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Green batteries for clean skies

Sustainability assessment of lithium-sulfur all-solid-state batteries for electric aircraft

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Abstract

The use of novel battery technologies in short-haul electric aircraft can support the aviation sector in achieving its goals for a sustainable development. However, the production of the batteries is often associated with adverse environmental and socio-economic impacts, potentially leading to burden shifting. Therefore, this paper investigates alternative technologies for lithium-sulfur all-solid-state batteries (LiS-ASSBs) in terms of their contribution to the sustainable development goals (SDGs). We propose a new approach that builds on life cycle sustainability assessment and links the relevant impact categories to the related SDGs. The approach is applied to analyze four LiS-ASSB configurations with different solid electrolytes, designed for maximum specific energy using an electrochemical model. They are compared to a lithium-sulfur battery with a liquid electrolyte as a benchmark. The results of our cradle-to-gate analysis reveal that the new LiS-ASSB technologies generally have a positive contribution to SDG achievement. However, the battery configuration with the best technical characteristics is not the most promising in terms of SDG achievement. Especially variations from the technically optimal cathode thickness can improve the SDG contribution. A sensitivity analysis shows that the results are rather robust against the weighting factors within the SDG quantification method.

KEYWORDS

all-solid-state battery, electric aircraft, industrial ecology, life cycle sustainability assessment, prospective sustainability assessment, sustainable development goals

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1 | INTRODUCTION

1.1 | Climate impact of the air transport sector and importance of lithium-sulfur all-solid-state batteries

The air transport sector is a continuously growing industry with a predicted increase in flight volume of 3.6% to 4.5% annually (Airbus S.A.S., 2019; Boeing, 2019). What is desirable from an economic perspective is associated with adverse environmental impacts. Especially the emission of climate-damaging CO_2 and non- CO_2 emissions (nitrogen oxides, soot, water vapor, and sulfate aerosols) resulting from fossil kerosene combustion intensify global warming in the long term (EASA/EEA/EUROCONTROL, 2019; Lee et al., 2021). In 2018, the air transport sector was responsible for 2.4% of the global CO_2 emissions and accounted for 5% of the global anthropogenic climate forcing overall (Lee et al., 2021; Staples et al., 2018). Considering the predicted growth in flight volume and based on current aircraft configurations with kerosene-powered propulsion systems, the aviation-induced CO_2 and non- CO_2 emissions could triple by 2050 (Gnadt et al., 2019).

While minor reductions of climate-damaging emissions per passenger kilometer (pkm) traveled were already achieved by efficiency improvements of aircraft engines, further progress toward clean and sustainable aviation requires more radical technological innovations (Barke, Bley et al., 2022; ICAO, 2019; Schäfer et al., 2016). One important strategy is the development and deployment of battery–electric aircraft (Gnadt et al., 2019; Schäfer et al., 2019). Due to technical restrictions regarding the maximum take-off and landing weight, a high specific energy of the battery is crucial. A promising technology in this context is the all-solid-state battery (ASSB), where a solid ion conductor acts as separator and electrolyte (Varzi et al., 2016; Viswanathan et al., 2022). Especially the lithium–sulfur-ASSB (LiS-ASSB) enables considerably high specific energy of up to 472 Wh/kg at pack level, which corresponds to an increase in pack capacity of 70% to 80% compared to state-of-the-art lithium-ion (248 Wh/kg) and lithium– sulfur batteries (277 Wh/kg) (Randau et al., 2020; Winjobi et al., 2022; Xue et al., 2017). By carefully selecting materials and components, LiS-ASSBs suited for air travel are potentially achievable.

1.2 | Evaluating the contribution of batteries and electric aircraft toward more sustainable aviation

A recent literature review by Melo et al. (2020) on challenges, methods, and tools for the sustainability assessment and engineering of emerging aircraft technologies showed the increasing attention on electric propulsion concepts in aviation. While the reviewed articles focused primarily on alternative fuels and implied environmental and economic impacts, first sustainability studies have been conducted on electric aircraft concepts. These studies emphasize the influence of the battery on aircraft sustainability. Moreover, a doubling of the battery's specific energy compared to the state-of-the-art would be required to make electric flying viable on short-haul flights (Gnadt et al., 2019; Melo, Cerdas et al., 2020; Schäfer et al., 2019). Simultaneously, the electricity mix for recharging the battery affects the environmental impacts significantly. Renewable electricity can reduce greenhouse gas (GHG) emissions by 95% compared to fossil kerosene-powered aircraft during the use stage (Barke, Thies et al., 2022; Johanning & Scholz, 2015; Ploetner et al., 2016). However, these studies are feasibility studies, and detailed analyses of sustainability hotspots in the battery life cycle, especially in the production stage, are neglected.

Sustainability assessments of battery production are common practice, and several studies investigate the environmental and socio-economic impacts of lithium-ion and lithium-sulfur battery production (Barke et al., 2021; Cerdas et al., 2018; Chordia et al., 2021; Dai et al., 2019; Deng et al., 2017; Ellingsen et al., 2014; Kelly et al., 2020; Lopez et al., 2021; Peters & Weil, 2017). Key insights from selected studies are presented in supporting information S1-2. In addition, Peters et al. (2017) and Emilsson and Dahllöf (2019) provide an overview of existing studies in this field. However, most studies investigate the production of batteries with liquid electrolytes. Only a few studies address the impacts of ASSB production, primarily focusing on ASSBs for automotive applications and environmental impacts. The studies suggest that GHG emissions during production could be reduced by 25% to 65% by replacing the liquid electrolyte with a solid electrolyte, depending on the battery technology (Keshavarzmohammadian et al., 2018; Lastoskie & Dai, 2015; Troy et al., 2016). Regarding the economic dimension, first calculation models underline the need to scale-up ASSB production processes to mass production (Schnell et al., 2018, 2020). However, a detailed analysis of environmental and socio-economic impacts of ASSB production suitable for use in aviation is missing. Moreover, a new perspective on globally oriented environmental and socio-economic goals is needed to evaluate further progress toward clean and sustainable aviation in the future.

