



Activity analysis based modeling of global supply chains for sustainability assessment

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Abstract

Assessing the sustainability of products is an intricate task that requires a thorough understanding of the underlying supply chains. Prominent challenges are the integration of the environmental, the economic, and the social dimension of sustainability as well as the consideration of spatial heterogeneity with regard to technology, environment, markets, and society. This paper proposes a novel modeling approach based on activity analysis to facilitate spatially differentiated sustainability assessments of global supply chains. The production and transportation activities in the supply chain and the exchanges between activities and their natural, economic, and social environments are formalized by means of activity vectors. Linking the activities and exchanges to specific locations allows for the calculation of regionalized sustainability indicators. The approach is used to analyze the environmental, economic, and social impacts of lithium-ion batteries. The comparison of alternative supply chain configurations with the spatially differentiated approach reveals that the assessment results differ significantly from those of the global average supply chain. These insights offer new opportunities to advance the design of sustainable supply chains.

Keywords Sustainability assessment · Activity analysis · Spatial differentiation · Supply chain

JEL classification M11 · Q57 · C67

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1 Introduction

Sustainability has become a topic that receives increasing attention of corporate decision-makers. Driven by customer requirements, competitive pressures, regulatory pressures, and internal risk management, companies seek to reduce their environmental footprints and to improve their social impacts, without compromising their economic profitability (O'Rourke 2014). For example, major companies from different industries and countries have recently committed to reduce their carbon footprint and to align their businesses with science-based targets to limit the worst impacts of climate change (Science Based Targets initiative 2019). Furthermore, managers recognize the increasing importance of corporate social responsibility to create a competitive advantage and to secure the long-term success of their business (Porter and Kramer 2006).

To achieve improvements in sustainability, an effective management of the supply chain is important (Goldstein and Newell 2019). Due to increased outsourcing and globalization, the supply chains of many modern products have complex structures, comprising multiple stages that are scattered over many locations. For example, a modern car consists of around 10,000 parts, which are sourced from hundreds of suppliers in all parts of the world. In this context, the structure of the supply chain, as reflected by the selection of the suppliers, the locations of the production sites, and the distribution system, can have a substantial influence on the sustainability performance of the supply chain. In the case of cars, the location of the production facilities was found to be the most influential factor with regard to production costs and production-related emissions (Kannegiesser et al. 2014).

From a decision-making perspective, it is thus important that the consequences of such design decisions in the supply chain can be evaluated properly. Alternative configurations of the supply chain need to be assessed with regard to economic, environmental, and social sustainability criteria that are relevant to the decision-maker. Thereby, emphasis must be placed on the global nature of modern supply chains and the manifold tradeoffs involved in sustainability decision-making. Design decisions not only affect supply chain sustainability from a global perspective but also have local and regional effects. Furthermore, tradeoffs between the different sustainability criteria as well as tradeoffs between local and global sustainability aspects often occur. For example, relocating a production facility might improve profitability due to lower production costs but increase the emission of greenhouse gases due to a different electricity supply and additional transportation. In addition to these global effects, local implications such as different working conditions and local pollution need to be considered (Thies et al. 2018).

Systematic approaches for sustainability assessment can be found under the comprehensive framework of life cycle sustainability assessment (LCSA), which combines assessment methods from all sustainability dimensions such as environmental life cycle assessment, life cycle costing, and social life cycle assessment. Although there are some similarities, the nature of the particular assessment

methods is quite different and a consistent way of modeling is missing. A second challenge that arises especially when assessing global supply chains is the regional heterogeneity of technology, environment, markets, and society, resulting in the need for spatially differentiated modeling and assessment approaches. Moreover, the environmental and social aspects are often not integrated into management-oriented decision models. They are assessed complementarily to the technological and economic performance indicators as the assessment is based on different modeling approaches. Activity analysis, as an established method for the techno-economic modeling of production systems, can be used to integrate LSCA into a management-oriented decision support tool.

Therefore, the objective of this paper is the development of a quantitative modeling approach that facilitates the sustainability assessment of global supply chains by integrating environmental, economic, and social aspects of sustainability and by considering their global as well as local implications. To this end, we consider a situation in which the decision-maker is a focal company (e.g., a car manufacturer) who seeks to assess the sustainability of the supply chain of a particular product or service based on production, transportation, and storage activities scattered all over the world. For this supply chain, alternative configurations need to be evaluated. The application of activity analysis leads to spatially differentiated algebraic process models that take into account all economically, environmentally, and socially relevant resource flows. The resulting global supply chain models enable decision-makers to analyze and to compare decision alternatives by the consistent computation of regional and country-specific sustainability indicators. This way, we aim to contribute to the existing body of literature by extending activity analysis of multi-stage production systems in the context of sustainability assessment with a spatial dimension and by providing a common modeling approach for environmental, economic, and social sustainability aspects. This facilitates the integration of life cycle sustainability assessment into managerial decision support tools.

The remainder of this paper is organized as follows: an analysis of current approaches to sustainability assessment and an overview of the basic concepts of activity analysis are provided in Sect. 2. The basic model formulations for sustainability assessment is presented in Sect. 3 and extended by the spatial dimension in Sect. 4. In Sect. 5, a case study that illustrates the application of the proposed modeling approach using the example of lithium-ion batteries is provided. The paper concludes with a summary of the benefits and limitations, recommendations for decision-makers, and an outlook on avenues for further research in Sect. 6.

2 Literature: approaches to sustainability assessment and activity analysis

In this section, an overview of existing approaches and main challenges of sustainability assessment is given, and the general concepts and recent developments of activity analysis are summarized. This lays the foundation for our model formulation in Sect. 3.

2.1 Principles and challenges of sustainability assessment

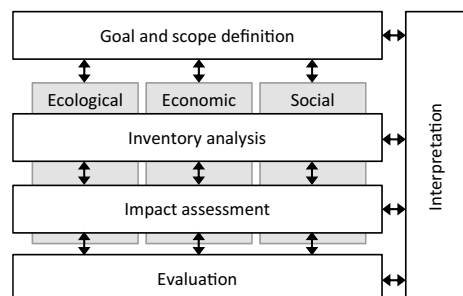
Sustainability assessment refers to the systematic compilation and evaluation of the environmental, economic, and social impacts of a system to provide information that supports improving it or comparing it to other systems. While sustainability assessments have been carried out for different systems, including countries, cities, industries, technologies, or companies (Costa et al. 2019; Singh et al. 2012), this paper focuses on the assessment of product systems (comprising goods and services) and their supply chains. In this context, the assessment methods are usually based on a life cycle perspective, considering the impacts in the various stages of the product's life cycle.

A comprehensive framework with life cycle oriented assessment methods for all three sustainability dimensions is life cycle sustainability assessment (LCSA). It combines the environmentally-oriented life cycle assessment (LCA) with economically- and socially-oriented assessment methods such as life cycle costing (LCC) and social life cycle assessment (SLCA) (Finkbeiner et al. 2010; Guinée et al. 2011; Kloepffer 2008; UNEP/SETAC 2011). While LCA is an established method with standardized procedures, the integration of economic and social aspects is a rather new endeavor for which the detailed procedures and computational methods have not been harmonized yet (Marvuglia et al. 2015).

The basic procedure of LCSA is derived from the ISO 14040/14044 standards (Fig. 1). A typical LCSA study starts with the definition of goal and scope. Next, inventory data describing the exchanges between activities in the product's life cycle and their executing organizations as well as the external environment is collected. In the subsequent impact assessment, the inventory data is assigned to environmental, economic, and social impact categories. Finally, an evaluation step integrates the various indicators from all three sustainability dimensions to support decision-making, taking into account the decision-makers' preferences and the underlying uncertainty (Grubert 2017; Keller et al. 2015). All steps are accompanied by interpretation and may be carried out in an iterative procedure (UNEP/SETAC 2011).

Life cycle assessment (LCA) addresses the environmental impacts of products. From the first studies dating back to the late 1960s, a sophisticated and comprehensive methodology for the assessment of a large set of environmental issues has evolved (Guinée et al. 2011). In inventory analysis, environmental interventions,

Fig. 1 Framework for life cycle sustainability assessment (adapted from ISO 14,040)



such as resource extractions, emissions, land use, and water use, of all processes in the product life cycle are compiled. Next to primary data that is collected for the specific study, secondary data from publicly available inventory databases is integrated. Thereby, most databases comprise processes that are only valid for selected geographical regions or represent the global average of the production technology and supply conditions and thus do not allow for a regionalized assessment. In impact assessment, the inventory results are linked to potential impacts in different areas of protection (human health, ecosystems, and resources). To this end, endpoint indicators at the level of the areas of protection and midpoint indicators on the pathway between the emissions and the endpoints are defined (Finnveden et al. 2009). The characterization factors that are used to quantify the impacts are often defined on a global level, but regionalized impact assessment methods are emerging (Patouillard et al. 2018; Potting and Hauschild 2006).

An established method to assess the economic aspects of a product is life cycle costing (LCC). It was first used in the 1960s by the United States Department of Defense to assess not only the investments into new equipment but also the related costs for operation and maintenance during its lifetime (Neugebauer et al. 2016). LCC is not intended as a financial accounting method but rather as a cost management method with the goal of estimating the costs associated with the existence of a product with complimentary inclusion of externalities that are anticipated to be internalized in the decision-relevant future (Rebitzer and Hunkeler 2003). The focus on cost is criticized by Neugebauer et al. (2016), who argue that economic activities have a wide range of positive and negative consequences. They propose a novel concept called economic life cycle assessment (EcLCA) for representing the economic pillar within the LCSA framework. The concept uses an impact assessment method based on five economic midpoint indicators, namely, profitability, productivity, consumer satisfaction, business diversity, and long-term-investment. Finally, a pertinent concept when it comes to the economic analysis of the supply chain of products is the valued added, i.e., the difference of the revenues received from downstream stages minus the expenses paid to upstream stages in the supply chain (Heijungs et al. 2013; Moreau and Weidema 2015).

