Prospective Life Cycle Assessment of a Model Magnesium Battery

Sebastián P. Bautista, Marcel Weil, Manuel Baumann, and Claudia Tomasini Montenegro*

Energy-storage systems are considered as a key technology for energy and mobility transition. Because traditional batteries have many drawbacks, there are tremendous efforts to develop so-called postlithium systems. The magnesium–sulfur (MgS) battery emerges as one alternative. Previous studies of Mg–S batteries have addressed the environmental footprint of its production. However, the potential impacts of the use-phase are not considered yet, due to its premature stage of development. Herein, a first prospective look at the potential environmental performance of a theoretical Mg–S battery for different use-phase applications is given to fill this gap. By means of the life cycle assessment (LCA) methodology, an analysis of different scenarios and a comparison with other well-established technologies are conducted. The results suggest that the environmental footprint of the Mg–S is comparable with that of the commercially available counterparts and potentially outperforms them in several impact categories. However, this can only be achieved if a series of technical challenges are first overcome.

1. Introduction

The increased penetration of renewable energy technologies and large deployment of electric vehicles, pillars of energy transition for a sustainable future, have raised great interest on storage systems capable of mitigating the inherent challenges that arise with this paradigm shift. On the one hand, the intermittent nature of renewable systems such as solar and wind power poses a risk to grid stability. Energy storage during peak generation times with subsequent feedback during low generation times would provide flexibility to the grid by mitigating potential imbalances of generation and demand. At the same time, the development of e-mobility would benefit from safer battery packs exhibiting high energy densities. Battery development thus has become the subject of continuous research and development efforts, but a large-scale expansion of these technologies must comply with environmental, economic, and social sustainability criteria. This compliance shall be continuously addressed over the different stages of technology development, from initial concept design to final commercialization. The batteries' market has been dominated in the past few decades by well-established technologies such as lead acid (PbA) and more recently lithium-ion (LIB) systems, but environmental and socioeconomic concerns such as use of toxic and scarce materials among others have led to questioning the sustainability of these technologies, especially critical for a growing market.[1–6] The establishment of a recycling industry seeks to mitigate these issues, with achieved success for the PbA systems and ongoing efforts for the LIBs.[7] Nevertheless, research efforts have been made, aiming not only to lower the environmental hotspots of these technologies but also to provide new alternatives that are not bounded to these problems—so called postlithium batteries.[8] Ultimately, an integration of a broad variety of storage systems will grant robustness and enhanced efficiency to the future energy grid. Sodium- and magnesium-based batteries are considered as some of the most promising postlithium systems.[9,10] In particular, the magnesium–sulfur (Mg–S) battery emerges as a promising alternative, given its high theoretical capacity, its potential low costs, and lower associated safety concerns.[11] For the time being, this type of battery is found at a very early stage of development, with active research and ongoing proof of concepts on the laboratory scale. Therefore, it still has to overcome several technological challenges before being able to compete with other systems available in the market. However, first evaluations are already possible based on a tested pouch-cell prototype built within the framework of the Mag–S project, funded by the German Federal Ministry of Education and in cooperation with Custom Cells Itzehoe (CCI) GmbH in Germany.[12] The analysis herein conducted gives continuity to previous studies by Montenegro et al.,[13,14] which already evaluated the potential environmental impacts of the Mg–S battery production, extending the analysis to include the potential impacts of the use-phase of the battery. This extended approach becomes relevant due

Dr. M. Weil, Dr. M. Baumann
ITAS
Institute for Technology Assessment and Systems Analysis
Karlsruhe Institute of Technology
Karlsruhe, Germany
E-mail: marcel.weil@kit.edu

S. P. Bautista, Dr. M. Weil, Dr. C. T. Montenegro
HIU
Helmholtz-Institute for Electrochemical Energy Storage
Helmholtzstr. 11, Ulm 89081, Germany

The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/ente.202000964.

DOI: 10.1002/ente.202000964

to the complexities introduced when evaluating different application scenarios. An example of these complexities was described by Baumann et al.,[15] who conducted a multicriteria decision-making analysis of eight different battery-storage technologies for four different applications to estimate the overall suitability of these technologies. The results suggest great versatility from the LIBs, suitable for most applications, but also indicate high influence of the considered use case, as it was the case of PbA and vanadium redox flow batteries (VRFBs).

2. Previous Work on Mg–S Batteries

The Mg–S battery has been the subject of study over the past few years. Wang and Buchmeiser[16] conducted a comprehensive review about the state of the art of the Mg–S batteries. Some of the major existing challenges relate to the formation of magnesium polysulfide that lead to severe overcharging, loss of active material, and low sulfur utilization, which translates into a short cycle life and capacity fading. Another major challenge relates to the compatibility of electrodes and electrolyte, as the Mg anode reacts with traditional carbonate-based electrolytes like the ones used in Li batteries. This creates an impermeable layer on the Mg surface, which hinders Mg deposition and dissolution. Further research seeks to fully understand the reactions at the interfaces within the battery as well as the effect of temperature on the self-discharge rate and sulfide formation.[17] At the same time, new electrode and electrolyte materials are being tested with the goal of achieving enhanced conversion kinetics and better discharge capacities.[18,19]

The first environmental assessment for the Mg–S battery, to the best of the authors' knowledge, was conducted by Montenegro et al. (2019)[13] based on the first pouch-cell prototype for this type of battery.[12] The authors used the life cycle assessment (LCA) methodology to evaluate the potential environmental impacts of the battery manufacture stage, also called cradle-to-gate analysis. This methodology allows estimating the environmental burdens in several impact categories based on specific indicators and characterization factors. The authors conducted an evaluation of a baseline system in accordance with the prototype cell, which had an energy density of 57 Wh kg^{-1} on the cell level and an estimated 46 Wh kg^{-1} on the pack level. A hypothetical industrial-scale battery pack production was considered based on the actual manufacturing processes of LIBs. The outcome exhibits that this baseline system entails significantly a higher footprint than the other commercial systems, inherent to the cell design and let alone the actual electrochemical performance of the cells. The aluminum-containing pouch cell packaging was identified as the main hotspot for global warming potential, abiotic depletion, human toxicity, acidification, and photochemical oxidation potential. Given that this prototype was first conceived to test the electrochemical performance of these types of batteries without special attention to its environmental footprint, the mass composition had been overestimated (the mass share of the housing accounted for about 50% of the total cell mass), leading to the obtained footprint. A further assessment was conducted[14] with the goal to evaluate potential improvements of the baseline model. The authors, in a joint assessment with the cell developers, proposed hypothetically optimized and technically feasible versions of the battery, assuming the redesign of passive components in the form of mass reductions. Two models were proposed: MgS-Evo1 and MgS-Evo2. The first configuration assumed a pouch-cell mass share reduction from 45 wt% (baseline configuration) to 3 wt%. The second model assumed reduced separator thickness and correspondingly a mass share reduction from 10% to 2 wt% based on the state of the art for LIBs. It was found that these optimization processes could significantly reduce the production impacts of the Mg–S battery. In particular, the MgS-Evo2 configuration bears a significantly lower footprint in all of the assessed categories.

3. Life Cycle Environmental Analysis

The environmental assessment hereby conducted follows the guidelines of the LCA methodology defined in the ISO standards 14040/14044.[20,21] This standard procedure comprises four main steps in the execution of an LCA: goal and scope definition, life cycle inventory, impact assessment method, and interpretation of the results.

3.1. Goal and Scope Definition

The goal of the study is to measure the environmental footprint of a hypothetical Mg–S battery for different stationary applications, including the burdens of primary material acquisition, system manufacture, and use-phase. The end-of-life stage has not been included within the system boundaries due to high level of uncertainty arising from the lack of data from the industry and premature state of this technology. However, some indications of the potential impacts of recycling have been presented by Baumann et al.[15] and Mohr et al.[7] These impacts greatly depend on the technology assessed and may lead to a very different picture when included in the overall life cycle, as it is the case for PbA batteries. The environmental impacts are expressed in terms of a functional unit (FU), which in this study has been defined as unit of electricity in MWh stored and delivered by the system.

3.2. Methodology

The LCA provides a profile of the environmental burdens of the system under study during the production and use-phases for different impact categories. The production phase contemplates all the impacts of the supply chain, calculated according to the system size and number of replacements specific of each application. The use-phase impacts arise from the internal energy losses associated with the roundtrip efficiency of the battery, leaving out the production burdens of electricity. The sum of these impacts allows an understanding of the environmental performance of the technology from a comprehensive perspective and already suggests how suitable the battery is for a certain application. The premature state of the Mg–S battery introduces a great level of uncertainty associated with its technical performance. For such reason, it becomes necessary to conduct a sensitivity analysis that takes into account different performance levels to measure their criticality. For the specific case, the sensitivity to cycle life (+/−20%), calendrical life (+/−20%), efficiency (+/−10%), and energy density (+/−20%) will be measured.