In this regard, the sustainable development goals (SDGs) provide orientation for a more comprehensive assessment encompassing long-term objectives for economic, environmental, and social development (United Nations General Assembly, 2015). While life cycle sustainability assessment (LCSA) studies provide detailed insights into the environmental and socio-economic impacts of products, SDGs provide guidelines for long-term sustainable development globally. In order to analyze the extent to which innovative products, such as LiS-ASSBs, contribute to the achievement of the SDGs, a linkage is required. Initial approaches of linking LCSA and SDGs already exist in the scientific literature. For example, SDG-based LCSA indicators and methodologies have been developed for specific use cases (Castor et al., 2020; Haryati et al., 2021; Kühnen et al., 2019; Maier et al., 2016; Wang et al., 2018), or to determine the potential of contributing to a specific SDGs (Herrera Almanza & Corona, 2020; Omer & Noguchi, 2020; Sala & Castellani, 2019). In addition, more general frameworks for linking LCSA impact categories to SDGs have been proposed (Henzler et al., 2020; Weidema et al., 2018, 2020; Wulf et al., 2018). This linking is based on the targets and indicators used to describe the

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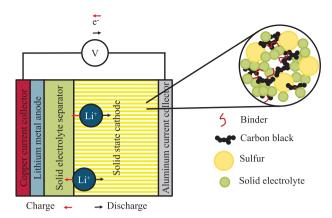


FIGURE 1 Scheme of the composition and structure of an lithium-sulfur all-solid-state battery cell.

17 goals. However, the existing studies leave uncertainties regarding how the linkage of LCSA impact categories and SDGs is conducted. In addition, the approaches for quantifying the contribution to SDG achievement developed so far often lead to a loss of information due to the development of highly simplified key figures.

1.3 | Objective and novelty of the study

This article aims to assess four configurations of innovative LiS-ASSB technologies that are potentially usable in electric aircraft regarding their contribution to a sustainable development of the aviation sector. We investigate whether battery configurations with desirable technical characteristics concerning maximized specific energy are also favorable from a sustainability perspective. To this end, we carry out an LCSA of LiS-ASSB configurations derived from an electrochemical model based on the requirements for use in short-haul aircraft. Moreover, we propose a novel approach for linking the LCSA impact categories to related SDGs and quantifying the contribution to their achievement. Here, this article focuses on the isolated analysis of SDGs 1 ("No poverty"), 10 ("Reduced inequality"), 12 ("Responsible consumption and production"), 13 ("Climate action"), and 15 ("Life on land") since their achievement is particularly affected by the environmental and socio-economic impacts of LiS-ASSB production. We demonstrate the application of the approach by evaluating the interdependencies between technical performance and sustainability of the batteries.

The intended contribution to the sustainability assessment literature is twofold: First, we seek to introduce a new perspective into the LCSA methodology by establishing the link to the SDGs. For this purpose, a characterization of the SDGs using LCSA impact categories is carried out before a novel approach for calculating the contribution of innovative products to the achievement of the SDGs is presented. Second, we seek to derive insights regarding the design of LiS-ASSB for future aviation. Therefore, we design optimal battery configurations in terms of maximized specific energy based on an electrochemical model and investigate to what extent the optimal battery configurations from a technical point of view also have the best characteristics in terms of sustainability aspects.

2 | METHOD AND SYSTEM DEFINITION

2.1 Specification of all-solid-state batteries for short-haul electric aircraft

The battery packs investigated in this article are characterized by the capability to provide a short-haul aircraft, developed in the cluster of excellence "SE²A – Sustainable and Energy-Efficient Aviation" with the required energy for a generic flight with a distance of 1000 km. This flight requires a battery capacity of 9.396 MWh (including a 5% safety margin) (Karpuk & Elham, 2021; Liu et al., 2018). Due to the restriction of the maximum take-off and landing weight of aircraft, high specific energy of the battery is crucial.

In this regard, LiS-ASSBs are a promising technology. The investigated LiS-ASSB cells consist of a cathode and an anode with a separator between them (see Figure 1). Current collectors enclose both sides of the battery cell and are connected to a power consumer. The separators are made of a solid electrolyte and a small amount of binder, providing better mechanical strength. As the separator's ionic resistance scales with its thickness, a very thin separator made of a solid electrolyte is desirable (Ates et al., 2019; Wang et al., 2020). Solid-state sulfur cathodes are composed of the solid electrolyte, the active material sulfur, and an additive to enable electric conductivity, usually carbon black. A high amount of active material is desirable for high specific energy. To facilitate sufficiently thick cathodes for the highest possible specific energy, a solid electrolyte with a high specific ionic conductivity and a low density must be chosen. Four high-performance solid electrolytes were selected based on these properties:

TABLE 1 Specifications of the lithium-sulfur all-solid-state batteries under study with different solid electrolytes

		LiS-ASSB[Ge]	LiS-ASSB[Sn]	LiS-ASSB[Si]	LiS-ASSB[CI]
Battery					
Mass	[kg]	19,919	22,910	24,728	25,166
Modules per pack	[items]	616	663	681	678
Cells per module	[items]	23	23	23	23
Layers per cell	[items]	34	43	49	52
Mean operating voltage	[V]	2	2	2	2
Total resistance	$[m\Omega m^2]$	2.6011	3.85	4.9989	5.4382
Cell density	[kg/m ³]	1697.15	1807.60	1837.8	1831.47
Specific energy at 0.5 C (cell level)	[Wh/kg]	813.28	707.11	655.13	643.66
Specific energy at 0.5 C (pack level)	[Wh/kg]	471.71	410.12	379.96	373.35
Anode					
Current collector thickness	[µm]	10	10	10	10
Active material thickness	[µm]	116.38	89.60	75.74	70.20
Cathode					
Current collector thickness	[µm]	20	20	20	20
Active material thickness	[µm]	126	97	82	76
Cathode resistance	$[m\Omega m^2]$	0.0184	0.0553	0.0961	0.1163
Separator					
Thickness	[µm]	21	21	21	21
Separator resistance	$[m\Omega m^2]$	2.5827	3.7957	4.9028	5.3218
Solid electrolyte					
Material		Li ₁₀ Ge(PS ₆) ₂	$Li_{10}Sn(PS_6)_2$	$Li_{10}Si(PS_6)_2$	Li ₆ PS ₅ Cl

 $Li_{10}Ge(PS_6)_2$, $Li_{10}Sn(PS_6)_2$, $Li_{10}Si(PS_6)_2$, and Li_6PS_5Cl . Further discussions on the battery properties are provided in supporting information S1-1.1 to S1-1.4.