Social life cycle assessment (S-LCA) is a method to analyze the potential positive and negative social impacts of products. First proposals to integrate social aspects into life cycle-oriented sustainability assessment methods have been made in the 1990s (O'Brien et al. 1996), followed by extensive discussions on the specific procedures, the development of social indicators, and the integration with other methods in the 2000s (Dreyer et al. 2006; Hauschild et al. 2008; Hunkeler 2006; Jørgensen et al. 2008; Norris 2006; Weidema 2006). The guidelines for social life cycle assessment (UNEP/SETAC 2009) and the methodological sheets for subcategories in S-LCA (UNEP/SETAC 2013) provide some guidance on how S-LCA studies should be carried out. In contrast to the focus of LCA on physical quantities of natural resources and emissions, S-LCA emphasizes the socio-economic interactions of the activities and analyzes their organizational and societal context in the supply chain. A common S-LCA procedure that is based on life cycle attribute assessment (Norris 2006) accounts for an activity variable (e.g., labor intensity) in the inventory analysis phase and links it to social indicators related to different stakeholders (e.g., workers,

consumers, local communities, value chain actors, society) in the impact assessment phase. It is important to note that due to the spatial heterogeneity of working conditions and socio-political situations, a spatially differentiated approach is specifically mandatory in S-LCA (Hauschild et al. 2008; Hunkeler 2006; Jørgensen et al. 2008).

Although the methods to assess the individual dimensions of sustainability are common in the industry and recognized in the scientific community, examples of full LCSA studies that seek to support the design of sustainable supply chains are still limited (Thies et al. 2019b). Next to the several unresolved problems and challenges in the particular assessment methods, a significant obstacle is the lack of an effective modeling approach that allows for a transparent analysis of all decision-relevant product flows as well as elementary flows and supports the consideration of environmental, economic and social sustainability aspects simultaneously (Fauzi et al. 2019; Guinée 2016; Petti et al. 2018; Reap et al. 2008a, b). Therefore, the computational models such as the matrix-based environmental life cycle assessment (Heijungs and Suh 2002; Yang and Heijungs 2017) need to be expanded by economic and social aspects, and the theoretical advancements in spatial differentiation (Mutel and Hellweg 2009; Patouillard et al. 2018; Potting and Hauschild 2006; Thies et al. 2018; Yang and Heijungs 2017) need to be integrated.

2.2 Foundations and applications of activity analysis

Activity analysis was first proposed by Koopmans (1951) and Debreu (1959) and deals with an algebraic modeling approach for the transformation of commodities by production and transportation processes. The central elements are activities and commodities. Activities describe “the combination of certain qualitatively defined commodities in fixed quantitative ratios as ‘inputs’ to produce as ‘outputs’ certain other commodities in fixed quantitative ratios to the inputs” (Koopmans 1951, pp. 35–36). In this context, the term commodities comprises production factors, intermediate products, and final products. The basic concept of activity analysis has been expanded in many ways to become a versatile modeling and assessment instrument in diverse economic settings. As activity analysis was initially developed as a general economic modeling approach, pertinent applications of activity analysis based models can be found in business economics, mainly in the field of production theory. The applications cover a wide range of planning tasks and industries (Table 1).

Most of these applications can be classified as linear activity analysis models. They are based on a finite set of basic activities describing the linearized input and output flows of real-world processes. By the introduction of non-negative or discrete activity levels, each stationary operation point of a transformation process (production, recycling, transportation, etc.) can be determined by a linear combination of the basic activities. If necessary, nonlinear input-output-relations, such as Gutenberg production functions, can be modeled (Fandel 2005; Hildenbrand 1966; Wittmann 1966). They can be approximated, for example, using several basic activities describing a piecewise linear function (Meyer et al.

Table 1 Overview of applications of activity analysis in business economics

Reference	Planning task	Industry
Fandel and François (1994)	Dynamic lot size planning	Information processing activities
Spengler (1994)	Disassembly and recycling planning	Building industry
Spengler et al. (1998)	Computation of material and energy balances	Chemical industry
Souren (2002)	Analysis of circular economy concepts	Packaging of consumer goods
Spengler et al. (2003)	Disassembly and bulk recycling planning	Electronic scrap
Walther and Spengler (2005)	Allocation of products and disassembly activities	Electronic scrap
Richter (2012)	Structural analysis of services	Knowledge-intensive services
Hoyer et al. (2015)	Technology and capacity planning	Recycling of lithium-ion batteries
Meyer et al. (2016)	Operative production planning	Metallurgical slag recycling
Kieckhäfer et al. (2017)	Technology assessment and strategic planning	Enhanced landfill mining

2016). The constant input-output-coefficients of the basic activities can be determined by publicly available databases, or even more specific by internal company data, such as bills of materials, process schedules, process flowsheets, or by sophisticated simulation studies. One big advantage of activity analysis is its capability to model joint production processes in which the production of a certain product always goes along with the production of one or several other joint products due to technical reasons, as described by Riebel (1955). Furthermore, linear activity analysis can be used for modeling quantitative input-output-relations in economic systems, introduced by Leontief (1936).

While the modeling of techno-economic relationships has been the predominant focus of activity analysis, first efforts to integrate environmental aspects have been made. For example, Freire et al. (2001) present Life cycle activity analysis (LCCA) based on a combination of activity analysis and life cycle assessment for the optimal allocations of resources and environmental impacts in the life cycles of products. Their approach features alternative activities for production technologies as well as product recovery strategies and is applied to investigate the Portuguese bottled water industry. Dyckhoff (2017) applies activity analysis to formulate a multi-criteria production theory (MCPT) as a generalization of traditional production theories that integrates concerns of sustainability and environmental protection. However, the integration of all three sustainability dimensions based on life cycle-oriented assessment methods and supporting spatial differentiation has not been considered in activity analysis so far. On the other hand, life cycle sustainability assessment is often seen as a complementary tool and lacks a systematic integration into decision-oriented supply chain planning frameworks (e.g., Foolmaun and Ramjeawon 2013; Keller et al. 2015; Schau 2012; Wulf et al. 2017).

3 Activity analysis based supply chain modeling approach for sustainability assessment

Building on the general concepts of linear activity analysis, a modeling approach for spatially differentiated sustainability assessment in supply chains is developed. We first introduce a basic model for sustainability assessment without spatial differentiation to illustrate the main concepts. The expansions to enable spatial differentiation will be explained in Sect. 4.

3.1 General idea and main features

The general idea of the approach is illustrated in Fig. 2. It supports the spatially differentiated sustainability assessment of global supply chains and enables industrial and political decision-makers to analyze and to compare alternative supply chain configurations with regard to environmental, economic, and social criteria. While the modeling of production and transportation processes is based on linear activity analysis, the assessment follows the procedures of life cycle-oriented sustainability assessment methods. The linear formulation is appropriate for many practical applications (e.g., in the automotive industry or in the electronics industry) and can be expanded to account for nonlinear relationships if necessary. The approach has several advantages: First, with the capability to model technological, economic, environmental, and social relationships, activity analysis provides a common language for LCA, LCC, and S-LCA. In this regard, it expands the standard calculation schemes of matrix-based LCA. Second, the spatially differentiated modeling allows for the consideration of regional heterogeneity and for the integration of recent regionalized impact assessment methods. Finally, the approach facilitates the integration of well-founded sustainability assessment methods into decision-oriented supply chain planning frameworks. By this means, the economic, environmental, and social consequences of changes in the supply chain can be considered directly in the decision process.

3.2 System definition

The basic model comprises activities and exchanges (Fig. 3). Activities $\rho = 1, \dots, \pi$ describe the transformation of exchanges. They represent production processes

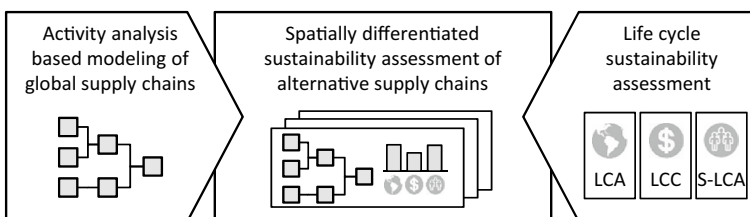


Fig. 2 General idea of the activity analysis based modeling approach for sustainability assessment

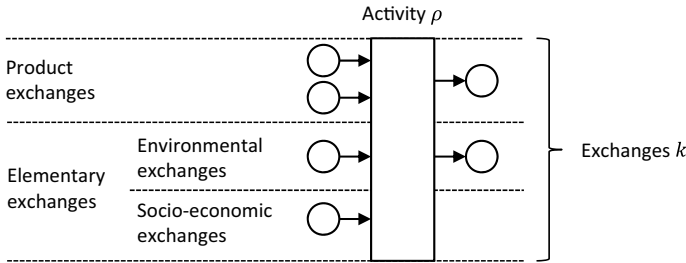


Fig. 3 Basic modeling of objects and activities

(qualitative transformation of exchanges), transportation processes (spatial transformation of exchanges), or storage processes (temporal transformation of exchanges). In the basic model, only production processes are considered. Exchanges $k = 1, \dots, \kappa$ constitute the inputs and outputs of activities. They can be categorized into product exchanges and elementary exchanges. Product exchanges refer to all man-made goods and services such as final products, intermediate products, and by-/waste-products. Elementary exchanges can be further distinguished into environmental exchanges and socio-economic exchanges. Environmental exchanges comprise resources from nature, emissions, or land. Socio-economic exchanges comprise, amongst others, human labor, knowledge, and capital. The term “exchanges” is used here as the English translation of “Objektarten” from the primarily German literature on activity analysis (e.g., Dyckhoff and Spengler 2010). The meaning is synonymous with objects, products, goods, or flows.