The assessment conducted in this study follows the approach described below. 1) Calculation of the production impacts per kg of battery based on the initial datasets. 2) Battery sizing for each application based on system performance and specific application requirements. 3) Calculation of the battery replacements based on calendrical life, cycle life, and application cyclability requirements. 4) Calculation of the production impacts per MWh of electricity stored and delivered normalized for a service life of 20 years based on n° of replacements. 5) Calculation of electricity losses and associated impacts of the use-phase based on battery roundtrip efficiency and electricity source. 6) Sensitivity Analysis for Different Technical Performance Levels.

3.3. System Description

3.3.1. Mg–S Battery

The system used for the analysis is the MgS-Evo2, a redesign of the original pouch-cell prototype proposed in joint assessment with the technology developers, based on the observed potential regarding its environmental performance.[14] This model strictly relates to a mass reduction of some passive components of the prototype, while still using the same materials as initially defined.

The anode is composed of a magnesium foil with a thickness of 100 µm. The composite cathode is prepared by mixing sulfur (50 wt.%), carbon black (40 wt.%), and a water-based carboxymethyl–cellulose/styrene–butadiene–rubber binder (CMC/SBR) (10 wt.%), cast on an aluminum current collector.[12] The development and synthesis of electrolyte has been presented by Zhao-Karger et al.,[22] consisting of a solution of magnesium tetrakis hexafluoroisopropyloxy borate, also referred to as $Mg[B(hfip)_4]_2$, with dimethoxyethane (DME) as the organic solvent. The production process for the ionic conductive salt is very robust and inexpensive, which is advantageous for practical scale-up. In addition, this solution is capable of reversible Mg plating/stripping with high Coulombic efficiencies. It is compatible with many cathode and anode materials, it is thermally stable (up to 150 °C), and also air and hydrolysis stable, making it safe in many applications. However, critical challenges for the MgS system remain, associated with poor cycle stability, low sulfur stabilization, and rapid self-discharge rates, product of a lack of understanding of the interfacial reactions between electrolyte and electrodes. These issues are reflected in potential hysteresis between charge and discharge, as well as degradation of both electrolyte and Mg anode caused by polysulfide dissolution, similar to other metal–sulfur systems, which still hinder the performance of this battery configuration.[23] Nevertheless, the initial objective of the project aimed at achieving a cell capacity of 200 mAh g_{sulfur}^{-1} after 20 cycles. The prototype cell had an initial capacity of about 350 mAh g_{sulfur}^{-1} and was stable for about 20 cycles, reaching a capacity of 221 mAh g_{sulfur}^{-1} after 21 cycles and above 200 mAh g_{sulfur}^{-1} after 100 cycles.[12]

The composition in the pack level and the technical performance of the Mg–S battery herein described corresponds to a hybrid approach that takes into account the observations from the pouch-cell prototype as well as optimistic performance assumptions that do not yet reflect the actual state of the battery at the time when this study was conducted. These assumptions are based on the performance of lithium-based systems under the premise that, with further research, the Mg–S battery could reach such technological maturity and performance level. In particular, the energy density corresponds to a recalculation of the value first described for the Mg–S battery prototype, after having taken into account the mass reduction of the proposed redesign. The assumed cycle life corresponds to the performance described by Ellingsen et al.[24] for an average LIB, despite newer LIBs reporting cyclability as high as 4000 cycles.[25] The roundtrip efficiency, also understood as charge/discharge cycle efficiency, corresponds to the average value of a standard LIB battery.[26] **Table 1** shows the material and mass composition of the initial prototype (namely MgS-BL) and the proposed MgS-Evo2 model as presented in the base study[14] and hereby subject of further analysis. The battery pack has been modeled based on the average composition of LIBs and the inventories for the battery management system (BMS) of the MgS battery have been modeled based on the datasets from Ellingsen et al.[24] to ease comparability.

3.3.2. Reference Technologies

Different battery technologies have been modeled as the benchmark of the potential of the Mg–S system. These technologies include mature and commercial systems such as LIBs: 1) nickel–cobalt–manganese (NCM), 2) lithium–iron–phosphate (LFP), 3) the valve-regulated lead-acid battery (VRLA), and the 4) VRFB system. In addition, a 5) lithium–sulfur battery (LiS) developed on a pilot scale was included, given the broad attention that this emerging technology has recently received,[27] also serving as a benchmark for postlithium systems. The technical characterization for each of these technologies is shown in **Table 2** with reported values found in the literature from Ellingsen et al.,[24] Deng et al.,[27] Zackrisson et al.,[28] Majeau-Bettez et al.,[29] and Baumann et al.[25] A maximum depth of discharge (DOD) of 80% with the respective number of cycles to failure (cycle life) has been assumed for every technology. For the Mg–S battery, the energy density value has been extracted from the study by Montenegro et al.[14] Roundtrip efficiency, cycle life, and calendrical life have been optimistic assumptions made by the authors as initially clarified.

3.3.3. Use-Phase Applications

Different stationary application scenarios for the use-phase are here considered, each one with specific demands in terms of energy rating, cyclability, and source of electricity for a service life of 20 years. It is here assumed that the Mg–S battery is capable of complying with these criteria and thus it will be suitable for these applications; however, this applicability is yet to be evaluated in a further stage of development. For practical purposes, a battery DOD of 80% has been defined for every application. **Table 3** shows the specific demands of the modeled application scenarios, as described by Baumann et al.[25] and Hiremath et al.[26]

Table 1. Mass composition of the Mg–S battery for the prototype and as proposed for the MgS-Evo2 model.[14]

	Item	Material	MgS-BL		MgS-Evo2	
			Mass	%wt.	Mass	%wt.
Battery Cell	Anode	Mg foil	427 mg	6.4%	427 mg	29.0%
	Cathode	Sulfur	421 mg	6.3%	421 mg	28.7%
		Binder	5 mg	0.1%	5 mg	0.3%
		Carbon	5 mg	0.1%	5 mg	0.3%
		Al collector foil	88 mg	1.3%	88 mg	6.0%
	Separator	Polyolefin	700 mg	10.4%	29 mg	2.0%
	Electrolyte	$Mg[B(hfip)_4]_2$ DME	2060 mg	30.7%	451 mg	30.7%
	Housing	Al composite	3000 mg	44.7%	44 mg	3.0%
	Total (cell level)		6706 mg	100.0%	1470 mg	100.0%
	Energy density (cell level)		57 Wh kg^{-1}		259 Wh kg^{-1}	
Battery Pack (1 kg)	Battery cells		0.8 kg	80%	0.8 kg	80%
	Pack housing		0.145 kg	14.50%	0.145 kg	14.50%
	BMS		0.055 kg	5.50%	0.055 kg	5.50%
	Energy density (pack level)		46 Wh kg^{-1}		207 Wh kg^{-1}	
	Roundtrip efficiency		–		90%	
	Cycle life at 80% DOD		–		2600 cycles	
	Calendrical life		–		10 years	

Table 2. Characterization of the different battery technologies.[14,24–29]

Battery type	Roundtrip efficiency	Cycle life at 80% DOD	Energy density battery pack [Wh kg^{-1}]	Calendrical life [years]
LIB–NCM[24]	95	4000[a)]	130.3[b)]	10
LIB–LFP[29]	90	6000	113.8[b)]	10
VRLA[25]	77	1400	45	18
LiS[27]	90	2000	224[b)]	10
VRFB[25]	75	10000	17.0	15

[a)]Updated value from the study by Ellingsen et al.;[24] [b)]Adjusted values from the study by Montenegro et al.[14]

Table 3. Characterization of the application scenarios for a timeframe of 20 years.[25,26]

Application	Required power rating [MW]	Discharge duration [h]	Required energy rating [MWh]	Cycle frequency	
				[Cycles/day]	[Cycles applications]
Increase of self-consumption	0.0025	4	0.010	0.6	4380
EM (community scale)	0.1	2.5	0.25	2	14 600
T&D investment deferral	10	5	50	0.68	4964
Utility ETS	100	8	800	1	7300
SVR	1	0.25	0.25	0.68	4964
RS	2	10	20	1.12	8176

1) Complete utilization of batteries (CUB): baseline scenario. A predefined energy rating is assumed so that each battery has to comply with until end of life due to surpassing their respective cyclability. 2) Photovoltaic self-consumption (PVSC): Electricity from a household rooftop-photovoltaic installation is stored during generation peak times and consumed during low generation periods to reduce grid dependency and electricity costs. 3) Energy management (EM)–community scale: Storage is used to provide flexibility to the energy demand of a community and reduce grid stress during hours of peak demand. 4) Transmission and distribution investment deferral (T&D): Storage systems are used to extend the life of the existing T&D equipment by supporting peak demand times that would otherwise require system upgrades. In this way, investments can be avoided or deferred by a couple of years. 5) Utility energy time-shift (ETS): Storage systems can be used to decouple demand from the utility side over daily time scales. Electricity is stored during low-price generation times and discharged during times of high prices or peak-demand hours. 6) Support of voltage regulation (SVR): Energy storage can serve to support voltage regulation, necessary for proper operation of equipment and prevent damage due to sudden oscillations in the grid. 7) Renewables support (RS): Electricity generated from renewable energy systems such as wind turbines and photovoltaic systems can be stored during times of excess production and distributed during peak demand times to increase penetration of renewables.

