Chapter 18
Multicriteria Decision Analysis for Sustainability Assessment for Emerging Batteries

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18.1 Introduction

The origin of the concept of sustainability is commonly associated with the definition of sustainable development given by the Brundtland Report and the Rio Conference "Environment and Development" in 1992: "Sustainable development meets the needs of the present without compromising the ability of future generations to meet their own needs." From this, different concepts emerged to give better

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understanding to sustainability such as the triple bottom-line model [3], the Sustainable Development Goals (SDGs) [54], the Integrative Concept of Sustainable Development (ICoS) [32], etc.

However, defining and assessing sustainability in a specific context is a challenging task. Considering different dimensions and perspectives results in conflicting goals when trying to select the best solution. In the context of batteries, the development and implementation of sustainable technologies is especially challenged by aspects such as materials availability (resources and geographical location), economic feasibility, and technology readiness levels.

Going beyond techno-economic factors, these challenges require methodologies that comprehensively analyze the sustainability issues and allow discussion and interaction among relevant stakeholders, e.g., researchers, technology developers, and policymakers. Multicriteria decision analysis methods are an adequate tool to assess sustainability in different contexts given their flexibility and capability to integrate stakeholders in decision-making processes. The process of conducting MCDA sustainability assessment has important implications regarding the identification of sustainability criteria and indicators, selection of MCDA methods, and identification of stakeholders and their involvement in the assessment. The aim of this chapter is to provide an overview of the MCDA methodology and how this can be applied in the context of sustainability assessment of emerging batteries. First, the definition of important concepts in MCDA sustainability assessment is given. This is followed by a review of MCDA studies in the field of battery storage. Then, a use case for cathode material selection for sodium ion batteries is presented as example for the use of PROMETHEE II. Discussion on the results with a focus on the methodology and their meaning is presented. The chapter ends with conclusion and outlook for MCDA sustainability assessment for emerging storage technologies.

18.2 MCDA for Sustainability Assessment

Multiple criteria decision analysis (MCDA) is a technique that supports decision-making processes through the comparison of potential solutions or alternatives using relevant, often conflicting, criteria. The process of MCDA generally consists of the following steps: identification and involvement of stakeholders, problem definition, selection of criteria (and indicators), definition of alternatives, preference modeling (criteria weighting and aggregation), comparison and evaluation of alternatives, sensitivity/robustness analysis, and problem resolution [21].

The three main challenges for the application of MCDA methods in sustainability assessment are stakeholders' integration, selection of sustainability criteria and indicators, and selection of MCDA methods. They are briefly described in the following paragraphs.

18.2.1 Stakeholder Integration

Identification and involvement of relevant (and diverse) stakeholders is of great importance for MCDA sustainability assessment. Stakeholders should be involved in the construction of the model from definition of the problem and identification of sustainability issues to the evaluation of the results [33]. In practice, this has some drawbacks since it demands high amount of resources such as time, people, and money. Therefore, it is common to find applications or models in which stakeholders' integration is limited to weighting using different formats again depending on the resources available, e.g., workshops, online surveys, and interviews.

18.2.2 Sustainability Criteria and Indicators

Guidelines for general applications of MCDA methods indicate that criteria/indicators are required to be unambiguous, comprehensive, operational, and understandable [31]. In the context of sustainability assessment, they should as well reflect the concept of sustainability used (e.g., triple bottom-line model) and the sustainability issues related to the object of study [4, 22, 48]. At this point, the integration of stakeholders facilitates and strengthens the process of identifying sustainability issues. It is also important to consider the nature of the criteria/indicators for sustainability assessment. It is recommended that they include a life cycle perspective "not to divert some negative impacts from one stage to the other" [12].

18.2.3 Selection of MCDA Method

This subchapter is divided into two sections. First, a general description of MCDA methods is presented, including more detailed information about three selected methods to illustrate their capacities and differences. Second, the presentation and description of the requirements of the MCDA methods to conduct sustainability assessment and a brief comparison of how those three methods perform on these requirements.

18.2.4 Classification of MCDA Methods

MCDA methods can be distinguished into multi-objective decision-making (MODM), multi-attribute decision-making (MADM), and combinations of MODM and MADM [35]. MADM methods can be categorized into (i) elementary methods (e.g., weighted sum method), (ii) single synthesizing criterion (e.g., TOPSIS, AHP), (iii) outranking methods (e.g., PROMETHEE, ELECTRE), and (iv) mixed methods [23]. These methods have different strengths and weaknesses, and their application depends on the decision problem and type of information available [35]. For example, Cinelli, Kadzinski, Gonzalez, and Roman [13] and Wątróbski, Jankowski, Ziemba, Karczmarczyk, and Zioło [56] present "guidelines" to help users to select the most adequate method based on categories such as criteria structure (flat, hierarchical), capacity to handle missing information, and easiness of use. The following paragraphs include a brief description of three methods (WSM, TOPSIS, and PROMETHEE) commonly used in the context of energy management.