The quantitative relationships between the exchanges are formalized by means of activity vectors. An activity vector $\mathbf{z}^\rho = (z_1^\rho, \dots, z_k^\rho, \dots, z_\kappa^\rho)^T$ describes the quantities of exchanges k that are consumed or generated by activity ρ . If the sign of z_k^ρ is negative, then k is an input that is consumed by activity ρ . If the sign is positive, then k is an output of ρ . The quantities z_k^ρ depend on the level at which the activity is carried out. In the case of linear technology, they can be derived by scaling the so-called basic activity $\mathbf{a}^\rho = (a_1^\rho, \dots, a_k^\rho, \dots, a_\kappa^\rho)^T$, which is normalized to one unit of the reference product or to a certain time period (e.g., one day), with the activity level $\lambda^\rho \geq 0$ (or, for discrete processes, non-negative integer), which describes how often the activity is carried out (Eq. 1).

$$\mathbf{z}^\rho = \begin{pmatrix} z_1^\rho \\ \vdots \\ z_k^\rho \\ \vdots \\ z_\kappa^\rho \end{pmatrix} = \lambda^\rho * \begin{pmatrix} a_1^\rho \\ \vdots \\ a_k^\rho \\ \vdots \\ a_\kappa^\rho \end{pmatrix}; \lambda^\rho \geq 0 \tag{1}$$

A supply chain can be considered as a multi-stage system of activities as illustrated based on a highly simplified supply chain of battery cell production with four activities and 11 exchanges in Fig. 4. The activities are linked due to their dependency on common exchanges. This means that the output provided by one activity may be used as an input to another activity. For example, the activity $\rho = 2$

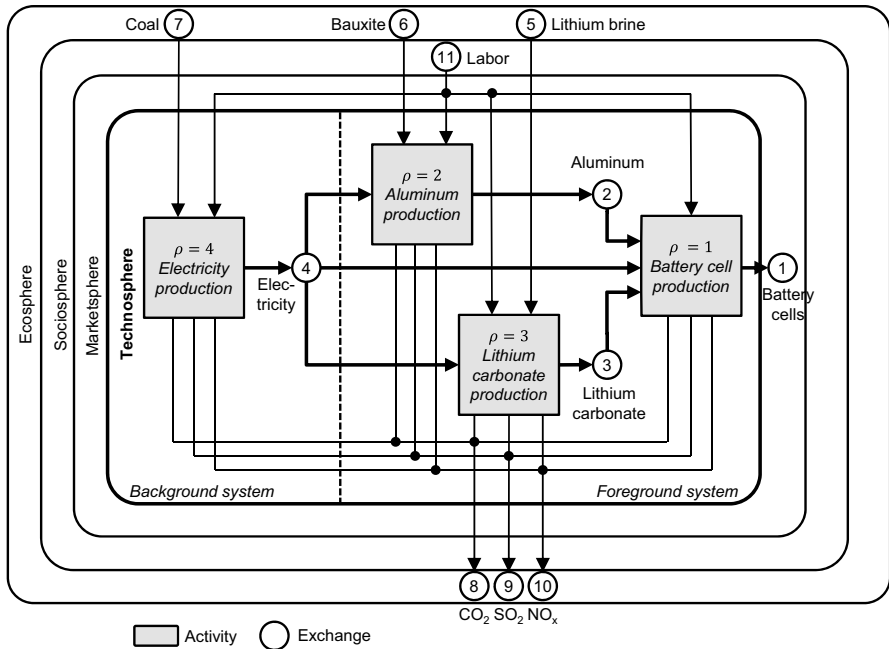


Fig. 4 Highly simplified supply chain of battery cell production

(“aluminum production”) has the exchange $k = 2$ (“aluminum”) as an output. This exchange is then used as an input to the activity ($\rho = 1$) “cell production”. Note that the quantities a_2^2 and a_2^1 of the corresponding basic activities may differ, e.g., $a_2^2 = 1$ and $a_2^1 = -0.8$ (i.e., 0.8 kg of aluminum is required to make one battery cell).

In life cycle assessment, the world is divided into a technosphere and an ecosphere (sometimes also called biosphere). While the technosphere includes everything that is intentionally man-made, the ecosphere represents the natural environment and includes everything that is not intentionally man-made (Bjørn et al. 2018). For a full sustainability assessment, a sociosphere comprising the human-beings in a society and a marketsphere for economic exchanges are integrated. While the ecosphere is the source and the sink of all environmental exchanges, the sociosphere and the marketsphere provide and receive all socio-economic exchanges (Fig. 4).

As supply chains of modern products often comprise many activities, it is useful to distinguish between a foreground system and a background system. The foreground system contains all activities that are of particular relevance for the conducted study. The background system contains all processes of a system that are not specific to it, i.e., auxiliary activities that are only of secondary interest for the conducted study (e.g., electricity generation). The definition of system boundaries also depends on the type of analysis. In a cradle-to-grave analysis, the system is set up in a way that only a non-material service leaves the system as a reference flow. All material flows are produced and treated inside the system. In a cradle-to-gate analysis, the reference flow is an output of a material product

with a positive economic value (Heijungs and Suh 2002). Guidance on defining appropriate system boundaries is given in Tillman et al. (1994), Li et al. (2014), and Bjørn et al. (2018).

The basic activity vectors can be adjoined to form the technology matrix $M = (a^1, \dots, a^\rho, \dots, a^\pi)$ of dimensions $\kappa \times \pi$. The columns of the technology matrix represent the activities, and the rows represent the exchanges. The technology matrix summarizes all relevant information about the supply chain and builds the quantitative base for the inventory analysis. It can be partitioned by the different types of exchanges. The submatrix A (called technosphere matrix) contains all rows of M with product exchanges and is usually square (assuming that each activity has exactly one reference product as output). The submatrix B (also referred to as biosphere matrix in LCA) contains all rows of M with elementary exchanges and is usually rectangular. The technology matrix M of the illustrative supply chain from Fig. 4 is formulated in Eq. (2).

$$M = \begin{pmatrix} \mathbf{A} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} \rho=1 & \rho=2 & \rho=3 & \rho=4 \\ 1 & 0 & 0 & 0 \\ -0.2 & 1 & 0 & 0 \\ -0.8 & 0 & 1 & 0 \\ -20 & -0.7 & -15 & 1 \\ \hline 0 & 0 & -10 & 0 \\ 0 & -5 & 0 & 0 \\ 0 & 0 & 0 & -0.5 \\ 0 & 0.1 & 2 & 0.5 \\ 0 & 0.01 & 0.05 & 0.01 \\ 0 & 0.001 & 0.008 & 0.002 \\ -1.2 & -0.1 & 0.05 & -0.01 \end{pmatrix} \begin{matrix} k=1 & \text{Battery cells [kg]} \\ k=2 & \text{Lithium carbonate [kg]} \\ k=3 & \text{Aluminum [kg]} \\ k=4 & \text{Electricity [kWh]} \\ \hline k=5 & \text{Bauxite [kg]} \\ k=6 & \text{Lithium brine [kg]} \\ k=7 & \text{Coal [kg]} \\ k=8 & \text{CO}_2 \text{ [kg]} \\ k=9 & \text{SO}_2 \text{ [kg]} \\ k=10 & \text{NO}_x \text{ [kg]} \\ k=11 & \text{Labor [h]} \end{matrix} \tag{2}$$

3.3 Inventory analysis

In inventory analysis, a vector that quantifies the exchanges that are associated with the provision of the good or service is computed. Based on the functional unit specifying the function of the good or service (e.g., provide energy storage of 50 kWh over 1000 charging and discharging cycles), the reference flow specifying how much of the product exchanges is needed to fulfill that function (e.g., 350 kg of battery cells) is determined. The reference flow is expressed in the demand vector f . Typically, f contains only one element with a value greater than zero (the final product), while the values for all intermediate products are zero. For the illustrative example, let the reference flow be 350 kg of battery cells. The corresponding demand vector is $f = (350, 0, 0, 0)^T$.

To compute the total life cycle inventory z , the activity levels λ^ρ of all activities ρ need to be determined. For a given technosphere matrix A and demand vector f , this is done by solving the system of equations $A\lambda = f$. If A is non-singular, then exactly one solution exists, which can be obtained by using the inverse A^{-1} of the

technosphere matrix. The respective equation is $\lambda = A^{-1}f$. For the illustrative example, the resulting vector of activity levels is given in Eq. (3).

$$\lambda = (350 \ 70 \ 280 \ 9,310)^T \tag{3}$$

Multiplying the basic activity vectors a^ρ with the respective activity levels λ^ρ yields the activity vectors z^ρ (Eq. 1). Summing up the activity vectors over all activities ρ leads to the total life cycle inventory z (Eq. 4). This decomposed calculation is useful in analyzing the contribution of individual activities. The total inventory can also be obtained in a more aggregated way by multiplying the technology matrix M and the vector of activity levels λ .

$$z = \sum_{\rho=1}^{\pi} z^\rho = M \times \lambda \tag{4}$$

The resulting inventory vector z of the illustrative example is calculated in Eq. (5).

$$z = \begin{pmatrix} 350 \\ -70 \\ -280 \\ -7,000 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -420 \end{pmatrix} + \begin{pmatrix} 0 \\ 70 \\ 0 \\ -350 \\ 0 \\ 0 \\ 210 \\ 0.1 \\ 0.5 \\ -21 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 280 \\ -1,960 \\ -2,800 \\ 0 \\ 0 \\ 0.3 \\ 16.8 \\ -56 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 9,310 \\ 0 \\ 0 \\ -1,862 \\ 4,655 \\ 18.6 \\ 9.3 \\ -93 \end{pmatrix} = \begin{pmatrix} 350 \\ 0 \\ 0 \\ 0 \\ -2,800 \\ -350 \\ -1,862 \\ 7,105 \\ 19.0 \\ 26.6 \\ -590 \end{pmatrix} \begin{matrix} k=1 & \text{Battery cells [kg]} \\ k=2 & \text{Lithium carbonate [kg]} \\ k=3 & \text{Aluminum [kg]} \\ k=4 & \text{Electricity [kWh]} \\ k=5 & \text{Bauxite [kg]} \\ k=6 & \text{Lithium brine [kg]} \\ k=7 & \text{Coal [kg]} \\ k=8 & \text{CO}_2 \text{ [kg]} \\ k=9 & \text{SO}_2 \text{ [kg]} \\ k=10 & \text{NO}_x \text{ [kg]} \\ k=11 & \text{Labor [h]} \end{matrix} \tag{5}$$