3.4. Data Sources and Assumptions

The inventories of the Mg–S battery have been extracted directly from the study by Montenegro et al.[14] The inventories for the other types of batteries have been built based on the literature shown in Table 2. Regarding the electricity mix, the scenarios CUB, EM, T&D, ETS, and SVR have been modeled based on predictions of the German mix for 2030 and under the Business-as-Usual projections estimated by Agora Energiewende.[30] The previous consideration has been made under the assumption that this projection represents the average mix between 2020 and 2040 (for an application and use-phase of 20 years), with a higher penetration of renewables than the present-time mix. Regarding the PVSC scenario, electricity from photovoltaics (PV) has been modeled following the Life Cycle Inventories developed by the International Energy Agency[31] and for a slanted-roof multicrystalline silicon system installed in Germany (annual solar irradiance of 1088 $kWh\,m^{-2}\,a^{-1}$). The scenario RS refers to an electricity mix of PV and wind power with a 50–50 ratio in Germany. The inventories of the foreground processes, those that are not the focus of study, have been extracted from the Ecoinvent 3.5 database. The system boundaries are delimited by the battery pack, which is composed of cells, packaging, and BMS, leaving out additional Balance of Plant (BOP) components such as inverters and external cabling.

3.5. Impact Assessment Method

The impact assessment method selected is the ReCiPe midpoint with hierarchist perspective. This method comprises a set of 18 impact categories evaluated over a time span of 100 years.[32] For practical purposes, a detailed analysis of five of these categories is presented. The chosen categories are "climate change" (kg CO_2-eq), "fossil depletion" (kg oil-eq), "human toxicity" (kg 1,4-dichlorobenzene-eq), "metal depletion" (kg Fe-eq), and "particulate matter formation," (kg PM10-eq) which have been selected based on the perceived relevance that each of the associated topics has in present times. A complete view of all the categories is presented in Supporting Information of this document. An estimation of the cumulative energy demand (CED), expressed as $MJ\,MWh^{-1}$, is also offered. The ReCiPe methodology has its own limitations, especially when measuring the criticality of the material resources required to manufacture the batteries. This obeys a lack of characterization factors capable of measuring the depletion of abiotic resources such as lithium, which becomes especially critical when expecting a large deployment of energy-storage systems. For this reason, a detailed analysis of the "abiotic depletion potential" (ADP) is additionally conducted. This analysis has been made using the updated characterization factors presented in the study by van Oers et al.,[33] that takes into account the annual production and reported reserves of several materials and expresses them as a function of a reference resource (antimony). The modeling of the product systems (batteries and BMS) has been performed with the software OpenLCA.

4. Results

The first part of this section displays the overall performance of the different technologies analyzed in different application scenarios. This allows a direct comparison in each of the selected categories. Similarly, the second part relates to the sensitivity analysis conducted specifically for the Mg–S battery displayed for two main impact categories. As a rule, high values are associated with poor environmental performance. **Table 4** shows the impacts of production per kg of battery for the different systems in this study. It is worth noting that some values obtained for the prototype appear lower than those of the proposed redesign, but these do not take into account the energy density of the system. Therefore, these shall not be mistakenly understood as a better performance of this model.

4.1. Indicative Results

The results in this section are presented for seven different impact categories. A complete view of the 18 categories can be found in the appendix. Each of these is divided according to the different use-phase applications. For each application, the cumulated impact of each battery type is displayed. **Figure 1–7** show the calculated impacts distinguishing between the production and use-phase.

It has been found that the use-phase has a significant contribution to the total "CED" (Figure 1). In particular, the VRFB carries the highest CED in almost every application. Specifically, it has a high contribution of the use-phase associated with its low efficiency, which translates into a higher demand of electricity per MWh stored. On the contrary, the LIB–NMC has the lowest total impacts, even when the contributions of the production phase are higher than those from the production of other batteries. Its high efficiency leads to the lowest use-phase impacts giving it significant advantage over the other technologies. The Mg–S battery is found to be performing on comparable levels as the lithium-ion counterparts, with values of energy demand between

Table 4. Environmental impacts per kg of battery of the prototype and assessed technologies.

Indicator	MgS-BL	MgS-Evo2	LIB–NCM	LIB–LFP	LiS	VRLA	VRFB
CED [MJ]	2.59 E + 02	2.97 E + 02	2.34 E + 02	2.31 E + 02	8.70 E + 02	5.09 E + 01	9.65 E + 01
Climate change [kg CO_2-eq]	1.50 E + 01	1.82 E + 01	1.46 E + 01	1.65 E + 01	3.82 E + 01	3.14 E + 00	6.58 E + 00
Fossil depletion [kg oil-eq]	4.55 E + 00	5.44 E + 00	3.95 E + 00	3.96 E + 00	1.47 E + 01	9.19 E-01	2.10 E + 00
Human toxicity [kg 1,4-DCB-eq]	1.60 E + 01	1.26 E + 01	2.53 E + 01	3.40 E + 01	2.49 E + 01	1.75 E + 01	1.36 E + 01
Metal depletion [kg Fe-eq]	2.00 E + 00	2.25 E + 00	1.82 E + 01	6.01 E + 00	1.02 E + 01	8.99 E + 00	4.71 E + 00
Particulate matter formation [kg PM10-eq]	3.70 E-2	5.62 E-02	6.70 E-02	3.73 E-02	7.39 E-02	1.41 E-02	2.65 E-02
ADP [kg Sb-eq]	1.11 E-02	7.79 E-03	1.30 E-02	1.12 E-02	6.53 E-03	3.08 E-02	4.52 E-04

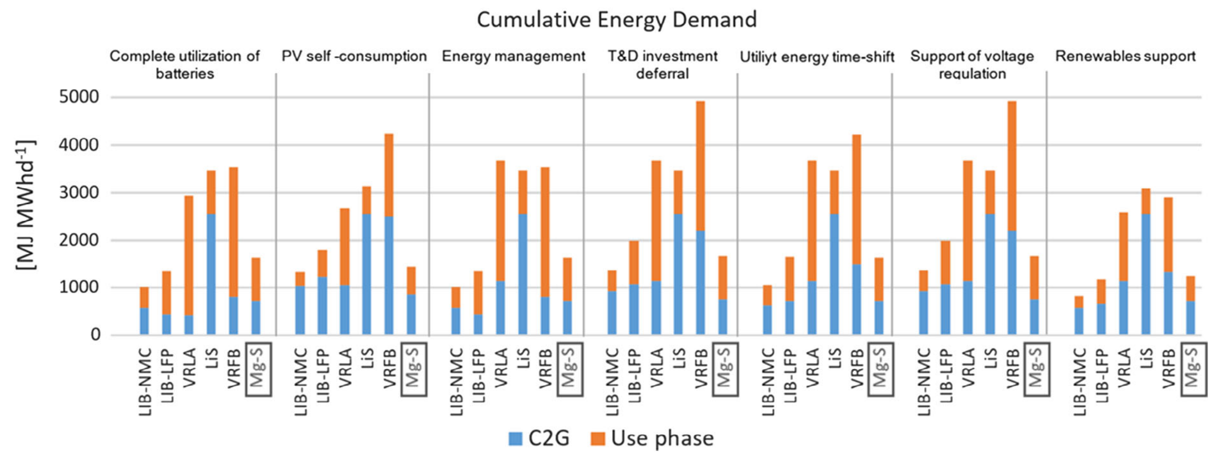

Figure 1. Contributions from the production and use-phase to the total CED.