The optimal cell composition concerning maximum specific energy is calculated using an electrochemical model and the properties of the components and materials as described in supporting information S1-1.5 and S1-1.6. The mass of the other battery components (e.g., casing and battery management system [BMS]) can be approximated to about 42% of the total mass of the battery pack (Zhao, 2018). The specifics of the LiS-ASSB under study are presented in Table 1. In the following, the term "LiS-ASSB[Ge]" is used for the LiS-ASSB with $Li_{10}Ge(PS_6)_2$, "LiS-ASSB[Sn]" for LiS-ASSB with $Li_{10}Sn(PS_6)_2$, "LiS-ASSB[Si]" for the LiS-ASSB with $Li_{10}Si(PS_6)_2$, and "LiS-ASSB[CI]" for LiS-ASSB with Li_6PS_5CI . Based on the technical properties, the LiS-ASSB[Ge] seems most promising for application in electric aircraft.

2.2 | Functional unit and system boundaries

The analysis is conducted from the cradle-to-gate perspective of a battery manufacturer, following the attributional modeling principles. The focus is on the production processes of the aforementioned LiS-ASSBs with the previously selected solid electrolytes as well as the supply chains of essential components and raw materials. Due to a lack of valid data regarding the use and end-of-life of the batteries, these life cycle phases are excluded in this study. The functional unit of this LCSA study corresponds to the production of one LiS-ASSB battery pack capable of providing the capacity of 9.396 MWh for a short-haul reference flight. All battery systems are designed for the same capacity. The investigated system and its boundaries are presented in Figure 2. The foreground system comprises the production of the battery pack, the battery cells, and their components, as well as the required materials and energy. The process-based life cycle inventories (LCIs) of the foreground system include 77 unit processes per LiS-ASSB configuration. They are linked to the ecoinvent 3.7.1 database with the system model "allocation, cut-off by classification" (Wernet et al., 2016) and the Social Hotspots Database (Benoît-Norris et al., 2012). Wherever necessary and possible, the unit processes in the foreground and background system are allocated using economic partitioning. The LCIs of the four LiS-ASSB configurations, as well as of the raw materials, electricity, and transports, can be found in supporting information S2-S9.

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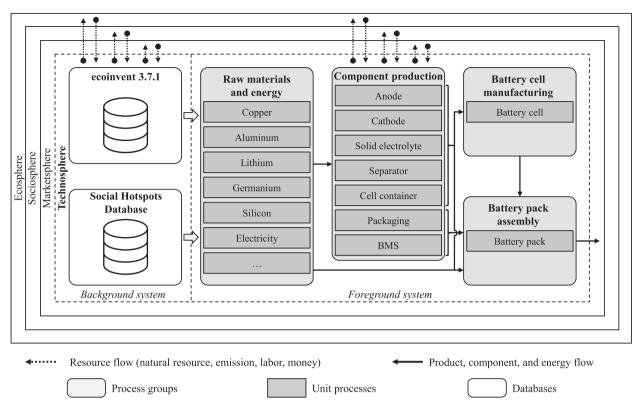


FIGURE 2 Foreground and background system within the system boundaries, including exchanges between technosphere, ecosphere, sociosphere, and marketsphere.

A detailed description of the production is provided in supporting information S1-3.1. It comprises the selection of background databases, specifications of production sites, materials used, energy requirements, transports, and production costs, which are mainly derived from scientific literature (Deng et al., 2017; Duffner et al., 2021; Ellingsen et al., 2014; Nelson et al., 2019; Peters et al., 2017; Schmuch et al., 2018; Schnell et al., 2020; Thies et al., 2021).

2.3 Evaluating the SDG contribution within life cycle sustainability assessment

To evaluate the contribution of innovative products to SDG achievement, a novel approach for linking LCSA impact categories to the SDGs and quantifying the progress in SDG achievement by a dimensionless indicator is introduced. It integrates into the LCSA procedure, derived from the ISO 14040/14044 standards (Singh et al., 2012). In essence, a new phase, *evaluation of contribution to SDGs* following the impact assessment, is added, but some particularities in the other phases need to be considered.

The concept requires the definition of a benchmark product in the *goal and scope definition* phase, which relates to the prevalent technology. For this benchmark product, inventory data within the same system boundaries must be collected, and impact scores must be calculated in the *inventory analysis* and *impact assessment* phases. The key idea of the new phase is now to analyze to what extent innovative products contribute to the progress toward particular SDGs. To this end, the impact scores of each product alternative are compared to the impact scores of the benchmark, and the relative performance in the impact categories related to the same SDG are aggregated. Since innovative products are often still in the development phase, the approach is developed against the background of a prospective life cycle assessment (LCA) (Bergerson et al., 2020; Hung et al., 2020; Sacchi et al., 2022) transferred to a prospective LCSA approach. The procedure is illustrated in Figure 3.

The subsequent description focuses on the concept of the new approach. Explanations of the basic LCSA approach or specific aspects can be found in the pertinent literature (Benoît-Norris et al., 2012; Heijungs et al., 2013; Hunkeler et al., 2008; Keller et al., 2015; Moreau & Weidema, 2015; Thies et al., 2019b, 2021; UNEP, 2020, 2021; UNEP/SETAC, 2011).

