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# Energy use and climate change improvements of Li/S batteries based on life cycle assessment

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## HIGHLIGHTS

- LCA showing how to improve energy use and climate change of Li/S cell production.
- Energy use and climate change impact can be reduced by 54 and 93%, respectively.
- Important to reduce cell production electricity and source renewable electricity.
- Best-case climate change is similar for Li/S and lithium ion batteries.

## ARTICLE INFO

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## ABSTRACT

We present a life cycle assessment (LCA) study of a lithium/sulfur (Li/S) cell regarding its energy use (in electricity equivalents, $kWh_{el}$) and climate change (in kg carbon dioxide equivalents, $CO_2$ eq) with the aim of identifying improvement potentials. Possible improvements are illustrated by departing from a base case of Li/S battery design, electricity from coal power, and heat from natural gas. In the base case, energy use is calculated at 580 $kWh_{el}$ $kWh^{-1}$ and climate change impact at 230 kg $CO_2$ eq $kWh^{-1}$ of storage capacity. The main contribution to energy use comes from the LiTFSI electrolyte salt production and the main contribution to climate change is electricity use during the cell production stage. By (i) reducing cell production electricity requirement, (ii) sourcing electricity and heat from renewable sources, (iii) improving the specific energy of the Li/S cell, and (iv) switching to carbon black for the cathode, energy use and climate change impact can be reduced by 54 and 93%, respectively. For climate change, our best-case result of 17 kg $CO_2$ eq $kWh^{-1}$ is of similar magnitude as the best-case literature results for lithium-ion batteries (LIBs). The lithium metal requirement of Li/S batteries and LIBs are also of similar magnitude.

## 1. Introduction

Hybrid and electric vehicles (xEVs) are an emerging technology with the potential to reduce the use of fossil fuels. Life cycle assessment (LCA) [1–3] has been used in a number of studies to compare electric vehicles to hybrid and fossil-fueled vehicles and to investigate whether such a replacement would in fact lead to reduced environmental impacts, with a positive result given electricity produced from renewable sources [4]. For xEVs, production of the vehicle and extraction of the required raw materials for the lithium-ion batteries (LIBs) used are then the dominating life cycle phases, in contrast to fossil-fueled vehicles where the use phase typically is most impacting. In particular, the production of the LIBs is a major contributor [4,5], and the potential increase in use of scarce metals in LIBs, such as lithium, cobalt and nickel, is problematic. Also natural graphite, the preferred LIB anode, might become scarce and is classified as critical to the European Union due to high supply risk [6]. Therefore, the development of batteries and battery concepts less dependent on scarce materials is warranted. The lithium-sulfur (Li/S) battery is one such promising technology requiring no scarce elements except for the lithium metal itself. In addition, it has a promise of higher specific energy densities (400–500 Wh $kg^{-1}$ at the cell level) than current LIBs (*ca.* 250 Wh $kg^{-1}$) [7,8].

While LIBs has been studied extensively by LCA [5,9–13], there is, to the best of our knowledge, only a single cradle-to-grave LCA study on

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Li/S batteries [14]. They considered a wide range of environmental impacts, including climate change, acidification and toxicity. Of the battery materials considered, the electrolyte was the largest contributor to the life cycle energy use (30%), but overall, different life cycle phases dominated different environmental impacts. Since a fossil-dominated electricity mix was assumed for the use phase, this phase dominated the climate change impacts.

Here, we perform an in-depth cradle-to-gate study on the Li/S battery cell, from the extraction of raw materials to the production of the cell. A cradle-to-gate approach is chosen over a cradle-to-grave since data on e.g. life-length and usage conditions are lacking, and hence the total energy throughput and similar parameters cannot yet be accurately estimated. Our aim is to guide Li/S cell developers and producers on how to improve environmental performance, much as Zackrisson et al. [10] did for LIBs. We consider a Li/S cell with typical current state-of-the-art materials choices [15–17]: (i) a lithium metal anode, (ii) a composite carbon/sulfur (C/S) cathode of mesoporous carbon and elemental sulfur, and (iii) a liquid organic solvent-based electrolyte.

## 2. Method and materials

All material and energy flows related to the cradle-to-gate production of a Li/S battery cell are quantified in terms of a functional unit (FU) reflecting the function of the product, in this case 1 kWh of specific energy storage. Flows crossing the boundary between the technosphere and the environment are calculated into environmental impact categories [18]:

$$I = \sum_{i,j} q_{i,j} C_i \tag{1}$$

where $I$ is the environmental impact, e.g. energy use or climate change [impact $FU^{-1}$]), $q$ is the quantity of emitted substance or resource used [amount $FU^{-1}$], $C$ is a characterization factor (CF) that reflects the impact of the emitted substance or resource used [impact $amount^{-1}$], $i$ is the emitted substance or resource type (e.g. carbon dioxide or hard coal), and $j$ is a process in the product's life cycle.