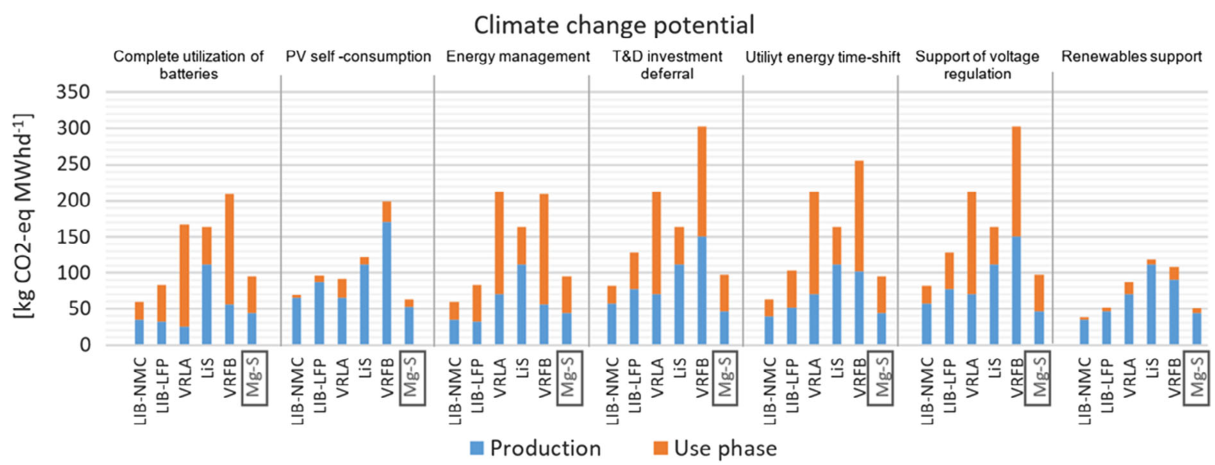

Figure 2. Life cycle impacts of each battery in the “climate change” impact category.

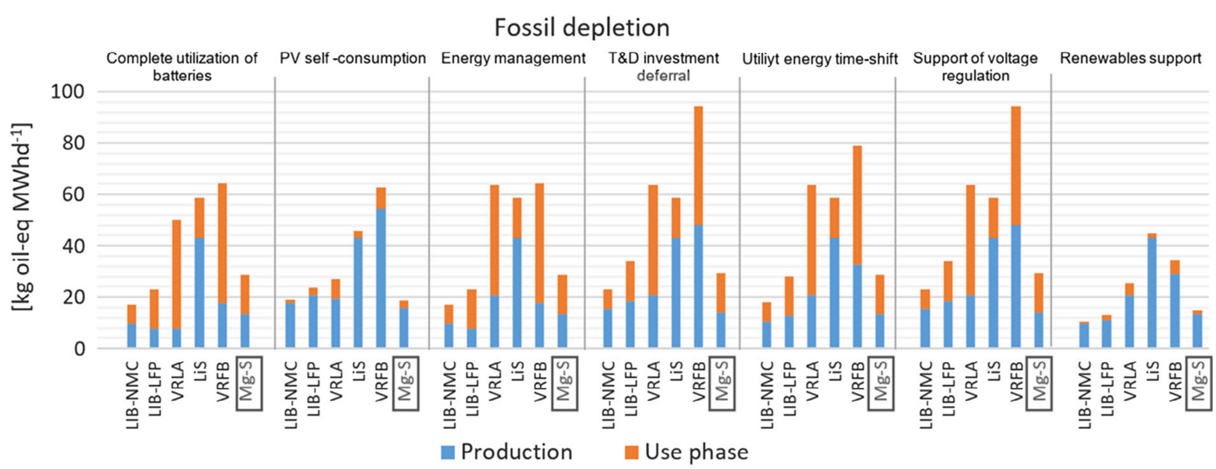

Figure 3. Life cycle impacts of each battery in the “fossil depletion potential” impact category.

1247 and 1670 MJ MWh^{-1}. The Mg–S battery also has an advantage over the LiS system, attributed to the lower energy demand during production. The modeling of the manufacture of the LiS battery corresponds to a pilot-scale model, which is, as reported in the referenced literature, very energy intensive. In addition, the production of the graphene–sulfur composite for the

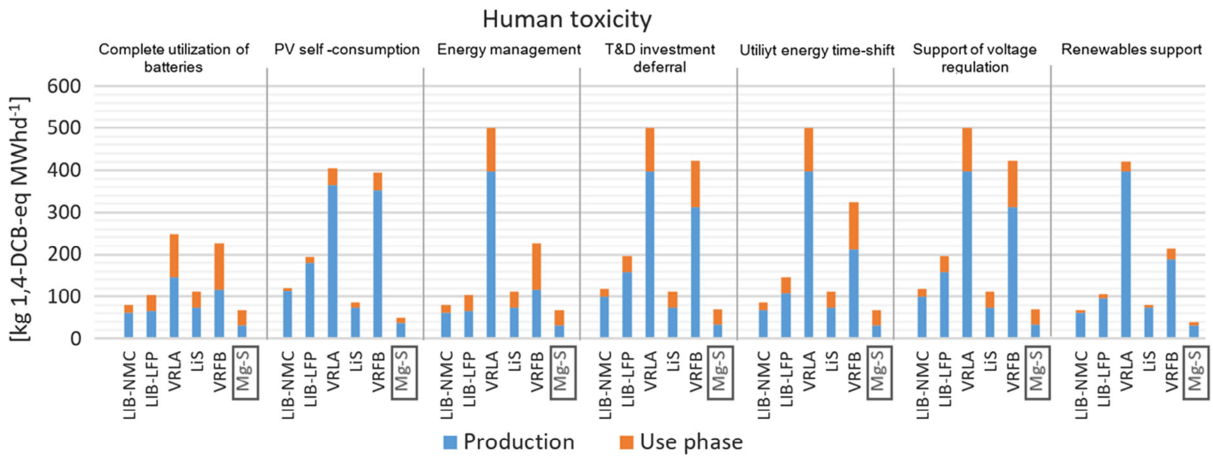

Figure 4. Life cycle impacts of each battery in the "human toxicity potential" impact category.

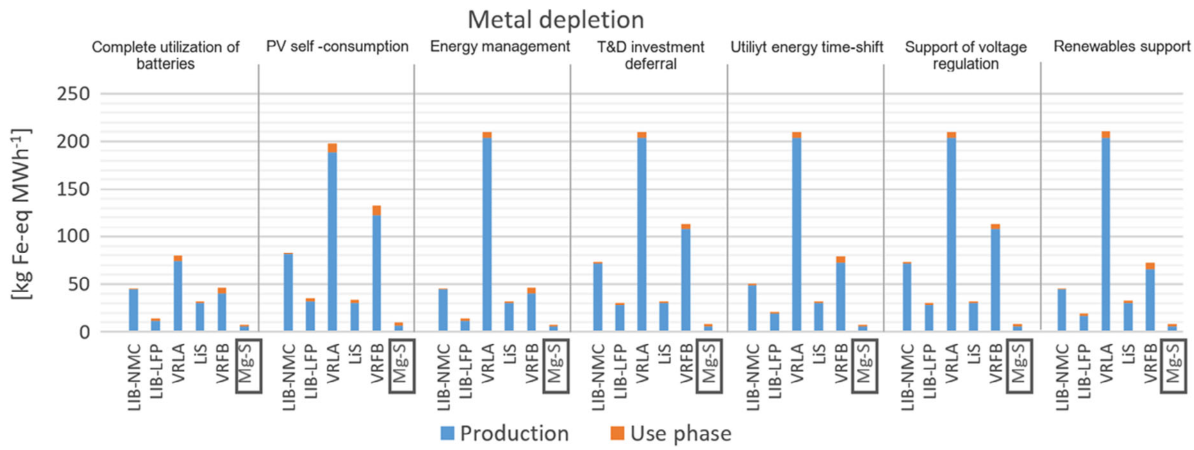

Figure 5. Life cycle impacts of each battery in the "metal depletion potential" impact category.