Within the new *evaluation of contribution to SDGs* phase, a calculation approach is developed for calculating the contribution to SDG achievement. The investigated product alternatives are described using the index p = 1, ..., P with the benchmark as p = 0. The SDGs are described via the index i = 1, ..., I and the LCSA impact categories via the index h = 1, ..., H. Each SDG i is characterized by a set L_i of LCSA impact categories, using the linking procedure described in supporting information S1-4.2. $y_{p,h}$ describes the computed impact scores for each product p and each impact

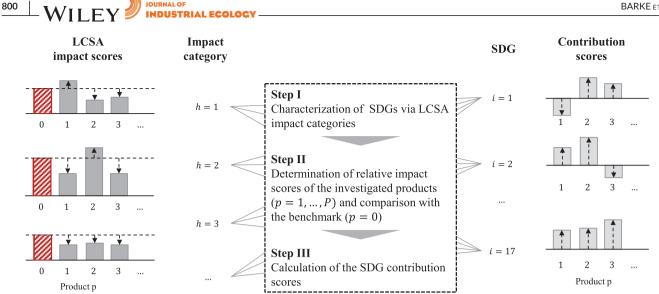


FIGURE 3 Procedure for the evaluation of contribution to sustainable development goals based on life cycle sustainability assessment impact scores.

category h. In this article, the ReCiPe Midpoint (H) V1.13 method (Goedkoop et al., 2013) is used for the environmental impact assessment, a costoriented approach accounting for the production cost (Hunkeler et al., 2008) is used for the economic assessment, and a risk-oriented method related to the Social Hotspots Database (Benoît-Norris et al., 2012) is used for the social assessment.

The contribution of product p to SDG i is calculated via the so-called SDG contribution score sp.i, which corresponds to the weighted sum of the product's relative performances $c_{p,h}$ compared to the benchmark over all impact categories h that are used to characterize the SDG i with the weighting factor w_{hi}:

$$s_{p,i} = \sum_{h \in L_i} w_{h,i} \cdot c_{p,h}(y_{p,h})$$
 (1)

The performance function $c_{p,h}(y_{p,h})$ describes the relative performance of product p compared to the benchmark (p = 0) concerning the expression of the impact $y_{p,h}$. It is defined to be zero if the product's performance equals the benchmark, positive if the performance is better than the benchmark, and negative if the performance is worse than the benchmark:

$$c_{p,h}(\gamma_{p,h}) = \begin{cases} \frac{\gamma_{0,h} - \gamma_{p,h}}{\gamma_{0,h}} , \text{ if smaller impact scores are preferable} \\ \frac{\gamma_{p,h} - \gamma_{0,h}}{\gamma_{0,h}} , \text{ if larger impact scores are preferable} \end{cases}$$
(2)

The weights $w_{h,i}$ of the LCSA impact categories h sum up to one for each SDG i. One possible approach is to use equal weights, i.e., $w_{h,i} = \frac{1}{|L_i|}$ Alternative approaches for weighting exist but are mostly subjective or involve a high loss of information. Further discussions on alternative weighting approaches are presented in supporting information \$1-4.4.

The calculated SDG contribution scores s_{ni} offer an alternative perspective on the interpretation of LCSA results. A positive SDG contribution score indicates that the product p is beneficial regarding the achievement of SDG i (compared to the benchmark). In contrast, a negative SDG contribution score indicates that the product counteracts progress toward that SDG.

3 RESULTS

3.1 Impact assessment results and contribution to SDG achievement

The analysis focuses on SDGs 1, 10, 12, 13, and 15 since their achievement is particularly affected by the environmental and socio-economic impacts of LiS-ASSB production. These SDGs are linked to the LCSA impact categories. Further explanations on the selection of SDGs and the linking procedure can be found in supporting information S1-4.1 to S1-4.3. The environmental and socio-economic impact scores related to the four LiS-ASSBs and the state-of-the-art lithium-sulfur battery with liquid electrolyte (benchmark) are presented in Table 2.

TABLE 2 Impact scores of the selected life cycle sustainability assessment impact categories linked to the relevant sustainable development goals for 1 kWh pack capacity

SDG	Impact category	Unit	Benchmark	LiS-ASSB[Ge]	LiS-ASSB[Si]	LiS-ASSB[Sn]	LiS-ASSB[CI]
1	Production costs	US-Dollar	101.6	61.8	31.1	29.7	31.0
	Risk of labor laws violation	Medium risk hour equivalents	392.7	349.5	51.9	45.3	42.6
	Risk of poverty	Medium risk hour equivalents	159.9	143.1	20.3	17.7	16.5
	Risk of absentee of social benefits	Medium risk hour equivalents	1802.8	1622.2	236.0	205.4	193.6
	Risk of unemployment	Medium risk hour equivalents	17.4	10.2	5.8	5.5	5.5
	Risk of low average wage	Medium risk hour equivalents	418.1	224.8	48.9	46.3	43.4
	Risk of non-communicable disease	Medium risk hour equivalents	1329.6	1175.9	176.9	154.2	145.6
	Risk of not having access to improved drinking water	Medium risk hour equivalents	94.1	70.4	14.5	12.9	12.5
	Risk of not having access to improved sanitation	Medium risk hour equivalents	344.6	311.2	43.4	37.8	34.9
	Risk of not having access to hospital beds	Medium risk hour equivalents	154.4	139.2	19.9	17.2	16.3
	Risk of children out of school	Medium risk hour equivalents	9.5	5.4	1.7	1.5	1.6
10	Production costs	US-Dollar	101.6	61.7	31.1	29.7	31.0
	Risk of high number of migrant workers	Medium risk hour equivalents	1133.3	1031.9	164.7	144.6	137.5
	Risk of poverty	Medium risk hour equivalents	159.9	143.1	20.3	17.7	16.5
	Risk of low average wage	Medium risk hour equivalents	418.1	224.8	48.9	46.3	43.4
	Risk of gender inequality	Medium risk hour equivalents	1388.4	1268.7	171.4	148.5	137.7
	Risk of indigenous rights infringements	Medium risk hour equivalents	392.3	433.7	51.7	43.1	40.0
12	Terrestrial acidification	$kg SO_2$ -equivalents	0.3192	0.3489	0.2801	0.2553	0.2841
	Freshwater eutrophication	kg P-equivalents	0.0695	0.0644	0.0833	0.0726	0.0879
	Marine eutrophication	kg N-quivalents	0.0277	0.0242	0.0260	0.0238	0.0265
	Freshwater ecotoxicity	kg 1,4-DCB-equivalents	21.2	19.1	28.2	23.5	30.5
	Human toxicity	kg 1,4-DCB-equivalents	71.4	101.8	85.5	76.8	90.9
	Marine ecotoxicity	kg 1,4-DCB-equivalents	18.4	17.9	24.3	20.3	26.3
	Terrestrial ecotoxicity	kg 1,4-DCB-equivalents	0.0058	0.2247	0.0042	0.0038	0.0042
	Fossil resource depletion	kg Fe-equivalents	19.1	22.2	17.6	16.3	17.5
	Mineral resource depletion	kg Oil-equivalents	23.7	22.9	30.0	141.7	32.4
	Water depletion	m ³ water	0.7921	0.9911	1.1065	0.7878	0.8229
	Risk of labor laws violation	Medium risk hour equivalents	392.7	349.5	51.9	45.3	42.6
	Risk of a repressive legal system	Medium risk hour equivalents	1124.0	1004.0	143.7	124.8	117.1
13	Climate change	$kg CO_2$ -equivalents	64.3	61.1	56.6	51.8	56.6
	Risk of non-communicable disease	Medium risk hour equivalents	1329.6	1175.9	176.9	154.2	145.6
	Risk of occupational injuries and deaths	Medium risk hour equivalents	163.2	140.4	26.1	23.2	22.8
15	Terrestrial acidification	kg SO ₂ -equivalents	0.3192	0.3489	0.2801	0.2553	0.2841
	Terrestrial ecotoxicity	kg 1,4-DCB-equivalents	0.0058	0.2247	0.0042	0.0038	0.0042