We perform an attributional LCA of the Li/S cell and of different improvements, effectively identical to a consequential LCA where only first-order (linear) physical flow consequences are considered [19] – or "a consequential LCA based on the attributional [LCA] framework" [20].

### 2.1. Technology studied and system boundaries

The Li/S cell material composition and balance (Table 1) was obtained from a cell developer, and hence no exact amounts and sources can be provided for confidentiality reasons. A generic organic liquid electrolyte of 1 M lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) in dioxalane/dimethoxyethane (DIOX/DME) with 0.2 M lithium nitrate ($LiNO_3$) as additive [15] was used. For the composite C/S cathode, a mesoporous carbon, CMK-3, and elemental sulfur [16] was employed. Other carbon materials are considered in a scenario analysis (Section 2.4). An aluminium foil is used as current collector for the cathode, a lithium metal foil is both active material and current collector for the anode, and the separator is a typical micro-porous polyolefin membrane made of polypropylene (PP) and polyethylene (PE) in a tri-layer configuration (PP-PE-PP). The two main differences as compared to the cell of Deng et al. [14] is that they employed a copper current collector for the anode and a C/S composite made from graphene oxide and sodium thiosulfate.

**Table 1**
Composition of the Li/S cell.

| Component | Material | Mass [g $cell^{-1}$] |
|---|---|---|
| Anode | Lithium foil | ~4 |
| Cathode + Current collector | C/S composite | ~4 |
| | Aluminium foil | ~3 |
| Electrolyte | DIOX | ~9 |
| | DME | ~11 |
| | LiTFSI | ~8 |
| | $LiNO_3$ | ~0.5 |
| Separator | Tri-layer PP-PE-PP membrane | ~6 |
| Total | | ~45 |

In this cradle-to-gate study, the gate is the exit of the battery cell production facility (Fig. 1). A cut-off limit of 1% of the main product mass was employed for each unit process. Water flows were excluded because of the low impact for water for the considered impact categories, e.g. ~0.0005 $kWh_{el}$ $kg^{-1}$ and ~0.001 kg $CO_2$ eq $kg^{-1}$ for deionised water produced in Europe [21].

### 2.2. Allocation

In the production system, by-products are produced, such as chlorine gas ($Cl_2$) during the production of lithium from lithium chloride (LiCl) and various by-products from petroleum refining (see the Supplementary data). Since economic value is the driver of most industrial processes [22,23], economic allocation based on price was applied to partition the environmental impact between products and by-products [24]:

$$P_i = \frac{n_i x_i}{\sum_i n_i x_i} \tag{2}$$

where $P_i$ is the partitioning factor of product $i$, $n_i$ is the mass of $i$ produced and $x_i$ is its price. Price data (2005) were obtained from the Ecoinvent database [21]. In addition to economic allocation, in a sensitivity analysis we apply allocation by mass and no allocation, i.e. allocating all impact to the main product. Mass allocation has been advocated because mass relationships are more fundamental than the prices of products [24]. The no-allocation approach is unconventional in LCA and can be seen as a worst case for the Li/S cell with regard to allocation.

### 2.3. Impact categories

Two key impact categories are considered: energy use and climate change. All energy used is re-calculated into electricity equivalents [$kWh_{el}$] to enable comparisons between different energy flows with electricity as a 'common currency' [25,26]: (i) electricity is added as is, (ii) heat is converted at an efficiency of 37% to represent an electricity-generating turbine [27], and (iii) chemical energy in the form of energy carriers (e.g. diesel) and materials (e.g. polyethylene) were traced back to their respective primary sources, both renewable and non-renewable, and converted at efficiencies of 43% for natural gas, 32% for coal and 33% for crude oil, biomass and uranium [28] (Fig. S1).

Climate change [kg $CO_2$ eq], sometimes referred to as global warming potential [29], is modelled according to the ReCiPe 2016 impact assessment method [30] with a 100-year time-frame.

In addition to these two key impact categories, due to the potential future scarcity of lithium [31], lithium use is quantified as input mass to the production system. Due to the ongoing discussion on the relevance of different methods for assessing mineral resource depletion [32,33], this impact category is not considered.

### 2.4. Scenario analysis and sensitivity

In addition to a base scenario (Table 1), we consider five improvement scenarios. First, battery cell production electricity requirement is reduced. Deng et al. [14] modelled an operational pilot-scale production facility and arrived at 47 kWh $kg^{-1}$ of Li/S cell, but also a potential future industrial-scale production with a *ca.* 77% reduction to 11 kWh $kg^{-1}$, which we apply. For the C/S composite cathode,

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