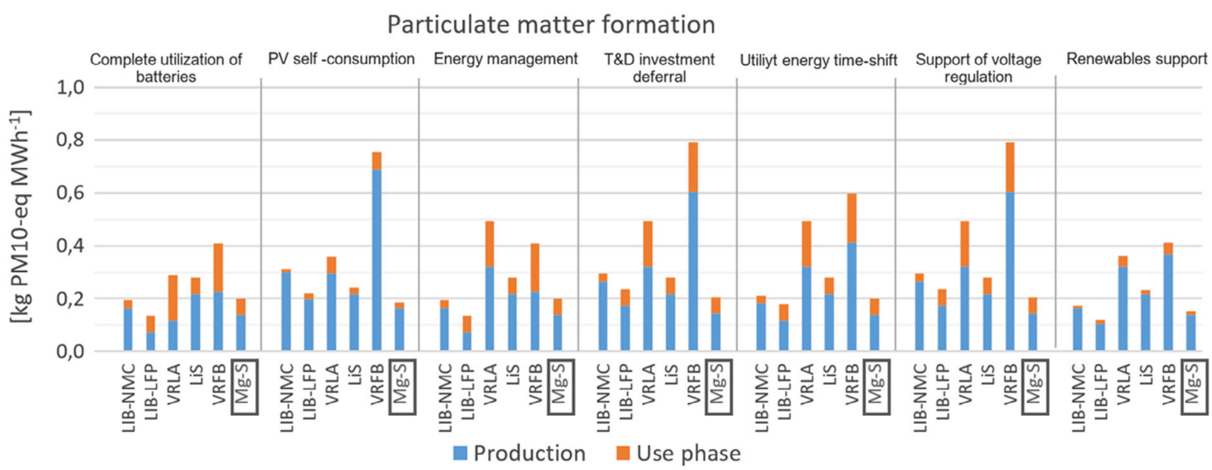

Figure 6. Life cycle impacts of each battery in the "particulate matter formation potential" impact category.

cathode has a large contribution within this category. Finally, the considered cycle life is lower than that of the Mg–S battery and at least half the value of the LIB, which increases the specific burdens per MWh of battery capacity. These leads to similar effects within the "climate change" and "fossil depletion" impact categories.

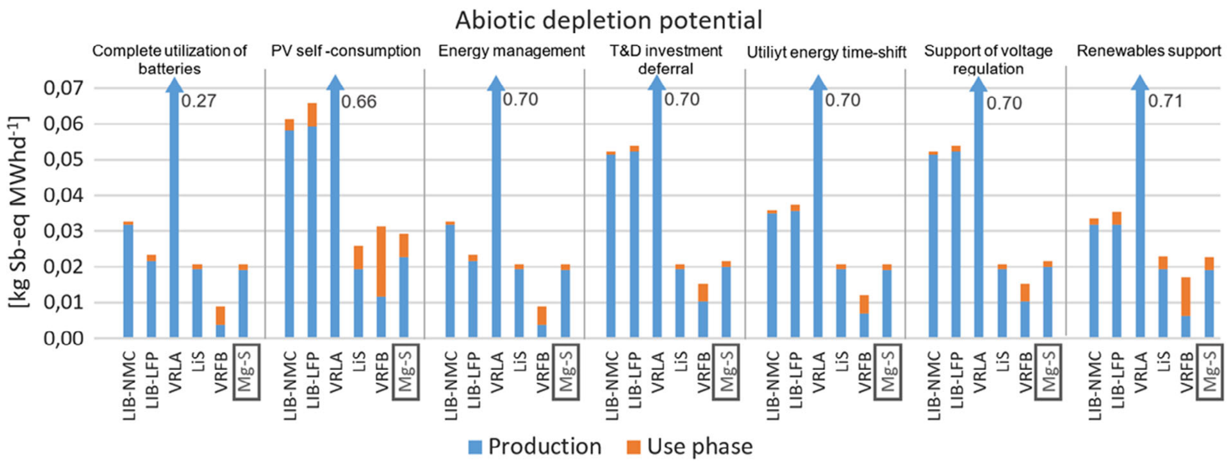

Figure 7. Life cycle impacts of each battery in the "ADP" impact category.

Regarding the "climate change potential," it is no surprise that the scenarios associated with higher levels of clean electricity experience a lower use-phase associated footprint than those using electricity from the traditional grid (even for the year 2030). This is strictly connected to the low CO_2 emissions of the production of electricity from renewables. As in CED, the Mg–S battery performs similarly to the LIBs, with impacts varying from around 50 kg CO_2-eq MWh^{-1} in the RS scenario and of about 98 kg CO_2-eq MWh^{-1} in support voltage regulation and T&D (Figure 2). The advantage of the Mg–S battery over LiS is the result of the lower energy demand in production, described in the previous category, and consequently lower greenhouse gases emissions. The vanadium battery leads negatively once again with the highest impacts in almost every application, despite renewable support where LiS has higher impacts. The high impacts of VRFB stem in all cases from its comparable low roundtrip efficiency.

Similar to "climate change potential," low use-phase impacts are found for the PVSC and RS scenarios within the "fossil depletion potential" category. The Mg–S battery performs with the lowest potential impact, of about 15 kg oil-eq MWh^{-1} in the RS scenario and a maximum potential impact of about 29 kg oil-eq MWh^{-1} for most other scenarios (Figure 3). It is worth mentioning that the impacts of the use-phase represent around half of the total in the scenarios using a more traditional grid.

In the case of "human toxicity potential," The Mg–S battery performs considerably better than the other systems. Even when the contribution from the use-phase is relatively similar between different technologies, the Mg–S battery has the lowest production impacts in every scenario, with a toxicity potential between 39 and 69 kg 1,4-DCB-eq MWh^{-1}, as shown in Figure 4. The lead-acid and vanadium batteries carry the highest impacts in every application within this category.

The "metal depletion potential" category shows a clear dominance of battery production over the total impacts of each battery. It is also shown in Figure 5 that the Mg–S battery displays an advantage over the alternatives. Given that the impacts of the use-phase are negligible, the low production-phase impacts of this battery entail it with the lowest footprint, on average around 9 kg Fe-eq MWh^{-1}. In contrast, the VRLA battery performs significantly worse in every scenario, in most cases up to around 200 kg Fe-eq MWh^{-1}. This can be explained due to the criticality of lead, which has a characterization factor higher than most other metals. It is worth mentioning that this category of the ReCiPe impact assessment method does not contain characterization factors for lithium and therefore, the impacts of the LIBs might be underestimated.

Regarding "particulate matter formation," the production impacts of the vanadium flow battery are far superior in every application, leading to the highest footprint up to about 0.8 kg PM10-eq MWh^{-1} in the most critical case (Figure 6). This can be attributed to the high burdens of the selected vanadium–pentoxide production method for the electrolyte. However, different production methods for this compound exist, potentially leading to different environmental profiles. Further evaluation of these methods is the fore necessary. The Mg–S battery has potential impacts between 0.15 and 0.21 kg PM10-eq MWh^{-1}, which are in most cases the lowest among all the systems.

Concerning the specific analysis of "ADP," the most critical potential impacts are found for the lead-acid battery and of about 0.61 kg Sb-eq MWh^{-1}, which is on a higher order of magnitude than the other batteries (Figure 7). Just as in "metal depletion," this can be attributed to the high value of the characterization factor of lead in comparison with other resources and the fact that the model contemplates consumption of primary materials. The potential benefits of recycling have not been considered due to the uncertainty regarding recycling of LIBs and the Mg–S battery, which precludes the expansion of the system boundaries for all the technologies. Nevertheless, for the specific case of PbA batteries, the high recycling rates already mitigate most of these impacts. In most applications, the LiS and the vanadium redox-flow battery have the lowest impacts, down to around 0008 kg Sb-eq MWh^{-1} for the latter. The potential impacts of the Mg–S battery oscillate between 0.021 and 0.029 kg Sb-eq MWh^{-1}, in most cases lower than the LIBs and attributed mostly to the electronics contained within the BMS. The LIBs carry, apart from the BMS, additional burdens due to the usage of other critical resources such as nickel and cobalt.

4.2. Sensitivity Analysis

The sensitivity analysis has been conducted exclusively for the Mg–S battery and by varying the cycle life, the energy density, and the calendrical life ±20% with respect to the original value. An additional scenario varying the roundtrip efficiency ±10% is also included. The results are presented individually, varying one parameter at a time while keeping the other parameters as in the baseline. It is expected that the negative percentages, in other words worsened technical performance, will lead to increased environmental burdens. These can be read on the upper end of the variation line. The lower end of the line reflects the effects of increased technical performance.