3.4 Impact assessment

Inventory analysis is followed by impact assessment, the procedure to evaluate the life cycle inventory by linking the exchanges to impact categories (classification) and by quantifying their potential impact in each impact category (characterization). Depending on the goal and the scope of the assessment, a set of impact categories $h = 1, \dots, \eta$ is defined. Although the impact categories may cover a wide range of sustainability issues, the impact calculations follow the same scheme. Usually, a linear relationship between inventory results z_k and impact indicators y_h is assumed. Hence, the inventory results are multiplied with so-called characterization factors q_{hk} , quantifying the potential contribution of exchange k to impact category h (Eq. 6).

$$y_h = \sum_{k=1}^{\kappa} (q_{hk} * z_k) \quad (6)$$

For the environmental impact assessment, all elementary exchanges crossing the boundary between the technosphere and the ecosphere are assessed. To this end, different impact assessment methods that are based on scientific models of environmental mechanisms are available. Each method comprises a set of characterization factors that represent the contribution per quantity of an exchange to a specific environmental impact category. The characterization factors of selected emissions for the impact categories climate change, terrestrial acidification, and particulate matter formation are illustrated in Table 2. Note that different emissions may contribute to the same impact category but with different magnitude. Typical impact categories at the midpoint level are climate change, stratospheric ozone depletion, acidification (terrestrial/freshwater), eutrophication (terrestrial/freshwater/marine), photochemical ozone formation, ecotoxicity (terrestrial/freshwater/marine), human toxicity (cancer/non-cancer), particulate matter formation, ionizing radiation, land use, water use and resource use (fossil/mineral). Common impact categories at the endpoint level are human health, ecosystem quality, and natural resources (Rosenbaum et al. 2018b). A comprehensive overview and a systematic comparison of environmental impact assessment methods are provided by Rosenbaum (2018a) and the best practice for selecting an appropriate method can be found in Hauschild et al. (2013).

The economic assessment can be carried out in different ways, depending on the stakeholders and the decisions that it is intended to support. Conventional LCC addresses a single-stakeholder perspective, typically that of the user of products with either long lifetimes or high maintenance costs, or both. This compilation of procurement cost, operating cost, maintenance cost, and end-of-life cost is particularly useful to support the user in purchase decisions if one product has to be selected from a set of alternatives. In this context, the specific costs of individual activities in the supply chain are not relevant as they are comprised in the product's price. In contrast, environmental LCC (Heijungs et al. 2013; Moreau and Weidema 2015) assesses all costs associated with the life cycle of a product, incurred by one or more actors, over the product's lifetime. In this context, the term "environmental" simply indicates that the economic assessment is made in a way that is consistent with the environmental assessment. This type of LCC provides useful results for analyzing cost hotspots in the product's supply chain and for improving the economic performance of the supply chain (Moreau and Weidema 2015).

The characterization factors in the economic assessment represent the market prices p_k of the exchanges. Desired exchanges (goods) usually have a positive price ($p_k > 0$) and undesired exchanges (bads) have a negative price ($p_k < 0$). Exchanges that are not relevant for the assessment are assigned a price of zero. Multiplying the prices p_k with the exchange quantities z_k^p yields the variable costs and revenues of the activity. The output ($z_k^p > 0$) of desired exchanges (usually, the final product) and the input ($z_k^p < 0$) of undesired exchanges (e.g., waste treatment) generate revenues, whereas the input of desired exchanges (e.g., precursor products) and the output of undesired exchanges (e.g., waste) incur costs. The

Table 2 Selected environmental characterization factors of the ReCiPe midpoint method for climate change, terrestrial acidification and particulate matter formation (Goedkoop et al. 2013)

	Ammonia	Carbon dioxide	Methane	Nitrogen oxides	Nitrogen fluoride	Particulates <2.5 µm	Particulates 2.5–10 µm	Sulfur dioxide
Climate change		1	25		17,200			
Terrestrial acidification	2.45			0.56				1
Particulate matter formation	0.32			0.22		1	1	0.2

sum of positive and negative contributions from all exchanges in an activity corresponds to the contribution margin of the activity. By subtracting the fixed cost of the activity, its profit is calculated (Dyckhoff and Spengler 2010). In the life cycle costing literature (e.g., Heijungs et al. 2013; Moreau and Weidema 2015), the sum of positive and negative contributions from the exchanges of a given activity is also interpreted as the activity's value added. This metric provides a useful means to analyze where economic value is generated in the supply chain. Furthermore, the sum of value added over all upstream activities that are involved in the creation of a particular (product) exchange corresponds to the price of that exchange. Thus, from the perspective of the final product, the total value added of all activities can be interpreted as the life cycle cost of the product (Moreau and Weidema 2015). Depending on the goal and scope of the assessment as well as data availability, this basic model focusing on value added can be substituted by more sophisticated approaches to evaluate the economic dimension, for example, by considering fixed costs, taxes, or varying exchange rates.

The social assessment can be carried out at the level of social risk, social performance, or social impact (Zamagni 2019). Social risk refers to the likelihood of adverse social effects on stakeholders due to the company's activities or business relationships. Social performance measures a feature of a practice or a situation (e.g., number of work accidents) in comparison to a reference value (e.g., international guidelines, standards, specifications for certification). Social impact describes the positive or negative consequences due to the causal relationship between an activity and an issue of concern relating to human well-being. While different impact categories and characterization factors may be used for each assessment level, the general procedure is usually similar. For example, the impact assessment method of the Social Hotspots Database assumes discrete levels of risk, which can be quantified based on the relative probability of an adverse situation to occur (Table 3). Within this method, "high risk" activity is five times more likely to cause an adverse situation than a "medium risk" activity if the activity variable (e.g., labor intensity expressed in work hours) is the same. From a computational perspective, the exchange "work hours" is multiplied with the characterization factor that quantifies the risk relative to the medium risk level. The resulting impact indicator represents the equivalent work hours at medium risk level.

Table 3 Characterization factors for different levels of social risk

Risk category	Characterization factor
No risk	0.0
Low risk	0.1
Medium risk	1.0
High risk	5.0
Very high risk	10.0

The characterization factors can be summarized in the matrix of characterization factors Q and the equation for impact assessment can be written in matrix form, i.e., $y = Q \times z$. To analyze the impact contributions from individual activities, the characterization factors can also be applied to the activity vectors z^p , i.e., $y^p = Q \times z^p$. For the illustrative example, the impact vector y is calculated in Eq. (8), using the characterization factors Q from Eq. (7). Note that the characterization factors for social risks (here: $h = 4$, child labor) has a negative sign, because the exchange ‘labor’ is modeled as an input and thus also has a negative sign.

$$Q = \begin{matrix} & \begin{matrix} \text{Battery cells [kg]} \\ \text{Li-Carbonate [kg]} \\ \text{Aluminum [kg]} \\ \text{Electricity [kWh]} \\ \text{Bauxite [kg]} \\ \text{Lithium brine [kg]} \\ \text{Coal [kg]} \\ \text{CO}_2 \text{ [kg]} \\ \text{SO}_2 \text{ [kg]} \\ \text{NO}_x \text{ [kg]} \\ \text{Labor [h]} \end{matrix} \\ \begin{matrix} k=1 \\ k=2 \\ k=3 \\ k=4 \\ k=5 \\ k=6 \\ k=7 \\ k=8 \\ k=9 \\ k=10 \\ k=11 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 0 \\ 20 & 8 & 3 & 0.1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \end{matrix} \begin{matrix} h=1 \text{ Climate change [kg CO}_2\text{-eq]} \\ h=2 \text{ Acidification [kg SO}_2\text{-eq]} \\ h=3 \text{ Value added [USD]} \\ h=4 \text{ Child labor [med. risk work hours]} \end{matrix} \tag{7}$$

$$y = \begin{pmatrix} 0 \\ 0 \\ 4,900 \\ 420 \end{pmatrix}^{y^1} + \begin{pmatrix} 210 \\ 1.1 \\ 525 \\ 21 \end{pmatrix}^{y^2} + \begin{pmatrix} 2,240 \\ 33.9 \\ 644 \\ 56 \end{pmatrix}^{y^3} + \begin{pmatrix} 4,655 \\ 37.2 \\ 931 \\ 93 \end{pmatrix}^{y^4} = \begin{pmatrix} 7,105 \\ 72.2 \\ 7,000 \\ 590 \end{pmatrix} \begin{matrix} h=1 \text{ Climate change [kg CO}_2\text{-eq]} \\ h=2 \text{ Acidification [kg SO}_2\text{-eq]} \\ h=3 \text{ Value added [USD]} \\ h=4 \text{ Child labor [med. risk work hours]} \end{matrix} \tag{8}$$

With the proposed model formulation, a life cycle sustainability assessment comprising all three sustainability dimensions can be carried out. It does not consider the geographical dispersion of the activities and the regional heterogeneity yet. Therefore, the formulation will be expanded in the next section.

4 Spatially differentiated modeling

To allow for spatially differentiated sustainability assessment, the model formulation is expanded by localizing the activities and exchanges, by integrating transportation activities, and by enabling regionalized impact assessment. To this end, a new index of locations $r = 1, \dots, \gamma$ is introduced. The locations usually represent

regions such as states, countries, or continents. However, more granular modeling where locations represent specific points on the map is also possible.

4.1 Localization of exchanges and activities

The localization of activities and exchanges follows Koopmans' idea that "in principle, flows of technically the same commodity in two different locations represent different commodities" (Koopmans 1951). Therefore, each activity ρ is assigned to a location r^ρ and its exchanges are specified with an additional index r . It is assumed that exchanges can only be consumed or produced at the location of the activity, i.e., $r = r^\rho$ (Eq. 9).

$$\mathbf{z}^\rho = \begin{pmatrix} z_{1,r}^\rho \\ \vdots \\ z_{k,r}^\rho \\ \vdots \\ z_{\kappa,r}^\rho \end{pmatrix} = \lambda^\rho * \begin{pmatrix} a_{1,r}^\rho \\ \vdots \\ a_{k,r}^\rho \\ \vdots \\ a_{\kappa,r}^\rho \end{pmatrix} \quad (9)$$

The integration of the new index r leads to an increased number of rows in the activity vectors \mathbf{z}^ρ and in the technology matrix \mathbf{M} . However, it may not be necessary, nor meaningful, to generate a data structure with all exchanges at all possible locations. Whether and to what extent localization should be carried out depends on the purpose of the analysis and the degree of detail and refinement required (Koopmans 1951).