18.2.5 WSM

The WSM (weighted sum method) is a way to combine criterion values according to their preferences into a ranking value for each alternative. Its main advantage lies in its simplicity, allowing stakeholders without background knowledge to understand how the ranking is achieved. WSM requires unitless criterion values of comparable scale and therefore usually operates on normalized criterion values, weighting them by normalized preference values and summing them up:

$$R_j = \sum w_i \cdot N_i(C_i) \text{ for } i$$

where R_j is the ranking value for alternative j, w_i the normalized weight for criterion i, and C_i the normalized criterion value for criterion i. The normalized criterion values must be profit oriented, i.e., higher values are better than lower ones. If this is not the case as for, e.g., costs, this can be achieved by an according normalization.

WSM is frequently chosen because it feels obvious and comes to stakeholders naturally.

18.2.6 TOPSIS

The Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) starts with the normalization and weighting of the input data [10]. With the normalized and weighted input data, the different alternatives can be interpreted as points depending on the chosen criteria. Besides, two theoretical points are calculated: a point that corresponds to the best values in each category over all considered alternatives (theoretical best alternative) and a point which corresponds to the worst value over all alternatives (theoretical worst alternative). With TOPSIS, the best alternative is calculated based on the shortest and farthest Euclidean distances from the theoretical best and the theoretical worst alternative, respectively (cf. Hwang and Yoon [28] and

García-Cascales and Lamata [18]). To determine the so-called performance value P_i of an alternative, the named distances are determined and related to each other:

$$P_i = S_i^- / (S_i^+ + S_i^-)$$

where S_i^- is the distance to the theoretical worst alternative and S_i^+ is the distance to the theoretical best alternative. TOPSIS requires a limited subjective input compared to other approaches, e.g., PROMETHEE. Its logic is rational and understandable, and the computation processes are straightforward [18].

18.2.7 PROMETHEE

The PROMETHEE family of outranking methods includes several versions which are suitable for different decision-making situations: PROMETHEE I and II, for partial and complete rankings, PROMETHEE III for interval order, PROMETHEE IV for continuous extensions, PROMETHEE V for problems with segmentation constraints, PROMETHEE VI for the human brain representation, and PROMETHEE Group Decision Support Systems (GDSS) for group decision-making [9]. The principle of PROMETHEE is based on pairwise comparisons of alternatives along each criterion. These pairwise comparisons depend on preference functions assigned to each criterion with the aim of translating the difference between two alternatives from the criterion scale to a 0–1 degree of preference. PROMETHEE I provides partial rankings of the alternatives with the outranking flows Φ + and Φ-. The higher Φ + and the lower Φ- are, the better is the overall rank of the analyzed option. PROMETHEE II adds a step to derive a complete ranking of the alternatives (outranking flow Φ) by calculating the difference between the two flows. The challenge or complexity associated with this method when compared to elementary or single synthetizing methods relies on the cognitive effort by the decision-maker to define parameters associated with the preference functions. The next paragraphs describe weighting and preference function selection for PROMETHEE II.

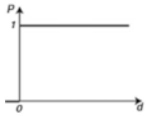
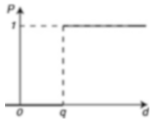
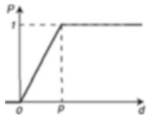
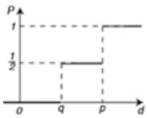
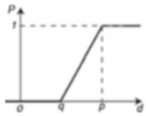
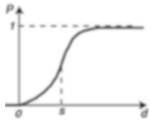
(a) Weighting

There is no specific methodology to determine the weights in PROMETHEE II, and commonly other methods are used for this task. An important consideration for the selection of weighting methods is that in PROMETHEE II the weights represent importance coefficient, i.e., the voting power of the criteria in the decision problem [11].

(b) Preference Function and Parameters

The selection of preference functions allows to identify the degree of preference among alternatives where 0 means indifference and 1 strict preference. Depending

Table 18.1 PROMETHEE preference functions [38]

Preference function	Thresholds	Graphical representation
Type I – Usual	None	
Type II – U-shape	q– Indifference	
Type III – V-shape	p– Preference	
Type IV – Level	q,p	
Type V – V-shape with indifference (linear)	q,p	
Type VI – Gaussian	S – Gaussian threshold	

on the type of function selected, preference thresholds (p) and/or indifference thresholds (q) can be defined. Q indicates the largest difference that can be neglected and p the smallest difference that represent a total preference [38]. Table 18.1 shows the six preference functions in PROMETHEE. PROMETHEE II is equivalent to the WSM when all criteria have the type III–V-shape preference function and the same value for the preference threshold P [19, 37].

The selection of the preference parameters P and Q is meant to be done by the decision-makers based on their perceptions on the decision problem [51]. However, this is commonly not a simple task, and several strategies or approaches have been proposed to simplify this in different contexts, e.g., uncertainty of life cycle impact assessment (LCIA) [58], and using the difference between the maximum and minimum value of each criterion and making then p and q equal to 10–30% and 5–15% of this difference, respectively [34].