The sensitivity to the earlier-mentioned parameters in "climate change potential" and "human toxicity potential" is shown in **Figures 8** and **9**. It is shown that variations of efficiency lead to the greatest differences with respect to the baseline in both cases. This is attributed to the high share of the use-phase within the total impacts. A look into the climate change category (Figure 8) suggests moderate sensitivity to cycle life, energy density, and calendrical life. These parameters are exclusively related to the production phase as they are necessary to determine the total mass of the battery required to comply with the specific application demands (including replacements during the defined application time). For the specific case of calendrical life, no sensitivity can be observed in the CUB, EM, ETS, and RS scenarios. When excluding the sensitivity to efficiency, the global warming potential could vary ≈±10 kg CO_2 MWh^{-1} from the baseline, which depending on the application may represent between 11 and 20% of the total impacts. The sensitivity to the efficiency oscillates in the most critical cases between −48/+59 kg CO_2 MWh^{-1} from the baseline accounting for around −50%/+62% of the total impacts.

When evaluating the human toxicity potential, the baseline impacts are ≈68 kg 1,4 DCB-eq for CUB, EM, T&D, ETS, and SVR and about 49–62 kg 1,4 DCB-eq for RS and PVSC, respectively (**Figure 10**). The deviations from the baseline adopt the same profile as in "climate change potential" with the maximum variations found again when varying the efficiency, with maximal percentages of around −50%/+62% of the baseline impacts.

To better understand the high sensitivity to roundtrip efficiency, Figure 10 shows the effects on the climate change potential if the system boundaries were expanded to account

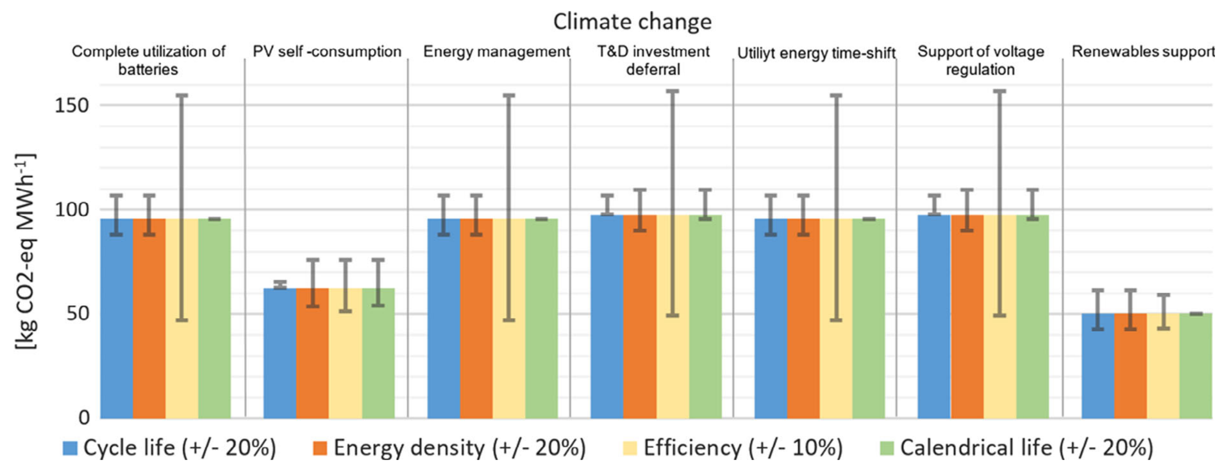

Figure 8. Results of the sensitivity analysis, "climate change" potential impact category.

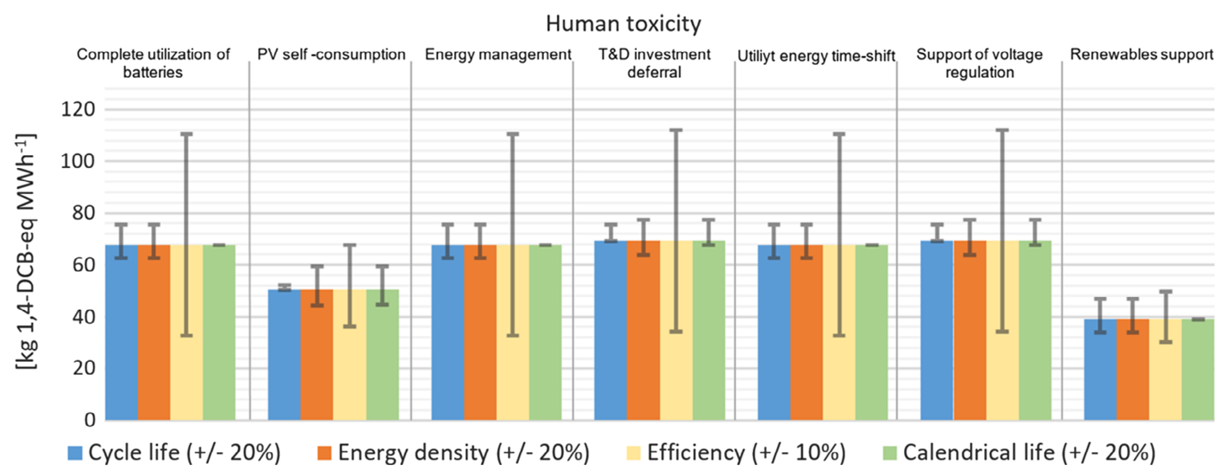

Figure 9. Results of the sensitivity analysis, "human toxicity" potential impact category.

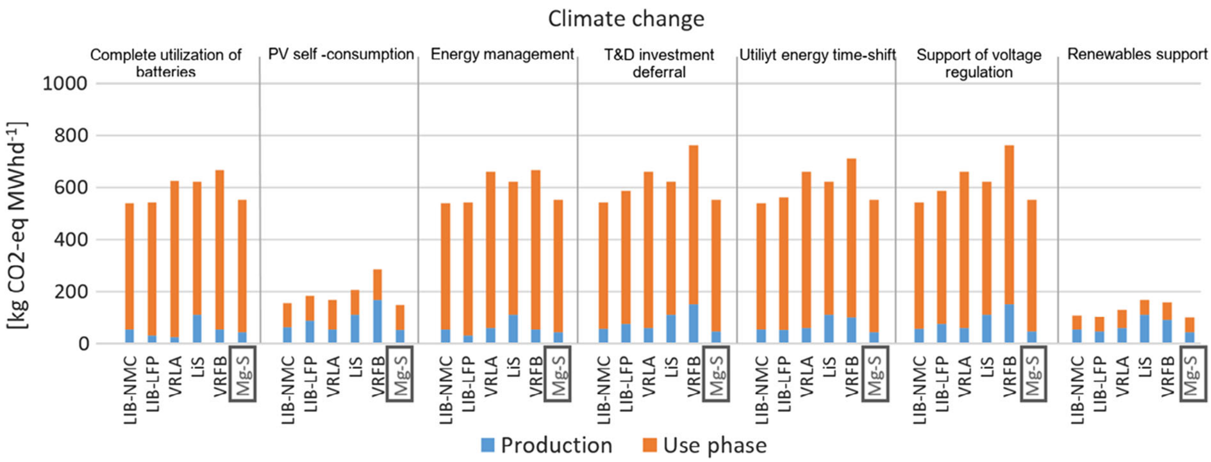

Figure 10. Climate change potential with modified use-phase boundaries.

for the total impacts of producing the electricity that each battery is meant to store during the use-phase. It is shown that the contributions from the use-phase are highly increased, leading now to a larger footprint. In our study, only a fraction of these impacts, related to the internal system losses during charge and discharge cycles, has been considered and allocated to the use-phase. The remaining fraction has not been taken into account because it is assumed to be allocated either to the grid or to the specific power generation technology (e.g. solar panels, windmills…). For such reason, Figure 2 shows in general significantly less contributions from the use-phase for every storage technology. These internal losses are calculated based on the defined roundtrip efficiency of each battery (e.g., 90% for the Mg–S battery). Different efficiency values, as shown in Figures 8 and 9 of the sensitivity analysis, require a recalculation of the system losses and associated impacts, which at the same time are bounded to a large footprint (as shown in Figure 10) and lead to large deviations from the baseline.

5. Discussion

It shall be emphasized that the Mg–S system hereby presented is an ideal model and that there are technological constraints that still have to be addressed with further research to reach the assumed technical performance level. For such reason, this is considered a prospective assessment and the obtained results shall be considered only in an indicative level. The parameters of electrochemical performance have been indicated as an optimistic goal based on a retrospective look to LIBs and are still subject to proof of feasibility. The composition of the battery pack was assumed the same as that of LIBs due to practical purposes and obeying a lack of available information in this matter. This already explains why the respective footprints are often found on similar levels. The sensitivity analysis contemplates scenarios with large deviations from the assumed values made to account for the high level of uncertainty of such assumptions. It is assumed that the technology development has the potential to bring the Mg–S system to the described level. Ultimately, the objective of the prospective assessment is to provide an insight into the potential of such technology by means of optimistic assumptions based on theoretical capacity, observations of the first prototype, and a retrospective view of the development of other reference systems. By doing so, and gaining attention for further research, development could be pushed further to overcome the existing challenges.