We extend the illustrative example and assume that cell production ($\rho = 1$) is located in China, aluminum production ($\rho = 2$) in Australia, and lithium carbonate production ($\rho = 3$) in Chile. Each of these countries has its own activity for electricity production ($\rho = 4, \dots, 6$). The extended example is illustrated in Fig. 5. It already includes transportation activities, which will be introduced in the following section.

At this point, it is not possible to find a solution to the equation $\mathbf{A}\lambda = \mathbf{f}$, as the technosphere matrix \mathbf{A} is not square anymore and some activities produce a product exchange k at location r_1 and that same exchange may be required by a subsequent activity at a different location r_2 . This issue is resolved by transportation activities that realize the necessary spatial transformations.

4.2 Integration of transportation activities

Transportation activities describe the spatial transformation of goods. A transportation activity is characterized by having product exchange k at location r_1 as input and the same product exchange k at a different location r_2 as output. Assuming that there are no losses during the transport, the respective quantities of k are of the same magnitude but have opposite signs, i.e., $-z_{k,r_1}^\rho = z_{k,r_2}^\rho$. In addition to the transported good k , transportation activities have further inputs and outputs such as fuel, labor, and emissions.

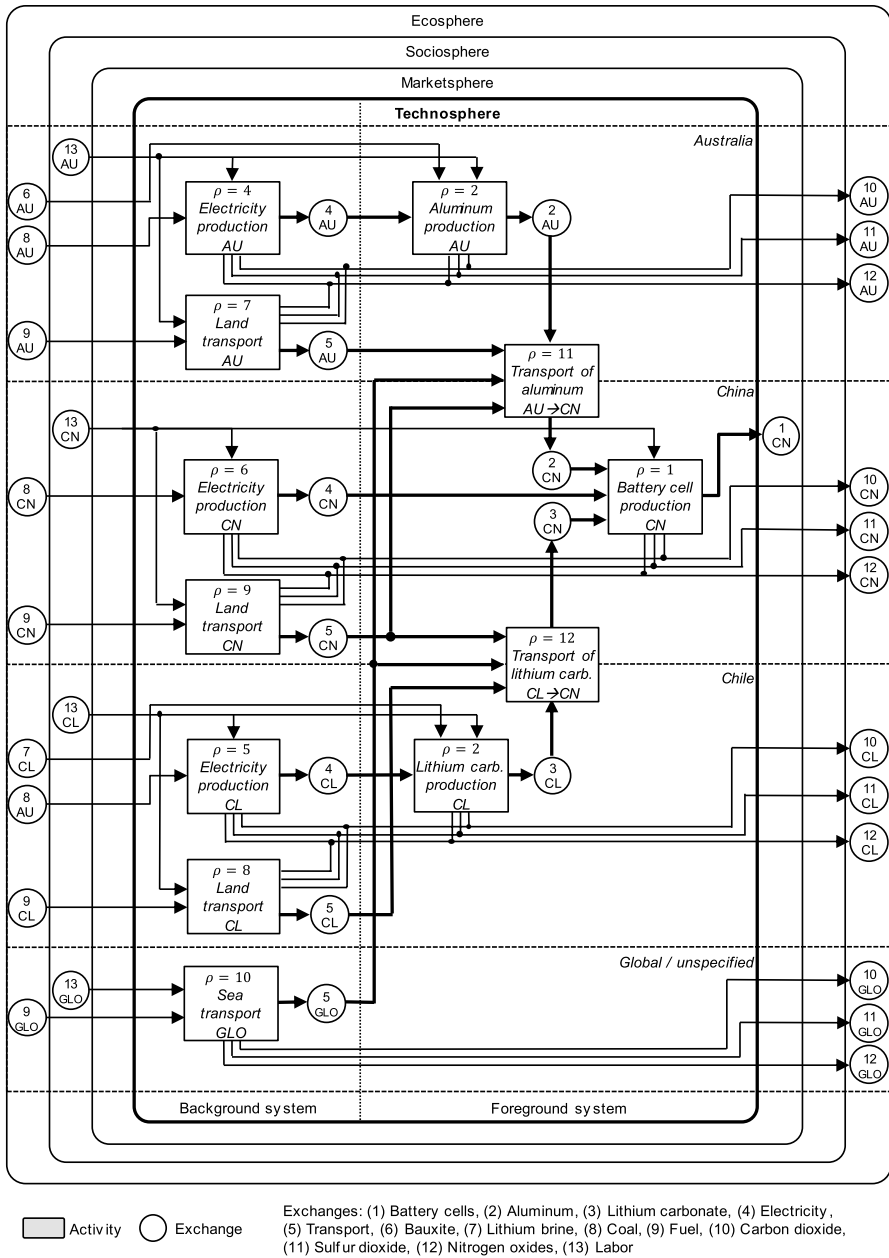


Fig. 5 Spatially differentiated model of the simplified supply chain for battery cell production

Unlike production activities that can be assigned to a specific location, transportation activities involve multiple locations, at least the origin and the destination of the transport but also locations on the route. We propose to address this issue in

5 Case study: sustainability assessment of lithium-ion batteries

As a key component in mobile and stationary energy storages, lithium-ion batteries are enablers for sustainable mobility and renewable energy systems. Despite the considerable benefits related to the use phase of lithium-ion batteries, there are significant impacts in their complex supply chain.

5.1 Supply chain of lithium-ion batteries

The main components of a lithium-ion battery pack in electric vehicles are the battery cells in which the electric energy is stored, the battery management system (BMS) to monitor and control the state of the cells, and the pack container with a cooling system to protect the cells from external influences. The battery cells consist of two electrodes, a separator, electrolyte, and a cell container with electric connectors. The composition of the electrodes is a major determinant of the performance and the cost of the battery system (Schmuck et al. 2018). For automotive applications, the cathode is typically made of an aluminum current collector and active material containing lithium, nickel, cobalt, and manganese (NMC). The anode is made of a copper current collector and graphite (G) as active material.

The raw materials that are used to make the components for the battery cells and the battery pack can be found in different locations. For some of them, geological reserves and production are concentrated in a few countries (Olivetti et al. 2017; USGS 2018): The largest producer of lithium is Australia, where it is extracted from the mineral spodumene. Other significant producers are Chile and Argentina, where the lithium is extracted from concentrated brines. The production of nickel is diversified geographically, with Indonesia, the Philippines, and Canada being the top three producers. Cobalt production is highly concentrated in DR Congo with a share of more than 60%. Minor producers of cobalt include Russia and Australia. Manganese production mainly takes place in South Africa, China, and Australia. Production of aluminum and graphite is concentrated to more than 50% in China, with minor shares in Russia and Canada for aluminum, and India and Brazil for graphite. The largest producers of copper are Chile and Peru, followed by China.

The raw materials are used as inputs for the production of intermediates such as lithium-cobalt-nickel-manganese oxide for the cathode active material, or lithium-hexafluorophosphate for the electrolyte. The production of these intermediates is usually done by specialty chemicals companies located in China (Olivetti et al. 2017).

The next stage of the supply chain is cell production. It involves electrode production, cell assembly, formation, and aging. Until 2015, Japan and South Korea were the leading countries with regard to production capacities for battery cells, but now China is the biggest producer, and its capacity is growing rapidly (Roland Berger and FKA 2019). With the operation of Tesla's Gigafactory, production has also started in the United States. Projects for European cell production in Sweden and Poland are underway (Davidsson Kurland 2020).

The assembly of battery packs is usually done by the car manufacturers in facilities that are located at or close to where the electric cars are built. The country with the highest production output of electric cars in 2017 was China with ca. 600,000 cars, followed by the United States with 200,000 cars and Germany with 145,000 cars (Roland Berger and FKA 2019).

5.2 Assessment setup and implementation

The goal of this case study is to analyze the sustainability impacts of lithium-ion batteries for electric cars. For that purpose, a representative state-of-the-art lithium-ion battery pack based on the NMC-G cell chemistry with a storage capacity of 52.9 kWh and a mass of 314.3 kg is considered. The underlying structure of the supply chain is displayed in Fig. 6. The foreground system comprises the principal activities of the stages materials production, components production, cell production, and pack production. They are linked to generic activities in different databases of the background system. The Ecoinvent 3.5 database is used for the environmental sustainability assessment, and the Social Hotspots Database (SHDB) is used for the social sustainability assessment.

The data that is needed to parametrize the activities is compiled from different sources. The composition of the battery system and the battery cells is mainly based

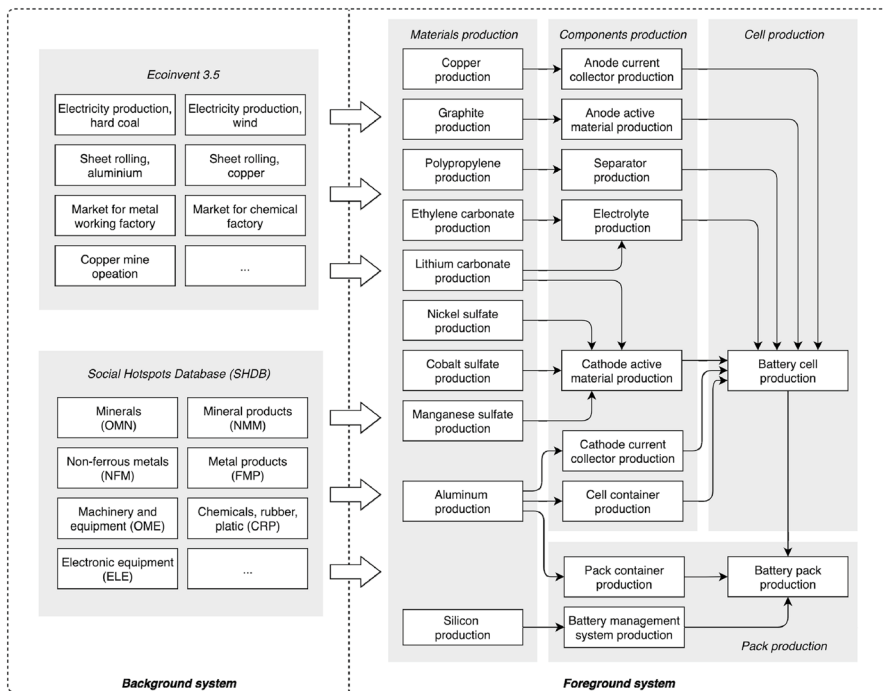


Fig. 6 Structure of the generic supply chain for lithium-ion batteries for electric cars

on the BatPaC model from Argonne National Lab (Nelson et al. 2018). The parametric model allows for the calculation of the material needs of different battery pack and battery cell configurations and contains information on the prices of individual components. As it focusses on the pack assembly and cell production stage, data on the upstream stages of component production and materials production is integrated from Ellingsen et al. (2014) and Ahmed et al. (2017).