Various LCSA impact categories are used to analyze the contribution to SDG achievement. The first analysis of the impact scores shows that the production of the most promising battery configuration concerning technical properties, the LiS-ASSB[Ge], does not perform best in terms of sustainability aspects (e.g., it shows high impact scores in SDGs 1 and 10). Thus, at least one battery configuration has a more favorable impact score for each impact category analyzed, except for *mineral resource depletion, marine ecotoxicity, freshwater ecotoxicity,* and *marine eutrophication*. Moreover, the preferability of particular LiS-ASSB configurations in terms of SDG achievement cannot be derived directly from the impact scores. For example, with respect to SDG 1, the production of LiS-ASSB[CI] performs best in six impact categories and that of LiS-ASSB[Sn] in five impact categories. Without additional information on the relevance of the impact categories concerning the SDG, no clear recommendation or preference for a particular LiS-ASSB technology can be derived. This is even more evident with regard to SDG 12, where the production of LiS-ASSB[Sn] is beneficial concerning five impact categories, the production of LiS-ASSB[Ge] concerning four impact categories, and the production of LiS-ASSB[CI] and the lithium–sulfur battery are beneficial in two and one impact categories, respectively.

To quantify the contribution of LiS-ASSB production to the achievement of the selected SDGs, the method presented in Section 2.3 is applied. The resulting SDG contribution scores are shown in Figure 4 and the underlying data are available in supporting information S10. Higher scores indicate a more favorable contribution of the respective LiS-ASSB configuration to the achievement of the respective SDG compared to the benchmark battery.

The results indicate that the production of LiS-ASSB is especially advantageous for the achievement of the socially oriented SDGs 1 and 10. Here, the contribution of LiS-ASSB production to SDG achievement ranges from +23% to +85% for SDG 1 and from +17 to +86% for SDG 10, whereby especially the production of LiS-ASSB[Si], LiS-ASSB[Sn], and LiS-ASSB[CI] stand out. This is due to the positive contribution in the individual impact categories, which ranges from +66% to +90% for SDG 1, and +69% to +90% for SDG 10, resulting from a lower impact associated with the cathode materials and the solid electrolyte. Regarding LiS-ASSB[Ge], the contribution is slightly lower. It ranges from +10% to +46% regarding SDG 10. Here, the extraction and processing of germanium in countries with questionable working conditions are responsible for the lower scores.

The situation is different regarding the environmentally oriented SDGs 12 and 15. Here, the production of LiS-ASSB[Ge] leads to a decrease in goal achievement of -317% for SDG 12 and -1888% for SDG 15. This deterioration in contribution to goal achievement is mainly due to the negative impacts of *fossil resource depletion, human toxicity,* and *terrestrial ecotoxicity,* which are related to the energy-intensive and harmful extraction and processing of germanium. While the production of LiS-ASSB[Sn] leads to deterioration in SDG 12 achievement of -23% as well, improvements of 4% to 5% occur due to the production of LiS-ASSB[Si] and LiS-ASSB[CI]. The negative or low positive impacts regarding SDG 12 achievement are due to the higher requirement of tin, copper, and lithium, which are primary drivers of the impact category *mineral resource depletion, freshwater ecotoxicity,* and *marine ecotoxicity.* However, concerning the achievement of SDG 15, the production of LiS-ASSB[Si], LiS-ASSB[Si], and LiS-ASSB[CI] has a positive contribution of +11% to +34%. Concerning SDG 13, the production of all LiS-ASSBs positively contributes from +10% to +65% to SDG achievement. The main contributor in the impact categories used to characterize the SDG is the cathode, but there are differences between the batteries. While for LiS-ASSB[Si], LiS-ASSB[Sn], and LiS-ASSB[CI], 44% to 45% of the impacts are due to the aluminum used in the cathode as well as the energy required for production; for LiS-ASSB[Ge], the cathode is responsible for 58% of the total impact. These differences in the impact are due to the production and processing of germanium. However, the impact is nevertheless lower than for the benchmark battery, which is also driven by the energy requirement during production as well as the extraction and processing of the materials copper and aluminum.