When comparing the different applications, it can be seen that T&D and SVR are the scenarios where the batteries have in overall the highest impacts per MWh in every category. On the contrary, RS has in most cases the smallest footprint per FU. When taking a detailed look at the different types of batteries, the lead-acid and the VRFBs stand out with the most critical performance in most categories. This can be partially attributed to the low efficiencies of these types of batteries, leading to high use-phase impacts within the selected application cases. For the same reason, the LIB–NCM (system with the highest efficiency) has a particular advantage over the other systems.

It has been found that different applications do not lead to significant discrepancies of the environmental performance of the Mg–S battery. Slightly better performance is found under renewable energy applications, attributed to the low impacts of the electricity stored and consequently, low impacts of the internal losses. The analysis is made under the premise that this battery complies with the technical requirements of each application case, which is not yet the case. Real suitability has to be subject of further research.

The specific end-of-life management approach that each battery is expected to experience after failure has the potential to modify to a great extent the overall environmental profile of each battery. The analysis conducted displays great criticality for the lead-acid battery in the “ADP” category. This is because the characterization factor for lead is several orders of magnitude higher than most other materials. However, the system is modeled with the high consumption of primary raw materials and does not take into account potential benefits of the recycling process. For this specific type of battery, there is a well-established recycling industry, which has reported recovery rates of about 99%,[34] already mitigating this problem. Similarly, the low integration of the VRFB eases recovery of the electrolyte and its overall recyclability, potentially reducing its environmental burdens.[35] In contrast, there is plenty of room for development of the recycling industry of LIBs before reaching large-scale deployment, thus adding potential criticality to the ADP in the meantime. For the Mg–S battery, little can be said at this stage about a prospective recycling model, which would greatly depend on its final layout and composition. In addition, the ADP of the Mg–S battery is dominated by the BMS, which contributes with about 96% of the total impacts per kg of battery. This dominance is explained due to the low contributions from other components, unlike for LIBs, where the use of more critical resources introduces additional burdens beyond those related to the BMS. The BMS incorporates gold-containing electronics for which a different recycling model exists. The resource criticality on the cell level is therefore very low. Nevertheless, the quantification of the benefits and burdens of the end-of-life management (namely recycling and other disposal methods) demands for an expansion of the system boundaries, which is outside of the scope of this work due to limited information available regarding LIBs and Mg–S batteries. Finally, the ADP analysis shows results based on estimated reserves but does not display criticalities arising from sociopolitic constraints, which could be relevant for resources unevenly distributed over the planet. This is particularly relevant for magnesium, classified by the European Commission as critical material due to the high dependency of the supply chain on the primary production from China, which accounts for over 86% of the worldwide market share.[36] The resource criticality should therefore be further studied taking into account these constraints.

The relative small footprints observed in the PVSC and the RS applications can be attributed to the fact that electricity generated from renewable sources is already characterized by entailing low environmental impacts, thus making the use-phase less critical. On the contrary, the scenarios associated with storage of electricity from a conventional grid, such as CUB, EM, T&D, ETS, and SVR, entail large contributions of the use-phase in the categories "CED," "climate change potential," and "fossil depletion potential." Ideally, energy-storage systems will be connected to such systems. It has been assumed that the Mg–S battery performs with the same efficiency as the LIB–LFP, thus making the use-phase impacts the same for both technologies. Given that the LIBs are nowadays the leading technologies, overcoming the technological barrier associated with efficiency would most likely bring the Mg–S to a competitive level in terms of ecological footprint.

In particular, the Mg–S battery has very low toxicity potential; in fact, it is the lowest of all the systems studied here. This represents a relevant advantage, especially when considering the large deployment of battery systems that will be required to support the energy transition. The previous, in combination with an adequate collection network at the end of life, could make this technology an exemplary sustainable model.

Being this the first study considering the use-phase of the Mg–S battery, it is not possible to compare the findings with previous studies for this specific type of system. Nevertheless, a comparison is possible for the remaining technologies. Baumann et al.[25] focused on the climate change potential, which already displayed a similar profile as the one presented here. The VRLA and the VRFB are found to entail the highest burdens within this impact category. In particular, the authors registered higher CO_2 emissions per unit of electricity, between 400 and 700 kg CO_2-eq MWh^{-1} for the application "electricity time-shift," in contrast to the 60–250 kg CO_2-eq MWh^{-1} found in this study for the same category (Figure 3). The difference can be explained due to the different system boundaries considered, as the authors included the impacts of electricity production within the life cycle of the batteries. Nevertheless, the modified model shown in Figure 10 leads to very similar values of CO_2-eq emissions per MWh, with the LIBs entailing a smaller footprint. Similarly, Rossi et al.[37] conducted an analysis for a solar home system, comparable with the PVSC herein described. The authors presented the impacts of the solar installation including PV panels, batteries, and other Balance of System components. This relates again to the extended boundaries shown in Figure 10. The LIBs carry a similar CO_2 footprint in both cases, with higher burdens found in the study from Rossi et al. attributed to the capacity fade (aging effect) considered and which leads to worsened performance over the years. A significant difference of the footprint was found for the VRFB, entailing higher impacts in this study. This is explained because of the different energy densities considered in both studies, 28 Wh kg^{-1} in contrast to 17 Wh kg^{-1} assumed in this study. Hiremath et al.[26] also considered the impacts of electricity production within the system boundaries, as this allows comparability with specific generation systems. A comparison of the global warming potential is again possible with the results from the model with extended boundaries. The authors considered electricity production with the traditional German mix in most scenarios. In addition, a sensitivity analysis with solar-only and a 50–50 renewables mix was presented. The authors registered higher CO_2 footprints, oscillating between $750^{-1}160$ kg CO_2-eq MWh^{-1}, with the best performance found for the LIB. The VRFB leads to the highest impacts in the scenarios with traditional German electricity. In general, the authors assumed superior technical specifications for the batteries, which lead to moderate lower footprints in the solar-only and renewable mix scenarios than the ones found here. Nevertheless, the performance levels display a very similar pattern. The definition of the system boundaries plays a critical role in the results and must be clearly stated when conducting such types of assessments in order to ease comparability between different studies.

Regarding the sensitivity analysis, it can be seen that in some applications such as "PVSC" and "SVR," there is no potential reduction of the impacts when assuming a higher cyclability. This can be attributed to the fact that the calendrical life of the battery is the parameter conditioning the amount of battery replacements. In other words, higher cycle life does not necessarily lead to better environmental performance if the calendrical life becomes a limiting factor. Similarly, varying the calendrical life of the battery will not have any impact on the footprint if the battery replacements are conditioned by the cycle life, as is the case for the EM, ETS, and RS scenarios in both impact categories. In contrast, changing efficiency leads to significant deviations from the baseline. The roundtrip efficiency determines the amount of extra energy that is necessary to supply per unit of electricity delivered by the system. Given that these internal losses have the potential to worsen considerably the system's footprint, special attention shall be given to the technical developments that aim to increase the efficiency. It should therefore be a focus of research to ensure that the Mg–S system performs at efficiencies similar to those of the established technologies to make it not only economically viable but also a real sustainable alternative.