To enable a spatially differentiated sustainability assessment, all activities in the foreground system are duplicated multiple times to account for the different locations at which they are carried out. For each activity, the top five countries with regard to global production in 2017 are considered. Comprehensive data on materials production is compiled in the mineral commodity summaries of the U.S. Geological Survey (USGS 2018). The production shares in cell production, which are also used as a proxy for components production, are extracted from the E-mobility index 2018 (Roland Berger and FKA 2019). The production shares for pack production are approximated based on data on electric vehicle production from the aforementioned source. The regionalized activities in the foreground system are linked to regionalized activities in the background system where possible. While all datasets in the SHDB are regionalized on a country level, only a few datasets in Ecoinvent are regionalized comprehensively on a country level (mainly electricity markets). Most Ecoinvent datasets are available for selected countries only, for much coarser regions (e.g., Europe, Asia, 'Rest of World'), or on a global level. We regionalize all activities that contribute more than 1% to the total impact (calculated in a preliminary analysis) in at least one environmental impact category.

The characterization factors for the environmental impact assessment are drawn from the ReCiPe Midpoint (H) method (Goedkoop et al. 2013) as well as the LC-Impact method (Verones et al. 2016) for the spatially differentiated assessment. For the economic impact assessment, we calculate the value added as described in Sect. 3.4. The impact assessment in the social dimension focuses on social risks and makes use of the related impact indicators from the SHDB.

The model is implemented in Python 3.7, using the Brightway2 library for life cycle assessment (Mutel 2017). Brightway2 is a powerful open-source framework that supports the import of inventory databases, the manipulation of activities, the generation of the technology matrix, and the calculations for inventory analysis and impact assessment. The framework is modified to support the integration of economic and social aspects and to enable spatially differentiated calculations. The technology matrix M of the case study has about 25,600 rows (exchanges) and 22,800 columns (activities). However, the matrix is sparse as only 2.37 million of the more than 583 million possible entries have a value different from zero (sparsity 99.6%). Therefore, high-performance algorithms for the solution of large, sparse, nonsymmetric systems of linear equations, such as supernodal lower-upper decomposition (SuperLU, cf. Li 2003), can be applied, resulting in negligible computation times of a few seconds for a full assessment on a standard Windows 64 bit laptop.

5.3 Sustainability assessment results

The sustainability assessment results are discussed as follows. First, aggregate results that are calculated with the basic model without spatial differentiation are presented. Then, more detailed results from the extended model with spatial differentiation are provided. The comparison of the results allows for an evaluation of the benefits of the spatially differentiated model. For a better overview, six environmental indicators, one economic indicator, and three social indicators are selected for the discussion.

5.3.1 Assessment results from the basic model without spatial differentiation

The impact scores that are calculated using the basic model without spatial differentiation are shown in Table 4. The activities in the underlying supply chain are not regionalized and represent the global average of the technology. The scores are computed for different functional units to facilitate comparisons with results from other studies. For example, we calculate a climate change impact of 187.1 kg CO₂-eq per kWh of storage capacity. This is within the range of typical values (50–250 kg CO₂-eq per kWh) that have been reported for lithium-ion batteries with NMC-G chemistry in the review by Peters et al. (2017). This also holds for the other environmental indicators. The value added of 158.6 USD per kWh is at the lower end of the long-run costs for lithium-ion battery packs estimated by Nykvist and Nilsson (2015). This seems reasonable as our model only includes the variable costs. The scores of the social indicators are slightly lower but in the same order of magnitude as the results reported in Thies et al. (2019a), which can be explained by differences in the underlying supply chains. Although the comparison of absolute impact scores

Table 4 Impact scores for the production of one battery pack expressed for different functional units

Dimension	Indicator	Unit	Per battery pack (52.9 kWh, 314.3 kg)	Per kWh	Per kg
Environmental	Climate change	kg CO ₂ -eq	9898	187.1	31.5
	Terrestrial acidification	kg SO ₂ -eq	87.4	1.65	0.28
	Human toxicity	kg 1,4-DCB-eq	20,154	381.0	64.1
	Freshwater eutrophication	kg P-eq	11.9	0.23	0.037
	Ozone depletion	kg CFC-11-eq	0.00038	0.000007	0.000001
	Metal depletion	kg Fe-eq	5215	98.6	16.6
Economic	Value added	USD	8392	158.6	26.7
Social	Occupational injuries & deaths	Eq. med. risk hours	4760	90.0	15.1
	Corruption	Eq. med. risk hours	5525	104.4	17.6
	Child labor	Eq. med. risk hours	7963	150.5	25.3

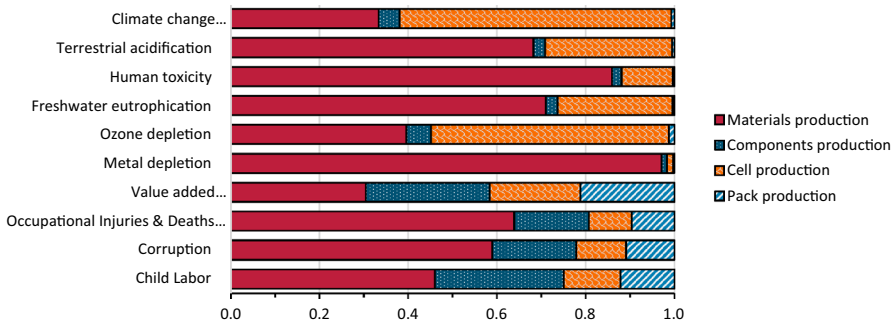


Fig. 7 Relative contributions of the supply chain stages to the total impact

to those from other studies must be interpreted with caution due to the different settings in each study, it may provide some indications for the validity of the model.

Analyzing the contributions of individual supply chain stages to the total impact (Fig. 7), considerable differences can be observed across the indicators. With regard to climate change, cell production accounts for 61% of the total impact. This is mainly due to the high electricity consumption of the dry rooms in the battery cell factory. The materials stage (33%) is the second-largest contributor to climate change, followed by the much smaller contributions from components production (5%) and pack production (1%). The distribution of impacts for ozone depletion is quite similar. For terrestrial acidification, freshwater eutrophication, and human toxicity, the most significant stage is materials production with contributions from 68 to 86% of the total impact. For metal depletion, the materials production stage is responsible for nearly the entire impact (97%), whereas the contributions from other stages are negligible. On the economic side, the value added is distributed almost evenly across all stages. For the social indicators, materials production is the stages with the largest impact (46–64%), followed by components production, cell production, and pack production. Overall, the analysis of impact contributions allows for a rough identification of sustainability hotspots in the supply chain.

To get a better understanding of the sustainability hotspots in the supply chain, the contributions of individual activities are analyzed. We focus our analysis on the climate change impact and on the materials production stage (Table 5). The top five activities in the materials production stage with the highest climate change impact are aluminum production, nickel sulfate production, cobalt sulfate production, copper production, and graphite production. These activities account for 28.4% of the total climate change impact of the battery back. The impact is driven by the activity level λ and the normalized impact per execution. For example, the activity level for aluminum production is $\lambda = 91.5$ and the normalized impact is 22.2 kg CO₂-eq. This means that 91.5 kg of aluminum is needed for the production of one battery pack, and the production of each kilogram of aluminum (primary, wrought alloy) has a climate change impact of 22.2 kg CO₂-eq. Note that the impact scores depend on the underlying process technologies. In the case of aluminum, the climate change impact of the more energy-efficient prebaked carbon anode technology is about 10%

Table 5 Top five activities in the materials production stage with the highest climate change impact

Activity	Impact contribution [%]	Absolute impact [kg CO ₂ -eq]	Activity level λ [# of executions]	Normalized impact [kg CO ₂ -eq per execution]
Aluminum production	20.5	2026	91.5	22.2
Nickel sulfate production	3.7	363	48.5	7.5
Cobalt sulfate production	1.6	163	48.5	3.4
Copper production	1.6	155	36.8	4.2
Graphite production	1.0	1	50.8	1.6

lower compared to the older Soderberg technology (Nunez and Jones 2016). For secondary aluminum, the score can be over 90% lower than for primary aluminum. We will show in the following that the normalized impact of each activity is also influenced substantially by the locations where the activities are carried out. To this end, the spatially differentiated model is applied.

5.3.2 Assessment results from the extended model with spatial differentiation

As a first result of the spatially differentiated model, the normalized climate change impact (kg CO₂-eq per execution of the activity) is compared for different locations where the activity is carried out (Fig. 8). For illustration, only the activity ‘battery cell production’ and the top five activities with the highest climate change impact in the materials production stage (Table 5) are displayed and discussed. For each activity, the normalized impact is compared for the five countries with the highest production in 2016. It can be seen that the normalized climate change impacts of the regionalized activities deviate from the values that are obtained using global average inventory data. For example, the climate change impact of battery cell production is 24.4 kg CO₂-eq per kg of battery cell for the global average dataset. If the battery cells are produced in China (CN), the impact increases to 29.9 kg CO₂-eq per kg, and if the battery cells are produced in Germany (DE), the impact reduces to 19.7 kg CO₂-eq per kg. These variations can be explained by technological heterogeneity, particularly with regard to the electricity mix in each country.