18.3 Properties of MCDA Methods for Sustainability Assessment

In the context of sustainability assessment, there is a set of desirable properties when selecting an MCDA method [12, 45]:

- Handling qualitative and quantitative data: when conducting sustainability assessment, different information can be obtained in different forms, i.e., ordinal, cardinal, or mixed.
- Type of weights: within an MCDA model, there are two types of weights: trade-offs when the weights reflect intensity of preference and importance coefficients which represent voting power [44]. In the case of sustainability assessment, the weights should be modeled as importance coefficients. Therefore, special attention should be paid when selecting the methods for preference elicitation.
- Partial/null compensation between criteria: compensation implies the existence of trade-offs in the aggregation of criteria, i.e., the extent to which bad performance of one criterion can be offset by good performance of another. Compensation is associated with the concept of weak sustainability and low compensation with strong sustainability (a more detailed description can be found in Ziemba [60]).
- Threshold values: these can be useful in complex preference models where not all preferences have the same intensity or relevancy.
- Ease of use: simple structure facilitates the experience of the users. Some methods are commonly preferred because of their simplicity. For example, full compensatory methods such WSM are easier to implement compared to low-compensatory methods that could require high cognitive effort such ELECTRE III or PROMETHEE II. However, it is a task of the analyst to properly understand the methods and be able to explain it to stakeholders.
- Handling uncertainty: sustainability issues are inherently related to uncertainty. In order to account for this imprecision or vagueness in the information, the multicriteria evaluation needs to either model the uncertainty of the input data, i.e., stochastic analysis, or include sensitivity analysis [42].
- Software support and graphical representation: several software exist that facilitate the implementation of different MCDA methods. Given their importance on the implementation of MCDA methods, an additional subchapter is dedicated to this topic.

Table 18.2 presents the performance of commonly used MCDA methods related to the desired properties for sustainability assessment in the context of energy technologies. It can be seen why outranking methods are more suitable for sustainability-related decision-making problems. Their ability to offer thorough understanding of how the problem is structured to accurately represent the decision-maker's preferences, and to account for uncertain information using techniques like probability distributions, fuzzy sets, and threshold values, makes them highly valuable [25].

Table 18.2 MCDA method performance with respect to the desired properties for sustainability assessment [12, 14]

	MADM methods		
	Elementary methods	Single synthesizing criteria	Outranking methods
Properties/characteristics for sustainability assessment	WSM	TOPSIS	PROMETHEE II
Handle qualitative and quantitative data	Quantitative	Quantitative	Quantitative, qualitative
Weights as importance coefficients	Trade-offs	Trade-offs	Relative importance coefficients
Threshold values	No	No	Preference, indifference
Partial/null compensation between criteria	Full	Full	Null, partial
Handling uncertainty	Yes	Yes	Yes
Ease of use	High	High	Medium
Software support and graphical representation	Definite [30], MCDA KIT Tool [43], diviz [41]	Triptych, PyTOPS [59], MCDA KIT Tool [43], diviz [41]	Visual PROMETHEE [39], D-Sight [27], MCDA KIT Tool [43], diviz [41]

18.4 MCDA Software

MCDA software supports users through decision-making processes by providing different methods. High diversity of MCDA software is available to match the various needs of the different users which could depend on characteristics such as MCDA methods available, structuring of preferences, graphical representation, usability, platform (desktop, website), and last but not least type of license (commercial, free). Inventory of some available MCDA software can be found in Beekman [8], International Society on MCDM [29], and Weistroffer and Li [57]. Commercial MCDA software stand out for offering good technical support and documentation. However, a great deal of MCDA software has been developed by the scientific community to meet specific needs (e.g., specific MCDA methods, context-based software) or simply to eliminate the barriers that licenses impose. The following subchapter presents the freely available software MCDA KIT tool, originally developed by the Karlsruhe Institute of Technology to support decision-making processes in the context of nuclear emergency management, yet with the original goal to avoid specific constraints and to provide a broadly applicable tool for both the scientific and the operational communities. This tool is still continuously improved in the context of the projects where it is applied, e.g., by adding a specific plug-in to meet the requirements of sustainability assessment.

18.4.1 MCDA KIT Tool

The MCDA KIT tool is a standalone java desktop application with the goals to teach and demonstrate multiple available MCDA methods as well as to apply MCDA in an operational environment. The former manifests in a flexible design which allows for easy and fast integration of new methods resulting in an already comprehensive collection. The latter leads to a clear and user-friendly graphical interface, displaying analyses and results in various ways. The MCDA KIT tool provides many interactive possibilities to edit and analyze an MCDA task. Figure 18.1 shows some of the more common interactions beginning from top left rank bar chart, normalization, report, stability analysis, values, and direct weighting.