Overall, these results confirm the indications from Table 2. The best LiS-ASSB configuration concerning technical properties (LiS-ASSB[Ge]) is not the best in terms of contribution to SDG achievement. In this respect, LiS-ASSB[Si], LiS-ASSB[Sn], and LiS-ASSB[CI] show great potential.

3.2 | Influence of cathode thickness on the contribution of LiS-ASSB production concerning SDG achievements

The previous analyses considered battery configurations optimized for maximum specific energy. To investigate whether these configurations are also preferable regarding their contributing to SDG achievement, a sensitivity analysis concerning the cathode thickness, a key determinant of the battery's specific energy, is carried out. Too thin cathodes lead to a bad current collector to electrode coating ratio, and too thick cathodes lead to high internal resistance due to slowed ion transport. An optimal cathode thickness exists for each solid electrolyte in question. For the sensitivity analysis, the cathode thickness varies from -20% to +20% relative to the optimum. Further explanations can be found in supporting information S1-1.8.

In Figure 5, the improvements and deteriorations of the SDG contribution scores resulting from the variations of cathode thickness are presented. The underlying data are available in supporting information S10. The results show that the technologically optimal battery configurations do not necessarily have the best properties in terms of sustainability aspects. Although the LiS-ASSBs designed for maximum specific energy perform well in terms of their SDG contribution scores, further improvements toward sustainability can be achieved in individual cases (shown by positive trends of the curves).

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SDCRelated LCSA impact designedSUE contructionImpact designed by the straining of the stra	E et al.			RIAL ECOL	ocy W]	LEY⊥
Note: 	SDG	Related LCSA impact categories				
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	1 NO POVERTY	 Risk of labor laws violation Risk of poverty Risk of absentee of social benefits Risk of unemployment Risk of low average wage Risk of non-communicable disease Risk of not having access to improved drinking wat Risk of not having access to improved sanitation Risk of not having access to hospital beds 	er			
12 EXEMPTION CONSTRUCT CONSTRUCT CONSTRUCT CONSTRUCT 	10 REDUCED INEQUALITIES	 Risk of high number of migrant workers Risk of poverty Risk of low average wage Risk of gender inequality 				
13 CLIMATE Image 10% Image Image Image Image Image Image Image Image Image Image Image Image Image Image Image Image I	CONSUMPTION	 Freshwater eutrophication Marine eutrophication Freshwater ecotoxicity Human toxicity Marine ecotoxicity Terrestrial ecotoxicity Fossil resource depletion Mineral resource depletion Water depletion Water depletion Risk of labor laws violation 		*****	<u>222222</u>	222222
Terrestrial acidification Terrestrial ecotoxicity Ge Si Sn Cl Battery types	IJ ACTION	N Risk of non-communicable disease				
	15 LIFE ON LAND		-1,888%	<u>annan</u>		<u>ennenne</u>
Ge: LIS-ASSBIGET Si: LIS-ASSBISTE Sn: LIS-ASSBISnT CI: LIS-ASSBICTE	Battery types Ge: LiS-ASSB[Ge]	Si: LiS-ASSB[Si] Sn: LiS-ASSB[Sn] C	l: LiS-ASSB[Cl]			

FIGURE 4 Contribution of the production of the lithium-sulfur all-solid-state batteries to the achievement of the relevant sustainable development goal. Underlying data for this figure can be found in Supporting Information S10.

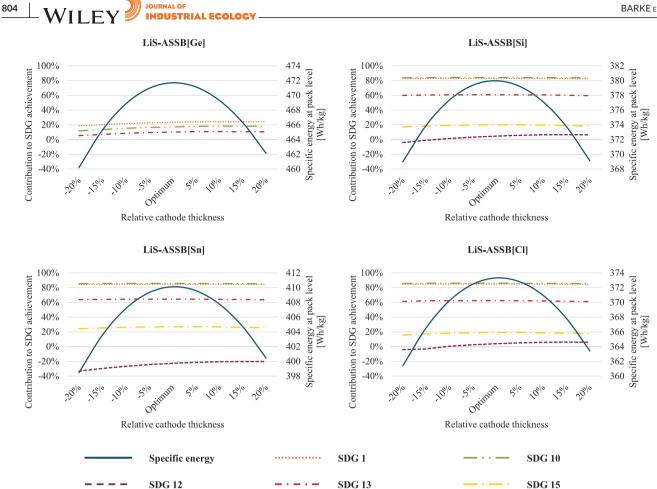


FIGURE 5 Influence of varying cathode thickness on the contribution to sustainable development goal achievement and the specific energy at pack level. Underlying data for this figure can be found in Supporting Information S10.

Concerning the LiS-ASSB[Ge], it is noticeable that a thicker cathode consistently improves the contribution to SDG achievement for all SDGs considered. This is because, with thicker cathodes, less of the material with negative impact is needed, as explained in the following: As an aircraft requires a fixed amount of energy for propulsion, a decrease in specific energy at pack level needs to be compensated by increasing the pack size by adding more cells. However, thicker cathodes result in significantly fewer cells installed per pack. The current collectors made of copper and aluminum and the germanium used in the solid electrolyte have the most decisive influence on the impact categories for characterizing the SDGs. Due to the change in battery configuration, the total share of these materials decreases at pack level, reducing the environmental and socio-economic impacts. Therefore, the LiS-ASSB[Ge] production positively contributes to SDG achievement by using thicker cathodes.

The results show that concerning the contribution to SDG 12, a thicker cathode consistently has a positive impact. Depending on the LiS-ASSB type, improvements of +1% to +8% can be gained to contribute to SDG achievement. Worse results in the impact categories mineral resource depletion, freshwater ecotoxicity, and marine ecotoxicity are mainly responsible for the negative contribution to SDG achievement. Here, tin, copper, and lithium are the primary drivers of the impact categories. A thicker cathode leads to the same effect as described above for the LiS-ASSB[Ge].