Based on the observation that some locations appear to perform better than the global average while others perform worse, we analyze the potential influence of the supply chain configuration on the total impact of the battery pack. To this end, we define two hypothetical supply chains: in the first supply chain, all activities are located in the country with the lowest climate change impact (BEST GWP), and in the second supply chain, the activities are located in the highest-impact countries (WORST GWP) among the countries analyzed. These two supply chain

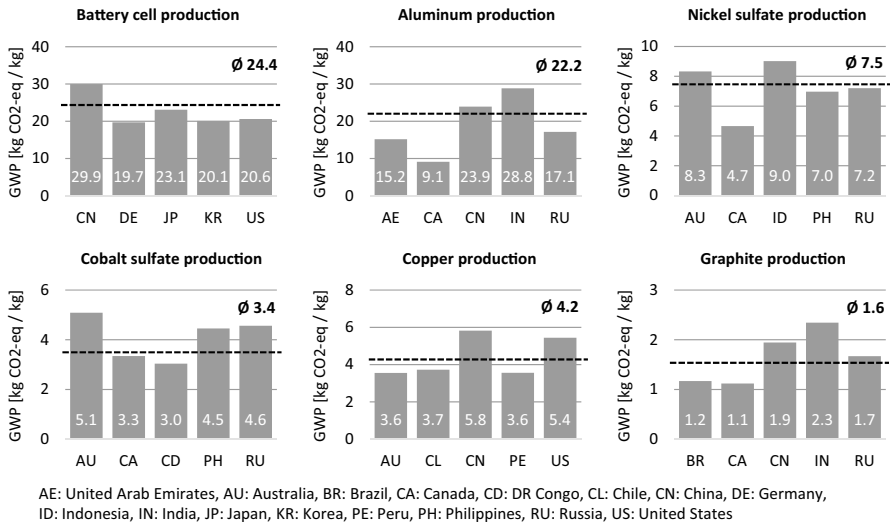


Fig. 8 Comparison of normalized GWP of top five contributing activities for different locations

configurations are compared to a supply chain representing the average global production mix (BASELINE).

The results of this comparison are shown in Fig. 9. As expected, the climate change impact of the BEST GWP supply chain with 7059 kg CO₂-eq per battery pack (133.4 kg CO₂-eq per kWh) is considerably lower (−28.7%) than the climate change impact of the BASELINE supply chain, and the climate change impact of the WORST GWP supply chain with 11,938 kg CO₂-eq per battery pack (225.7 kg CO₂-eq per kWh) is considerably higher (+20.6%). The BEST GWP supply chain also has the lowest impact in the categories human toxicity, metal depletion, corruption, and child labor. However, regarding terrestrial acidification, freshwater eutrophication, and occupational injuries & deaths, the BASELINE supply chain performs best, and regarding ozone depletion, the WORST GWP supply chain performs best. The total value added is identical for all three supply chain configurations. As explained in Sect. 3.4, it corresponds to the price of the final product and here, a globalized market for lithium-ion batteries without regional price differences is assumed. The composition of the total value added by country differs largely, however, because the supply chain configurations differ with regard to the countries where the activities are carried out. These results highlight the tradeoffs between the different sustainability indicators, i.e., the best-performing supply chain in terms of climate change is not necessarily the preferred choice in terms of other sustainability indicators. Furthermore, the results illustrate the potential range of impact scores that can be obtained from different supply chain configurations.

The final analysis in this case study addresses the environmental heterogeneity. To this end, we compare the application of regionalized characterization factors with the application of global average characterization factors (Fig. 10). The

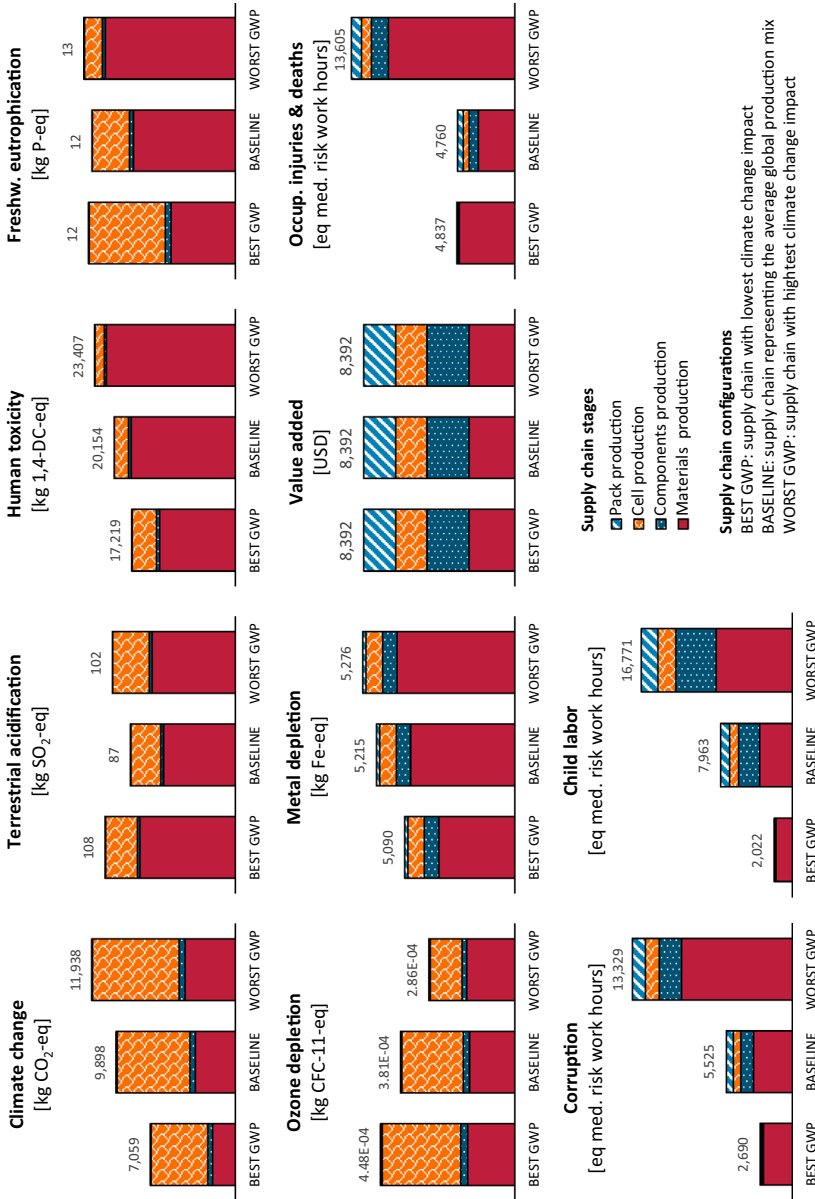


Fig. 9 Comparison of alternative supply chain configurations with regard to selected sustainability indicators

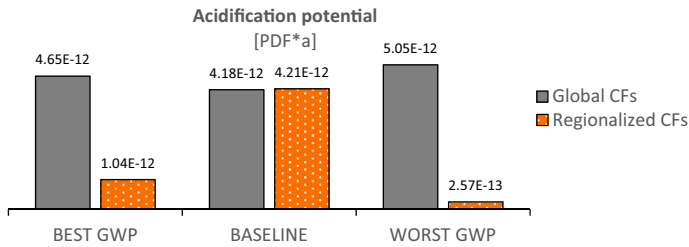


Fig. 10 Acidification potential for three supply chain configurations with standard LCIA and regionalized LCIA methods

analysis focuses on the acidification potential because the normalized impact in the context of lithium-ion batteries is rather high compared to other impact categories (Peters et al. 2017) and country-specific as well as global characterization factors are available within the LC-Impact method (Verones et al. 2016). These characterization factors are expressed on the endpoint level and have the unit “potentially disappeared fraction of species in a year” (PDF*a).

With the application of global average characterization factors, the impact scores of the BEST GWP and the WORST GWP supply chains are somewhat higher than the score of the BASELINE supply chain. In this case, the differences can be explained by technological heterogeneity (i.e., different processes with regard to sulfur dioxide, nitrogen oxides, and ammonia emissions). When the regionalized characterization factors are applied, the technological heterogeneity is superimposed by environmental heterogeneity (due to different characteristics of the environment as well as different initial levels of pollution), leading to significantly lower impact scores of the BEST GWP and the WORST GWP supply chains. This is due to lower characterization factors for most countries involved in these supply chains compared to the global characterization factors (Table 6).