The tool is designed in a modular and most generic way to allow combination and comparison of the different methods of the MCDA process. Many different algorithms have been implemented for the various tasks. Weights can be determined by the use of direct weighting, SMART, SWING, and AHP (analytical hierarchy process). Normalization is possible by many methods, starting with simple linear min-max functions up to nonlinear methods like Softmax or piecewise linear. So far, the method for aggregation can be chosen from WSM (weighted sum), WPM (weighted product), some voting methods, VIKOR, TOPSIS, or PROMETHEE. By design, other algorithms can be added easily, expanding the collection of methods over the course of time.

The software is also capable to address uncertainties, both in weights and values, by evaluation of ensembles. Uncertainties can be defined as histogram distributions, naturally supporting stakeholder surveys, or probability distributions with the need to specify the distributions and their parameters. Furthermore, the software features

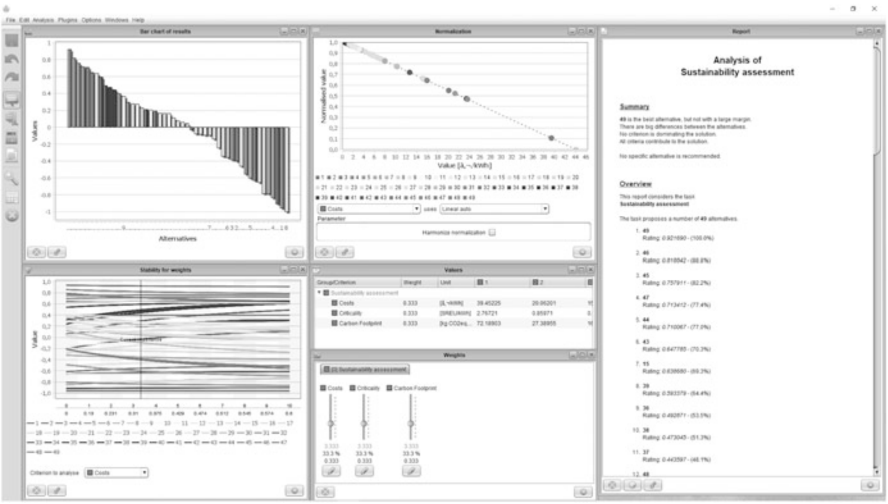


Fig. 18.1 Screenshot of MCDA KIT tool

the generation of documents which textual outline the input conditions, the applied MCDA methods and parameters, and the results as well as analyses like stability estimates and potential correlations. Several import and export methods allow to connect to other tools like MS Excel. A plug-in interface allows third parties to easily add functionality. The tool is also translated in several languages and provides different modes to address color blindness.

18.5 MCDA for Sustainability Assessment in the Field of Batteries

There are several MCDA studies available in the field of batteries, aiming at different technologies (different Li-based chemistries, redox-flow, or high-temperature batteries), as well as different applications reaching from stationary to mobile applications. Depending on the specific scope, corresponding methods and criteria are selected for the assessment of batteries as indicated in Table 18.3. This is not intended to be an exhaustive review but to provide some example of applications and perhaps identify common practices. A wide range of MCDA methods are applied in the selected studies, including mostly compensatory approaches. Criteria selected include mostly LCA indicators. In addition to that, some studies include a wide set of stakeholders, while others do not include any in their assessments. A major factor that should also be kept in mind is that technologies that are being compared might have different technology readiness levels. This can be challenging as some technologies already experienced a large learning curve, while others are just being presently developed. Having this heterogeneity in mind makes it difficult to directly compare the results of different studies. Consequently, it is not possible to determine the best technology via a single study.

18.6 Use Case MCDA Sustainability Assessment for Early-Stage Cathode Materials for Sodium Ion Batteries

In this chapter, the MCDA process (problem definition, selection of criteria, definition of alternatives, and preference modeling) for sustainability assessment is illustrated based on an example of early-stage cathode material screening for sodium ion batteries. The assumptions and calculations here presented correspond to the ones made by the authors in the original publication [6], except for the application of the MCDA method for which PROMETHEE II is used instead of WSM. More details on the made assumptions, considered chemistries, and used data can be found in Baumann et al. [6].

Table 18.3 Overview of selected MCDA studies in the field of battery storage with different chemistries, applications, criteria, and stakeholder involvement

Source	Technologies / alternatives	Application	Criteria	MCDA methods (w = weighting, a = aggregation)	Number and categories of stakeholders involved (participant/category description)	Results
Haase et al. [24]	Battery electric vehicle (BEV), fuel cell electric vehicle (FCEV), internal combustion engine vehicle (ICEV)	Electric vehicles	Environmental (LCA) Economic (total costs) Social (domestic value added)	TOPSIS (a)	None	Under given assumptions, the BEV with wind power was assessed as most sustainable option in 2020 as well as in 2050
Domingues, Marques, Garcia, Freire, and Dias [16]	BEV, FCEV, ICEV, plug-in hybrid (PHEV)	Electric vehicles	Life cycle impact assessment	ELECTRE TRI (a)	None	BEV and PHEV are the only vehicles that can achieve the top class
Baumann, Peters, and Weil [7]	Lithium–iron–phosphate (LFP), lithium–iron–phosphate/lithium titanate (LFP–LTO), lithium–manganese oxide (LMO), nickel–cobalt–aluminum oxide (NCA), and nickel–cobalt–manganese oxide (NMC)	Utility scale Battery storage technologies: Primary regulation, energy time shifting, wind energy support, decentralized grid	Environmental (damage to ecosystem DE, damage to human health DHH, damage of resources availability DRA) Economic (life cycle costs LCC) Social (socioeconomic values, acceptance, regulation, and frame) Technological (maturity, technology performance, tech. flexibility)	AHP (w), TOPSIS (a)	72 people/civil society, regulation, policymakers, researchers (university), municipal utility, network operator, utility company, RES production/retail, automotive sector, battery manufacturer, energy storage business	LIBs seem to be the most Recommendable technology among the evaluated BESS for most application areas (with exception of the LIB–LTO, which is only suitable for low E/P ratios)