6. Conclusion

The analysis herein conducted is based on a series of assumptions that do not yet reflect the actual status of the battery. Instead, these describe an ideal performance that is assumed as reachable with further research and development, yet to be proved. This prospective LCA offers an insight into the potential environmental footprint of a model Mg–S battery with an extended discussion of the use-phase of such technology. The model studied corresponds to the redesign of a prototype cell, namely model MgS-Evo2, which entails reduced mass fractions considered technically feasible by the technology developers and is proposed in a previous study. It was found that this sole action could already lead to a lower footprint of the cell, but the technical challenges of performance need still to be addressed in further research. An analysis distinguishing the contributions of the production phase and the use-phase under different application scenarios has allowed identifying the criticality entailed by the source of electricity that the system is meant to store. At the same time, a comparison with other commercially available technologies already suggests that Mg–S has the potential to become an interesting alternative when it comes to environmental performance. After a careful examination of the footprint from the different systems, the Mg–S battery could potentially perform at the same level as its commercial counterparts and could even outperform them in some impact categories. High sensitivity to the roundtrip efficiency has been observed, providing the battery with great potential but also conditioning its viability. These results are subject to high uncertainty and therefore should be considered on an indicative level only. The described environmental performance and eventual large deployment of this technology will therefore be feasible if the technical challenges found at the current stage of development are overcome. This would make this type of battery a very attractive alternative to lithium-based battery systems. Finally, further development of this system will most likely lead to the inclusion of new elements and materials, for instance, by introducing additives to the electrolyte to improve the interfacial behaviors with the electrodes.[38] Such modifications will have a direct impact on the environmental footprint, thus making it necessary to conducts continuous assessments to ensure that the final product complies with suitable sustainability criteria.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

Acknowledgements

This work contributes to the research conducted at Center for Electrochemical Energy Storage Ulm-Karlsruhe (CELEST). It was funded by the German Research Foundation (DFG) under project ID 422053626 (POLiS Cluster of Excellence) and it was supported by the Initiative and Networking Fund of the Helmholtz Association within the Network of Excellence on postlithium batteries (ExNet-0035). Open access funding enabled and organized by Projekt DEAL.

Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that supports the findings of this study are available in the supplementary material of this article.

Keywords

energy storage, environmental impacts, life cycle assessments, magnesium batteries, prospective assessments, renewable energy systems, sustainability

Received: November 4, 2020
Revised: January 15, 2021
Published online:

[1] J. Zhang, C. Chen, X. Zhang, S. Liu, *Procedia Environ. Sci.* **2016**, *31*, 873.
[2] J. Sutanto, Environmental Study of Lead Acid Batteries Technologies, https://www.grin.com/document/179643 (accessed: October 2020).
[3] A. Shanika, S. Jay, S. Brian, *Application of Life Cycle Assessment to Nanoscale Technology: Lithium-Ion Batteries for Electric Vehicles*, Tech. Rep. EPA 744-R-12-001, United States Environmental Protection Agency, Washington, DC, USA **2013**.
[4] D. Agusdinata, W. Liu, H. Eakin, H. Romero, *Environ. Res. Lett.* **2018**, *13*, 123001.
[5] H. E. Melin, *Analysis of the Climate Impact of Lithium-ion Batteries and How to Measure it*, Circular Energy Storage Research and Consulting, London **2019**.
[6] A. Leader, G. Gaustad, C. Babbitt, *Mater. Renew. Sustain. Energy* **2019**, *8*, 8.
[7] M. Mohr, J. Peters, M. Baumann, M. Weil, *J. Ind. Ecol.* **2020**, *24*, 1310.
[8] J. Choi, D. Aurbach, *Nat. Rev. Mater.* **2016**, *1*, 1601.
[9] B. L. Ellis, L. F. Nazar, *Curr. Opin. Solid State Mater. Sci.* **2012**, *16*, 168.
[10] D. Aurbach, Y. Gofer, Z. Lu, A. Schechter, O. Chusid, H. Gizbar, Y. Cohen, V. Ashkenazi, M. Moshkovich, R. Turgeman, *J. Power Source* **2001**, *97*, 28.
[11] M. Fichtner, in *Magnesium Batteries: Research and Applications*, Royal Society of Chemistry, Cambridge, UK **2019**.
[12] N. Wagner, M. Fichtner, H. G. Bremes, C. Wolter, I. Zwanziger, J. Remmlinger, *Entwicklung und Herstellung von Wiederaufladbaren Magnesium-Schwefel Batterien „MagS“*, **2019**, https://doi.org/10.2314/KXP:1680881833 (German).
[13] C. T. Montenegro, J. Peters, Z. Zhao-Karger, C. Wolter, M. Weil, in *Magnesium Batteries: Research and Applications*, Royal Society of Chemistry, Cambridge, UK **2019**.
[14] C. T. Montenegro, J. Peters, M. Baumann, Z. Zhao-Karger, C. Wolter, M. Weil, *J. Energy Storage*, Unpublished.
[15] M. Baumann, J. Peters, M. Weil, *Energy Technol.* **2019**, *8*, 1901019.
[16] P. Wang, M. Buchmeiser, *Adv. Funct. Mater.* **2019**, *29*, 1905248.

[17] J. Häcker, C. Danner, B. Sievert, I. Biswas, Z. Zhao-Karger, N. Wagner, K. A. Friedrich, *Electrochim. Acta* **2020**, *338*, 135787.
[18] P. Wang, J. Kappler, J. Häcker, K. Küster, B. Sievert, I. Biswas, U. Starke, F. Ziegler, M. R. Buchmeiser, *Electrochim. Acta* **2020**, *361*, 137024.
[19] B. Lee, J. Choi, N. Subin, D. J. Yoo, J. Kim, B. W. Cho, Y. Kim, T. Yim, J. Choi, S. H. Oh, *Appl. Surf. Sci.* **2019**, *484*, 933.
[20] ISO, *Environmental Management: Life Cycle Assessment – Principles and Framework*, ISO 14040, British Standards Institution, London **2006**.
[21] ISO, *Environmental Management: Life Cycle Assessment – Requirements and Guidelines*, ISO 14044, British Standards Institution, London **2006**.
[22] Z. Zhao-Karger, R. Liu, W. Dai, Z. Li, T. Diemant, B. P. Vinayan, C. B. Minella, X. Yu, A. Manthiram, R. J. Behm, M. Ruben, M. Fichtner, *ACS Energy Lett.* **2018**, *3*, 2005.
[23] Z. Zhao-Karger, M. Fichtner, *Front. Chem.* **2019**, *6*, 656.
[24] L. A. W. Ellingsen, G. Majeau-Bettez, B. Singh, A. K. Srivastava, L. O. Valøen, A. H. Strømman, *J. Ind. Ecol.* **2014**, *18*, 113.
[25] M. Baumann, J. F. Peters, M. Weil, A. Grunwald, *Energy Technol.* **2017**, *5*, 1071.
[26] M. Hiremath, K. Derendorf, T. Vogt, *Environ. Sci. Technol.* **2015**, *49*, 4825.
[27] Y. Deng, J. Li, T. Li, X. Gao, C. Yuan, *J. Power Sources* **2017**, *343*, 284.
[28] M. Zackrisson, K. Fransson, J. Hildenbrand, G. Lampic, C. O'Dwyer, *J. Cleaner Prod.* **2016**, *135*, 299.
[29] G. Majeau-Bettez, T. R. Hawkins, A. H. Strømman, *Environ. Sci. Technol.* **2011**, *45*, 4548.
[30] Agora Energiewende, *Die Energiewende im Stromsektor: Stand der Dinge 2019: Rückblick auf die wesentlichen Entwicklungen sowie Ausblick auf 2020*, Agora Energiewende, Berlin **2020**.
[31] R. Frischknecht, R. Itten, P. Sinha, M. de Wild-Scholten, J. Zhang, V. Fthenakis, H. C. Kim, M. Raugei, M. Stucki, *Life Cycle Inventories and Life Cycle Assessment of Photovoltaic Systems*, PVPS Task 12, Report T12-04:2015, International Energy Agency (IEA), Paris **2015**.
[32] M. A. Huijbregts, Z. J. N. Steinmann, P. M. F. Elshout, G. Stam, F. Verones, M. Vieira, M. Zijp, A. Hollander, R. van Zelm, *Int. J. Life Cycle Assess.* **2017**, *22*, 138.
[33] L. Van Oers, J. B. Guinée, R. Heijungs, *Int. J. Life Cycle Assess.* **2020**, *25*, 294.
[34] Battery Council International, *National Recycling Rate Study*, SmithBucklinStatistics Group, Chicago, IL **2019**. https://cdn.ymaws.com/batterycouncil.org/resource/resmgr/2020/BCI_482347-20_2019-Study.pdf (accessed: September 2020).
[35] S. Weber, J. Peters, M. Baumann, M. Weil, *Environ. Sci. Technol.* **2018**, *52*, 10864.
[36] European Commission, *Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee and the Committee of the Regions: On the Review of the List of Critical Raw Materials for the EU and the Implementation of the Raw Materials Initiative*, European Commission, Brussels **2014**.
[37] F. Rossi, M. Parisi, S. Greven, R. Basosi, A. Sinicropi, *Energies* **2020**, *13*, 3454.
[38] V. B. Parambath, Z. Zhao-Karger, T. Diemant, M. Jäckle, Z. Li, T. Scherer, A. Gross, R. J. Behmacand, M. Fichtner, *J. Mater. Chem. A* **2020**, *8*, 22998.