5.3.3 Influence of modeling choices and uncertain parameters on assessment results

The above results represent a specific operating point of the supply chain and are potentially influenced by modeling choices and uncertain parameters. The pertinent methods to analyze the resulting variability include sensitivity analysis, Monte-Carlo simulation, discernibility analysis, overlap area of probability distributions, and null hypothesis significance testing (Mendoza Beltran et al. 2018). Here, a sensitivity analysis is carried out for selected parameters in order to quantify their influence on the climate change score. It focuses on the battery cell production process, which was identified as the main contributor towards climate change (over 50% of total impact, cf. Figure 7). The influence of the capacity of the battery cell production plant is shown in Fig. 11a. The electricity use and, consequently, the climate change score, are nonlinear functions of the production capacity due to economies of scale mainly with regard to drying processes and technical building services (Thomitzek et al. 2019). The impact scores range from 13,727 kg CO₂-eq per battery pack for

Table 6 Regionalized inventory results (BASELINE supply chain) and characterization factors for acidification (based on Verones et al. 2016)

Location	Inventory results [kg]			Characterization factors [PDF*a/kg]		
	Sulfur dioxide	Nitrogen oxides	Ammonia	Sulfur dioxide	Nitrogen oxides	Ammonia
AE	0.234	0.115	0.001	4.53E-12	2.62E-12	4.83E-13
AR	0.084	0.055	0.008	1.27E-15	1.11E-15	3.15E-16
AU	7.853	0.705	0.084	2.12E-14	6.09E-14	8.41E-15
BR	0.120	0.022	0.001	5.54E-15	3.30E-15	7.27E-15
CA	4.129	0.401	0.041	2.28E-16	3.77E-17	3.02E-17
CD	0.401	1.266	0.160	2.86E-16	2.25E-16	3.03E-16
CL	5.872	0.967	0.144	6.66E-14	9.48E-15	2.94E-14
CN	20.207	16.423	0.269	5.04E-16	6.75E-16	2.32E-15
DE	1.309	1.143	1.230	3.57E-16	2.30E-16	5.39E-16
GA	0.144	0.009	0.000	5.53E-16	5.37E-16	6.25E-16
ID	7.724	0.671	0.059	8.72E-16	1.03E-15	9.22E-16
IN	0.648	0.454	0.011	6.55E-16	3.21E-16	1.50E-15
JP	1.357	0.897	0.026	1.74E-15	4.31E-16	1.41E-15
KR	0.459	0.664	0.038	1.57E-17	7.37E-18	4.55E-17
PE	2.500	0.349	0.054	8.40E-13	2.49E-14	1.31E-13
PH	4.494	0.431	0.042	9.77E-15	1.34E-14	2.85E-14
RU	3.868	0.554	0.041	1.02E-15	1.32E-15	1.53E-15
US	4.191	1.921	0.254	6.76E-16	3.22E-16	3.03E-16
ZA	0.511	0.059	0.002	3.39E-14	8.56E-14	2.40E-13
ZW	0.028	0.013	0.002	1.18E-16	3.62E-16	6.02E-16
GLO	66.134	27.121	2.465	5.27E-14	2.46E-14	1.04E-14

a production capacity of 5 GWh/a to 9420 kg CO₂-eq for a 50 GWh/a plant. In the BASELINE configuration, an impact score of 9898 kg CO₂-eq was obtained based on a 35 GWh/a plant, which is comparable to Tesla's Gigafactory 1 (Davidsson Kurland 2020). In Fig. 11b, the influence of the electricity mix at the location of battery cell production is investigated. With a high share of renewable energies in the electricity mix (usually < 50 g CO₂-eq/kWh_{el}), the impact scores are just above 6000 kg CO₂-eq per battery pack. With a primarily coal-based electricity supply (> 1000 g CO₂-eq/kWh_{el}), the impact scores increase to over 10,000 kg CO₂-eq. Therefore, locating battery cell production in countries with a low-carbon electricity mix (e.g., Norway, Sweden, France) or securing a renewable energy supply for the production plants (e.g., own windparks or photovoltaic fields) can have a big influence on the climate change score. Overall, the sensitivity analysis shows that the influence of modeling choices, such as the assumption of linearity, and uncertain parameters needs to be investigated carefully.

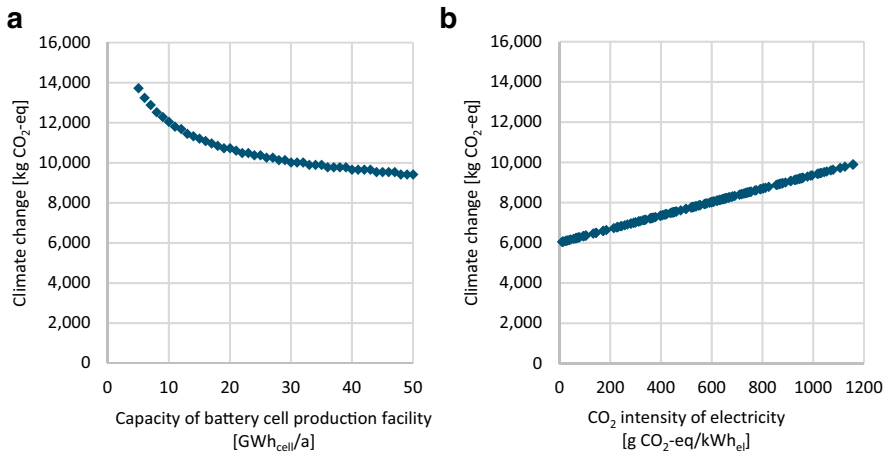


Fig. 11 Sensitivity of climate change impact of the battery pack with regard to **a** capacity of battery cell production facility and **b** CO₂ intensity of electricity at the location of battery cell production

5.3.4 Comparison and benefits of the spatially differentiated supply chain model

The sustainability assessment results for lithium-ion batteries depend on the underlying supply chain configuration. If a supply chain based on the average global production mix is assumed and the assessment is carried out without spatial differentiation, the results are within the typical range of values that have been reported in literature. However, considerable variability in the impact scores can be observed if technological heterogeneity is taken into account. In this case study, the environmental impact scores of the extreme supply chain configurations (BEST GWP and WORST GWP) vary up to 30% above and below the score of the BASELINE supply chain. For the social indicators, the variation is even higher (−75% to +185%). For the economic indicator “value added”, the total score does not depend on the supply chain configuration, but the contribution of the countries changes.

Environmental heterogeneity is found to be an additional source of variability. With the application of regionalized characterization factors, the impact scores for acidification can be up to 95% lower than the respective scores based on global characterization factors, dependent on the supply chain configuration. It should be noted, however, that these big differences are specific to the supply chain of lithium-ion batteries because most countries in this supply chain have characterization factors that are significantly lower than the global characterization factors.

While it was shown in the case study that the consideration of spatial heterogeneity has notable effects on the assessment results, the influence of process technologies, modeling choices, and uncertain parameters should not be neglected as they may superimpose the observed variability. For example, the influence of single parameters, such as the production technology of aluminum, the capacity of the battery production plant, or the carbon intensity of the electricity mix can lead to

variations in the climate change score that are in the range of the variations due to regional heterogeneity.

6 Conclusions

This paper proposes a novel modeling approach to facilitate the sustainability assessment of global supply chains. It addresses two important challenges of life cycle sustainability assessment, namely the integration of all three sustainability dimensions and the spatially differentiated modeling to account for regional heterogeneity. The approach builds on the foundations of activity analysis, a well-established method in production economics.

6.1 Potentials and limitations of the approach

The proposed approach offers the possibility to analyze a variety of impact and risk indicators in all three sustainability dimensions. It provides a consistent way of modeling environmental, economic, and social sustainability aspects. Following the principles of the ISO 14040/14044 standards and providing the possibility to establish links to existing life cycle inventory databases, it can be a useful modeling tool for life cycle sustainability assessment.

The approach not only enables sustainability assessments from a global perspective but also supports spatially differentiated assessments. This allows for the analysis of tradeoffs between global and local sustainability indicators. One advantage of the approach is its flexibility regarding the level of regionalization. While the regionalization is often done on a country level, the approach also supports coarser and finer levels of regionalization. The use of supplier-specific data would be particularly important if the situation at a specific supplier (e.g., the social conditions or the electricity mix) deviate significantly from the national average. Moreover, only the most relevant activities can be regionalized to reduce the computational complexity and data needs. The explicit modeling of the supply chain allows for the evaluation of strategic decisions regarding the selection of suppliers, the locations of production sites, or the configuration of the distribution system. For example, the sustainability impacts of a production process can be compared for different locations. The results of such analyses can be used to guide decisions towards sustainable supply chains.

Several limitations of the approach can be identified. First, the linear model formulation provides an appropriate approximation for many practical applications in which the effects of nonlinearities, for example due to economies of scale in production, are negligible. If the approximation error gets too large, suitable approaches to account for nonlinearities should be adopted. Second, the impacts related to the setup of production facilities are allocated over their expected lifetime output (attributional approach). This procedure is only valid for the comparison of stationary supply chain configurations for which transient effects can be neglected. Third, apart from spatial variability, the inherent

uncertainties in sustainability assessments are not addressed explicitly. Fourth, there are no restrictions on the possible range of activity levels. Considering the potentially limited supply and production capacities, the feasibility of the results must be validated. Finally, the supply chain configurations have to be pre-defined for the analysis. The method can only be used to compare alternative supply chain configurations but not to generate the optimal design for the supply chain. These limitations should be the subject of future work.

6.2 Recommendations for decision-makers

Despite the inherent uncertainties, several general recommendations for decision-makers can be derived. As illustrated in the case study on lithium-ion batteries, the impact scores differ considerably, depending on whether a spatially differentiated assessment approach is used or not. The spatially differentiated approach generates more granular results that allow for a better analysis of sustainability hotspots in the supply chain. Moreover, the impact scores are also influenced by the specific configuration of the supply chain. Therefore, manufacturers should carefully consider where to locate their production facilities and where to source the necessary components and materials.

The regional variability of sustainability impacts can also be seen as a chance for decision-makers to improve their supply chains. For example, a new production facility could be located at a site that leads to the best sustainability performance. The implications of such decisions should be analyzed carefully, however, as improvements in one impact category may lead to worse results in another impact category. Furthermore, improvements in global sustainability performance may come along with local degradations at some locations. Such tradeoffs, along with the potential degrees of freedom regarding the location of the activities, should be addressed in a systematic way by formulating a multi-criteria design problem.

6.3 Outlook

To handle the large number of feasible supply chain configurations in practical decision situations and to identify those configurations that match best with the preferences of the decision-maker, the activity analysis based assessment model needs to be transformed into a supply chain design problem. To this end, activities for the alternative production and transportation processes at different locations need to be defined. By treating the activity levels λ as decision variables and the provision of the functional unit as a demand constraint, the resulting problem can be solved by means of multi-objective optimization techniques. Such optimization models could also support the selection of process technologies, production capacities, and operating points, which are defined as alternative basic activities based on empirical observations or flowsheeting simulations. With the definition of additional binary variables, the impacts of setup activities that are independent of the activity level can be addressed. Furthermore, additional

constraints addressing supply limitations and production capacities can be integrated to capture the requirements of the practical planning problem and to provide decision support towards the design of sustainable supply chains. This would also allow for sustainability assessments in a consequential manner. To ensure robust decision-making, the supply chain design model should systematically incorporate the inherent uncertainties of sustainability assessment.

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