(continued)

Table 18.3 (continued)

Source	Technologies / alternatives	Application	Criteria	MCDA methods (w = weighting, a = aggregation)	Number and categories of stakeholders involved (participant/category description)	Results
Ma et al. [36]	Nas battery, lead-acid (LA) battery, NiMH battery, and Li-ion battery (LIB)	Electrochemical energy storage for renewable energy-based power generation stations	Environmental (CO_2 intensity) Economic (capital intensity and operation cost) Social (social acceptance and electric power system reserve capacity reduction) Technological (cycle life, energy efficiency, and self-discharge rate)	Bayesian BMW (w), TOPSIS (a)	Five people/experts	LIB is the optimal solution
Albawab, Ghenai, Bettayeb, and Janajreh [1]	LA batteries, LIBs, super-capacitors, hydrogen storage, compressed air energy storage, pumped hydro, and thermal energy storage	Not given	Environment (area and material intensities, energy, CO_2, and capital intensities of the construction, life cycle greenhouse gas emissions) Economic (operating cost, current installed capacity, growth rate) Social indicators (health and safety issues)	Extended SWARA (w)/ ARAS (a)	Three people/experts from engineering, energy storage, sustainability, energy and climate change, renewable energy	Ranking: (1) thermal energy storage, (2) compressed air, (3) LIBs, (4) pumped hydro, (5) LA batteries, (6) hydrogen storage (onboard), and (7) supercapacitors

			Technological: cycle lifetime, cycle efficiency, discharge time at rated power, and adaptability for mobile systems Resource (specific energy, specific power, energy density)			
Salameh et al. [49]	PV-BES based on nickel–iron (Ni–Fe), LIB, and LA battery technologies at different depths of discharges (DOD)	PV/battery technology microgrid system for a desalination plant	SDG 7: Affordable and clean energy (round-trip efficiency, energy density, number of life cycles, lifetime years, storage duration) SDG 8: Decent work and economic growth SDG 15: Life on land (environmental impact) Economic (annual levelized cost, levelized cost of energy) Size: NPV, NBAT	TOPSIS, WSM, NEW (a)	None	The PV-LIB at 50% DOD was the best option among all cases

(continued)

Table 18.3 (continued)

Source	Technologies / alternatives	Application	Criteria	MCDA methods (w = weighting, a = aggregation)	Number and categories of stakeholders involved (participant/category description)	Results
Murrant and Radcliffe [46]	Power to gas, a distributed battery system, battery storage integrated with solar PV and demand from an airport, liquid air energy storage, battery storage integrated with wave energy, and thermal energy storage at a new residential development	Energy storage projects	Environmental co-benefits Economic growth (innovation), economic viability, increasing self-consumption, economic co-benefits Deferral of grid upgrades, technology viability	MAVT (w,a)	18 people/local and national businesses, academia, community energy groups, and CC	Top-ranking project: Battery storage integrated with solar PV and demand from an airport

18.6.1 Stakeholder Integration

Material researchers from KIT were selected as relevant stakeholders given the scope of the analysis (screening of early-stage cathode materials). Their integration includes the stages of problem definition, selection of criteria, and alternatives and excludes weighting of criteria. In the following subchapters, these will be referred as stakeholders.

18.6.2 Problem Definition

Sodium ion batteries (SIBs) are considered as promising, sustainable alternative to lithium ion batteries (LIBs) regarding the use of critical and expensive materials and the high carbon footprint of the same [6]. Although there is a wide set of different cathode active materials (CAMs) available for SIB, they are considered to be in a lower technology readiness level (TRL) than CAMs for LIB, which are a state-of-the-art technology. Under these uncertainties, how to determine the most sustainable cathode types that are under development and to prioritize certain electrodes types becomes a challenge.

18.6.3 Selection of Criteria

The MCDA is based on a comprehensive bottom-up screening approach using three different criteria: (1) CAM cost, (2) raw material criticality, and (3) carbon footprint. These were selected considering the sustainability issues mentioned in Sect. 18.6.2, a literature review and workshops with stakeholders. Table 18.4 presents the information related to the criteria, indicators, and sources of the data.

