumptions. The weight factors (a:b) is set to be 45%:55%, which is the distance ratio of local and highway driving under the U.S. national average [48]. Finally, the nominal capacity of the Li-S battery pack, with 85% accessible fraction by user (UR), is calculated as the ratio between the amount of energy discharged from the battery pack and the battery discharging efficiency (($\eta_{discharging}$), while the total energy drawn from the wall outlet can be calculated as the ratio of the stored energy (E_{stored}) over the product of battery charging (($\eta_{charing}$) and charger efficiencies. The vehicle mass (M), as required for $E_{traction}$