In some cases, minimal improvements in the contribution to the achievement of SDGs 1, 10, 13, and 15 of +0.01% to +0.03% occur for the production of LiS-ASSB[Sn] and LiS-ASSB[Cl], which can be attributed to the changes in battery configuration. In addition, the results of the sensitivity analysis for the LiS-ASSB[Ge] in terms of contribution to SDG 12 and 15 achievements are neglected in Figure 5 since the negative contribution to SDG achievement is extremely large. Changes in cathode thickness make only a marginal difference.

3.3 Importance of weighting factors for the calculation of SDG contribution scores

The previous analyses show that a technically optimal battery configuration does not necessarily perform best concerning sustainability in terms of contribution to SDG achievement. However, the equal weighting factors used to calculate the SDG contribution scores are a simplification. Therefore, the influence of the weighting factors on the SDG contribution score is analyzed using Monte Carlo simulation (MCS). The analysis focuses on **TABLE 3** Empirical probability P' in which alternative p_1 has a higher SDG contribution score than alternative p_2 concerning the SDGs investigated

SDG 1					SDG 10							
$\overline{P'(s_1^{p_1}>s}$	^p ₂)	p ₂					$P'(s_{10}^{p_1} > s_{10}^{p_2})$		p ₂			
		Ge	Si	Sn	CI				Ge	Si	Sn	Cl
p_1	Ge		0%	0%	0%		p_1	Ge		0%	0%	0%
	Si	100%		0%	0%			Si	100%		0%	0%
	Sn	100%	100%		1.4%			Sn	100%	100%		2.5%
	CI	100%	100%	98.6%				Cl	100%	100%	97.5%	

SDG 12						SDG 13							
$P'(s_{12}^{p_1} > s_{12}^{p_2}) \qquad p_2$							$P'(s_{13}^{p_1} > s_{13}^{p_2}) \qquad p_2$						
		Ge	Si	Sn	Cl					Ge	Si	Sn	Cl
p_1	Ge		0.1%	3.8%	0.2%			p_1	Ge		0%	0%	0%
	Si	99.9%		84.9%	62.2%				Si	100%		0%	0%
	Sn	96.2%	15.1%		15.4%				Sn	100%	100%		93.7%
	CI	99.8%	37.8%	84.6%					Cl	100%	100%	6.3%	

		5	5DG 15				
$P'(s_{15}^{p_1} > s_{15})$	$P'(s_{15}^{p_1} > s_{15}^{p_2}) \qquad p_2$						
		Ge	Si	Sn	CI		
p_1	Ge		0%	0%	0%		
	Si	100%		0%	100%		
	Sn	100%	100%		100%		
	CI	100%	0%	0%			

the SDGs and impact categories described in Table 2, for which the SDG contribution scores are calculated. The weighting factors for the calculation are drawn randomly from a uniform distribution on the interval [0,1] and normalized so that the sum over all weighting factors per SDG equals one. Within each of the 10,000 MCS iterations, the SDG contribution scores are calculated for each LiS-ASSB configuration, and pairwise comparisons of the LiS-ASSB configurations are made. In Table 3, the empirical probability P' in which a LiS-ASSB configuration p_1 has a higher SDG contribution score s than a configuration p_2 is analyzed.

The results show that although the weighting factors affect the SDG contribution scores, the advantageousness of specific battery configurations is mainly independent of the weighting factors. In 21 of the pairwise comparisons, a specific LiS-ASSB configuration p_1 has a higher SDG contribution score than another configuration p_2 in all 10,000 MCS iterations. This is because LiS-ASSB[Ge] and LiS-ASSB[Si] have higher negative impact scores than LiS-ASSB[Sn] and LiS-ASSB[Cl] in most impact categories. The situation differs when comparing LiS-ASSB[Sn] and LiS-ASSB[Cl]. Here, the LiS-ASSB[Cl] is advantageous in three pairwise comparisons, and the LiS-ASSB[Cl] is better in two pairwise comparisons. This is because neither one of these configurations is dominated by the other in the considered impact categories. Hence, the choice of weighting factors has an influence on the advantageousness of these two configurations in terms of contribution to the achievement of SDGs 1, 10, 12, and 13. Concerning SDGs 1, 10, and 13, the influence of the weighting factors on the SDG contribution scores appears to be much smaller than the influence of the LCSA impact scores in this analysis. Only concerning SDG 12, the choice of the weighting factors can significantly influence the SDG contribution scores and thus the advantageousness of a LiS-ASSB configuration, which is due to very similar LCSA impact scores.

4 | DISCUSSION

The results of this study confirm that LiS-ASSBs should be regarded as a promising energy storage technology for electric aircraft. Their technical properties of achievable specific energy are clearly superior to lithium-sulfur batteries with liquid electrolytes. Also, from a sustainability perspective, the LiS-ASSBs have several advantages in terms of their environmental and socio-economic impacts compared to state-of-the-art battery technologies. This is partially due to the higher specific energy, implying a lower material and energy demand for a certain storage capacity, but JOURNAL OF

also results from the different materials used, which can be extracted and processed with less environmental impacts and under less critical socioeconomic conditions. Especially compared to currently available lithium-ion batteries, significant reductions in the LCSA scores can be achieved, ranging from 71% to 89% for environmental impacts (Dai et al., 2019; Deng et al., 2017; Ellingsen et al., 2014; Kallitsis et al., 2020; Kelly et al., 2020) and from 82% to 99% for socio-economic impacts (Barke et al., 2021; Thies et al., 2021).

As the development of LiS-ASSBs for electric aircraft is at an early stage, there are various degrees of freedom regarding their specific configuration. The assessment shows that the most promising battery configuration from a technical perspective, the LiS-ASSB[Ge], is not necessarily the most promising configuration in terms of sustainability. Instead, the LiS-ASSB[Si], LiS-ASSB[Sn], and LiS-ASSB[CI] are preferable regarding the investigated impact categories and SDGs. The LiS-ASSB[Sn] has the highest SDG contribution score concerning three of the five analyzed SDGs, whereas the LiS-ASSB[Si] and the LiS-ASSB[CI] are each advantageous for one SDG. Therefore, these configurations should also be considered in further research. These findings are supported by a sensitivity analysis with varying cathode thicknesses. It demonstrates that combining promising technical properties (e.g., maximum specific energy) with beneficial environmental and socio-economic impacts can be complicated. Both are equally needed to ensure long-term sustainable development of the aviation sector.