18.6.4 Definition of Alternatives

The alternatives consist of 49 CAMs selected using literature screening and from workshops conducted with stakeholders. An overview of the used SIB CAMs and their properties as well as results for the three different criteria is provided in Table 18.5. Here, each SIB CAM chemistry is benchmarked to eight selected LIB CAMs (Nos. 1 to 7 and No. 30 in Table 18.4). From this, lithium–nickel–manganese–cobalt (No. 5) and lithium–iron–phosphate (No. 30) are among the most prominent CAMs. All CAMs are separated into oxidic and polyanionic cathode types for a more differentiated comparison.

Table 18.4 Overview of used criteria for SIB cathode evaluation

Sustainability issues	Criteria	Indicator	Unit	Description	Methods for quantification/ source of data
Resource management (global supply concentration, country governance, import reliance, trade restriction, recycling)	Raw material criticality (criticality)	Supply risk (SR) for the EU	SREU/ kWh	Collective term describing the economic value and dependency on certain materials as well as the probability of supply chain disruptions [50]	SR for Europe [17]
Global warming, emissions to air and water	Carbon footprint (CF)	GHG emissions	kg CO_2eq./ Wh	Greenhouse gas emissions of the CAM precursors and their synthesis process	LCA
Competitiveness	CAM cost (cost)	Costs	€/kWh	Costs of raw materials and precursor materials	Literature and market search inflations and inflation adjusted median values of costs from the last 11 years

A major challenge is to gather the specific mass composition of all cathodes on a common functional unit, here the specific energy of the CAM without an anode. This was realized via a literature review, complemented by laboratory data and stoichiometric calculations for a reference case without anode. All criteria are calculated on a Wh base.

18.6.5 Preference Modeling

PROMETHEE II is selected to model preferences in this chapter based on the description and requirements for sustainability assessment presented in Table 18.2.

18.6.6 Weighting

There is no direct involvement of stakeholders for the weighting process as stakeholders preferred the use of equal weights in combination with a sensitivity analysis with different weighting sets.

Table 18.5 Overview of assessed CAM and corresponding results for the three assessment criteria

No.	CAM name	Theoretic capacity (mAh/g)	Reversible capacity (mAh/g)	Reversible specific energy without anode (Wh/kg)	Cost (€/kWh)	Criticality (SREU/kWh)	CF (kg CO_2eq.-kWh)
Layered oxide materials							
1	$LiCoO_2$	274	150	585	39.45	2.77	72.19
2	$LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA)	279	188	696	20.06	0.86	27.39
3	$LiNi_{0.5}Mn_{0.5}O_2$	280	150	585	15.98	0.90	16.51
4	$LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (NMC111)	278	160	592	23.62	1.51	34.92
5	$LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622)	276	170	629	21.25	1.12	29.40
6	$LiMn_2O_4$ (LMO)	148	110	472	8.01	1.29	5.04
7	$LiNi_{0.5}Mn_{1.5}O_4$ (LNMO)	147	140	644	10.33	0.67	10.62
8	P2-$Na_{0.67}CoO_2$	168	115	369	44.06	3.76	99.05
9	a-$NaMnO_2$	244	185	509	1.97	0.88	2.16
10	ß-$NaMnO_2$	244	190	523	1.92	1.14	2.77
11	$Na_{0.44}MnO_2$	122	120	336	3.22	1.52	2.86
12	P2-$Na_{0.67}MnO_2$	175	175	490	2.14	0.99	2.08
13	P2-$Na_{0.67}Mn_{0.72}Mg_{0.28}O_2$	191	220	572	1.74	1.16	2.23
14	P2-$Na_{0.67}Mn_{0.95}$ $Mg_{0.05}$ O_2	177	175	455	2.29	1.13	2.33
15	P2-$Na_{0.67}Mn_{0.5}$ $Fe_{0.5}O_2$	174	190	523	1.26	0.72	1.51
16	O3-$NaMn_{0.5}Fe_{0.5}O_2$	243	110	303	2.12	1.16	2.92
17	P2-$Na_{0.67}Ni_{0.33}$ $Mn_{0.67}O_2$	173	161	596	5.16	0.69	7.78
18	P2-$Na_{0.8}Li_{0.12}Ni_{0.22}$ $Mn_{0.66}O_2$	214	118	415	7.14	0.97	9.26

(continued)

Table 18.5 (continued)

No.	CAM name	Theoretic capacity (mAh/g)	Reversible capacity (mAh/g)	Reversible specific energy without anode (Wh/kg)	Cost (€/kWh)	Criticality (SREU/kWh)	CF (kg CO_2eq.-kWh)
19	P2-$Na_{0.83}Li_{0.07}Ni_{0.31}Mn_{0.62}O_2$	214	140	490	6.60	0.80	9.40
20	P2-$Na_{0.83}Li_{0.25}$ $Mn_{0.75}$ O_2	237	185	500	4.35	0.85	3.54
21	O3-$NaFe_{0.5}Co_{0.5}O_2$	238	160	502	15.61	1.55	35.18
22	O3-$NaNi_{0.33}Co_{0.33}Fe_{0.33}O_2$	238	165	487	15.12	1.24	31.68
23	O3-$NaNi_{0.5}Mn_{0.5}O_2$	240	125	377	10.13	0.93	16.28
24	$Na[Mn_{0.4}Fe_{0.5}Ti_{0.1}]O_2$	244	110	308	2.38	1.18	6.30
25	$NaMn_{0.33}Fe_{0.33}Ni_{0.33}O_2$	240	100	481	5.51	0.66	9.00
26	$Na_{0.6}Fe_{0.11}Mn_{0.66}Ni_{0.22}O_2$	159	120	324	7.25	1.29	10.50
27	$NaMn_{0.3}Fe_{0.4}Ni_{0.3}O_2$	241	130	390	6.19	0.80	10.16
28	P2-$Na_{0.6}Fe_{0.2}Mn_{0.65}Ni_{0.15}O_2$	158	200	620	2.97	0.67	4.16
29	$Na_{0.6}Ni_{0.22}Al_{0.11}Mn_{0.66}O_2$	164	225	675	3.63	0.62	5.33
Polyanionic materials							
30	$LiFePO_4$ (LFP)	170	165	569	5.70	0.81	5.08
31	$Na_3V_2(PO_4)_3$	118	110	381	15.33	1.59	34.99
32	$Na_4MnV(PO_4)_3$	111	110	380 [a)]	8.01	1.30	18.79
33	$Na_3MnTi(PO_4)_3$*	117	114	410[a]	1.87	1.14	5.55
34	$Na_3MnTi(PO_4)_3$**	176	172	506[b]	1.51	0.93	4.50
35	$Na_3MnZr(PO_4)_3$	107	110	402[b]	1.41	1.12	3.23
36	$NaFePO_4$	154	152	410	0.57	0.87	3.06
37	$Na_{1.7}0_2Fe_3(PO_4)_3$	87	140	406	0.55	0.93	2.95
38	$Na_4Fe_3(PO_4)P_2O_7$**	152	129	406	0.62	0.87	3.27

39	Na_2MnPO_4F*	249	178	651	0.99	0.76	2.29
40	$NaV(PO_4)F$	143	82	303	23.42	2.52	51.79
41	$Na_{1.5}VPO_{4.8}F_{0.7}$	130	134	509	12.69	1.30	28.27
42	$Na_2Fe(PO_4)F$	124	110	360	0.78	1.09	3.52
43	$Na_3MnPO_4CO_3$*	192	125	490	1.08	0.61	2.80
44	$Na_2MnFe(CN)_6$*	171	140	490	1.32	0.50	2.06
45	$Na_{0.61}Fe[Fe(CN)_6]_{0.94}$[1]	61	170	493	0.80	0.58	2.06
46	$Na_{0.81}Fe[Fe(CN)_6]_{0.79}$[1]	90	149	447	0.88	0.46	1.67
47	Na_2FeSiO_4*	276	181	724	0.87	0.44	3.14
48	Na_2MnSiO_4*	278	210	630	1.66	0.68	4.00
49	$Na_2Fe_2(SO_4)_3$*	120	102	418	0.40	0.45	0.87

Data based on Baumann et al. [6]
[a]Specific energy is directly from the literature and the average potential is calculated
[b]Specific energy is calculated from the integration of the potential capacity
*2Na exchange; **3Na exchange; [1]Prussian blue analogs

Table 18.6 Preference function and parameters selected for use case

Criteria	Cost (€/kWh)	Criticality (SREU/kWh)	CF (kg CO_2eq.-kWh)
Preference function	Linear	Linear	Linear
Maximum value	44.06	3.76	99.05
Minimum value	0.40	0.44	0.87
Q	0	0	0
P	0.89	0.07	2

18.6.7 Preference Function and Parameters

In this example, we use the type V-shape with indifference function (linear preference function) for each of the three criteria since they all have a continuous numerical scale, and while comparing them, very small differences can be neglected. P and Q are defined as suggested in Haralambopoulos and Polatidis [25], P being equal to the difference between the maximum and the minimum value for each criterion divided by n (49 CAMs) and Q being equal to zero (Table 18.6).

18.6.8 Results

In this section, the results of using the MCDA method PROMETHEE II for the aggregation of criteria and ranking of materials are presented. Additionally, sensitivity analyses of weights are carried out. All calculations are carried out using the MCDA KIT tool (see Sect. 18.2.4).