The proposed approach for assessing the alternative LiS-ASSB configurations regarding their contribution to SDG achievement offers a new perspective that complements the assessment based on LCSA impact categories. Establishing this link to the SDGs in sustainability assessment supports the target-oriented development of new products and technologies. Nevertheless, there are methodological aspects that deserve further attention. These comprise uncertainties regarding the parameters in the SDG classification and characterization procedures. While in the case of LiS-ASSBs, a MCS revealed that the weighting factors have a rather limited influence on the overall preferability of particular configurations, this does not necessarily hold for other types of products. Product-specific linking procedures could be a promising approach. In addition, the currently used linear weighted sum allows for the compensation of positive and negative contributions in different impact categories. This could be avoided by using a more differentiated approach as proposed by Kalbar et al. (2017) for characterizing endpoint indicators in LCA, alternative weighting factors (UNEP, 2020), or applying multi-criteria decision-making (MCDM) models (Triantaphyllou, 2000; Velasquez & Hester, 2013). In addition, such MCDM models can be used to select beneficial technologies or products for achieving several SDGs. The selection of an appropriate MCDM model can be conducted based on Guitouni and Martel (1998).

Uncertainty exists regarding the battery design for an electric aircraft. The battery capacity is taken from the scientific literature, but the battery systems differ in terms of their specific energy and, therefore, also in terms of their weight and volume. This leads to the need for a larger or smaller capacity, which in turn increases or decreases the weight of the battery system, which, in addition, leads to changes in the incidental aircraft design, further influencing the aircraft weight and required battery capacity. The required battery capacity would have to be calculated using an iterative model, taking these system-immanent complexities into account. An exact determination of the battery technology with the best technical properties does not necessarily have the best properties in terms of sustainability aspects will remain since the LiS-ASSB[Ge] has a 15% to 26% higher specific energy overall but is associated with much higher negative environmental and socio-economic impacts during production as well as weaker contributions to the achievement of the SDGs. Against this background, however, an extension of the scope of the study could be necessary to consider the additional environmental and socio-economic impacts associated with the use stage and end-of-life stage. In particular, the end-of-life stage can have a considerable impact, but significant research concerning the end-of-life of LiS-ASSB is missing so far.

Further uncertainties exist concerning the LiS-ASSBs. Because the technology is still in the development phase, several assumptions had to be made. A porosity of 0% was assumed for the cathode and separator, leading to an overestimation of the specific energy. In addition, no charge transfer resistances were considered, and the reaction-induced change of the interface between active material and solid electrolyte was neglected. Furthermore, the electrode structure on ionic and electrical conductivity was not considered, leading to the charge-dependent voltage profile being assumed not to be entirely accurate. The anode thickness was calculated to match the cathode's capacity. However, commercial lithium is not available in these thicknesses yet, and we assumed a perfect chemical and electrochemical compatibility between solid electrolyte and metallic lithium. To achieve this, novel surface coatings of the solid electrolyte particles or the metallic lithium are required.

5 | CONCLUSIONS AND OUTLOOK

In this article, the potential of LiS-ASSB as a key technology for the electrification of the aviation sector is analyzed. The study scrutinizes the environmental and socio-economic impacts related to LiS-ASSB production, identified as the decisive phase within the batteries' life cycle, and quantifies the contribution of the new technologies toward sustainable development, indicated by related SDGs.

It is shown that purely based on LCSA impact scores, no preferable LiS-ASSB configuration can be identified regarding its contribution to SDG achievement. The LCSA impact scores represent detailed analytical results, but their relationship to the SDGs has been unclear, and, in particular, quantification of their contribution to achieving the goals has not been possible. Therefore, a novel method for quantifying the contribution to SDG achievement is introduced. The results indicate that the battery configuration with the best technical characteristics is not the most promising in terms of sustainability aspects. Instead, the focus should be on the further development of LiS-ASSB[Sn], LiS-ASSB[Si], and LiS-ASSB[CI]. A



subsequent sensitivity analysis showed that a deviation from the technically optimal configuration to maximize the specific energy could generate further advantages in terms of sustainability aspects and thus contribute to achieving the SDGs.

This study should be a starting point for future research from technical and methodological perspectives. Battery development should take sustainability aspects into account in addition to technically optimal battery properties. Thus, by varying characteristics of battery components or by developing novel materials and production processes, technical properties may deteriorate, but further improvements in sustainability aspects and SDG achievement could be generated, which may be preferred in multidimensional system analysis. In future work, however, primary data from battery production must be used when it becomes available to make the process modeling more realistic and thus more scalable. Especially the determination of the production costs and the energy requirement during battery production must be revised carefully. Here, the underlying system model of the ecoinvent database should be changed to "substitution, consequential, long-term" to determine the impacts from the conversion to large-scale industrial production. Furthermore, if multi-output or recycling activities exist in the foreground system, it should be ensured that the allocation rules are consistent with those in the background system. In addition, a scope extension of the study, including the use stage and end-of-life stage, should be addressed to allow for comparison with conventional kerosene-powered aircraft. At the same time, the analysis method should be further elaborated. The linear weighted sum for calculating the SDG contribution scores should be adapted using alternative weighting factors or MCDM models to avoid compensating for negative impacts with positive ones. Furthermore, the method should be expanded to evaluate beneficial technologies or products regarding their contribution to achieving several SDGs.

Overall, this article expands the scientific literature by creating novel LCI datasets for LiS-ASSB production based on short-haul electric aircraft characteristics from an interdisciplinary research center and generated using an electrochemical model. In addition, the contribution to SDG achievement is determined by applying a novel method for quantifying the contribution to SDG achievement, and recommendations for the future development of batteries for electric aircraft are derived.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available in the Supporting Information.

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