18.6.9 Comparison and Evaluation of Alternatives (Ranking)

In Fig. 18.2, the resulting net flows of materials using the method PROMETHEE II are displayed for equal weighting of the three considered criteria. The higher the resulting net flow, the better the alternatives perform from a sustainability point of view. In Fig. 18.2a, alternatives are sorted from left to right according to their CAM number (see Table 18.5), whereas, in Fig. 18.2b, alternatives are sorted from left to right according to their net flows, i.e., ranking. Some trends can be observed in the ranking. First ranks are achieved by polyanionic SIB CAMs (Nos. 49, 46, 45, 47), from which Nos. 45 and 46 correspond to Prussian blue analogues (PBAs), and Nos. 49 and 47 to Si- and S-containing SIBs. Most LIB layered oxide materials (CAM Nos. 1–7) show negative net flows (ranks 32 and higher). Only LIB CAM LFP (CAM No. 30) has a positive net flow. CAMs containing cobalt or vanadium perform lower in the rank, whereas those that contain Mn show preferable rankings. A detailed overview on the results can be found in Baumann et al. [6]. It is important to notice that varying the energy densities can have a high impact on the results. Also, the performance on a cell level can be very different and has thus to be analyzed in detail for further assessments.

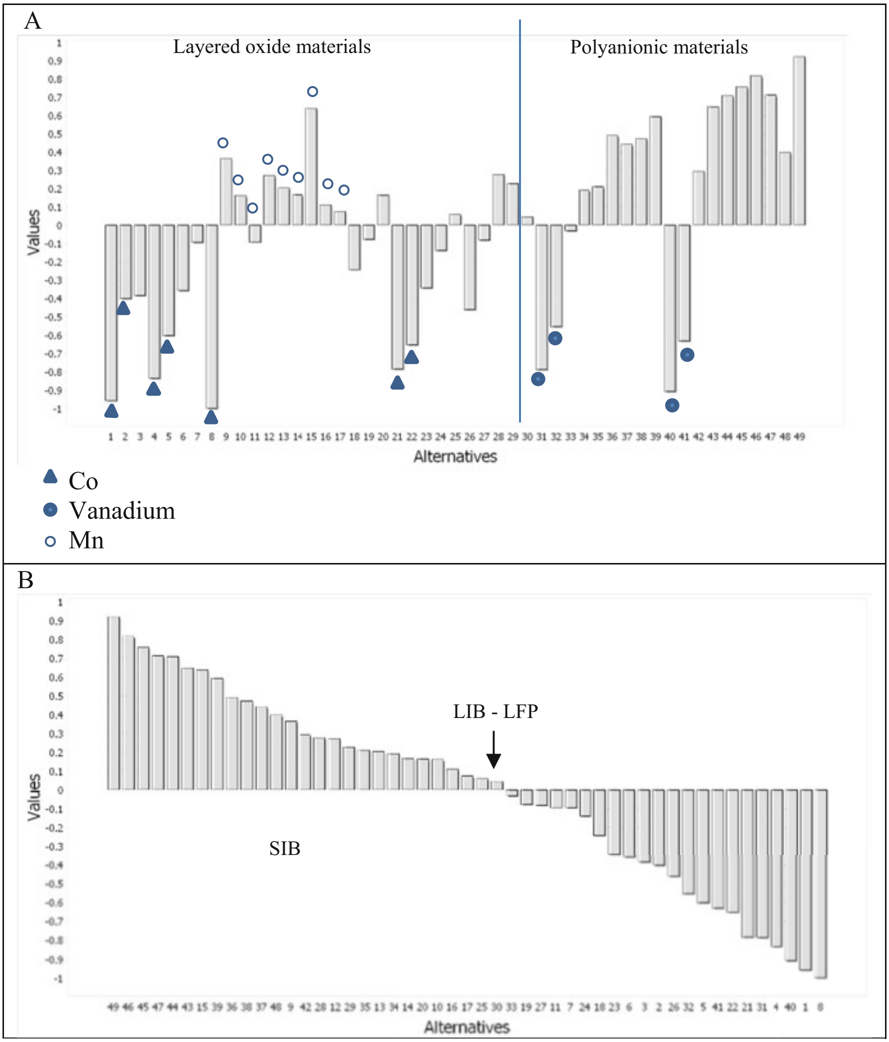


Fig. 18.2 Resulting net flows and rankings of CAMs using PROMETHEE with equal weighting of criteria, sorted according to material numbers (**a**) and rankings (**b**)

18.6.10 Sensitivity Analysis

Table 18.7 presents the rankings with different importance coefficients (weights) up to the 15th place for the cases of (i) equal weights for all criteria, (ii) higher importance to costs (25% criticality and 25% CF), (ii) higher importance to criticality (25% costs and 25%CF), and (iii) higher importance to CF (25% criticality and 25% costs). There is low variation in the ranking when considering different importance coefficients for the criteria.

Table 18.7 Net flows of cathode materials of first 15 ranks

	Equal weights (original case)			Sensitivity analysis		
				50% costs	50% criticality	50% CF
Rank	Net flow	CAM No.	CAM name	CAM No.		
1	0.921	49	$Na_2Fe_2(SO_4)_3$	49	49	49
2	0.818	46	Na0.81Fe[Fe(CN)6] 0.79[a]	46	46	46
3	0.757	45	Na0.61Fe[Fe(CN)6] 0.94[a]	45	47	45
4	0.713	47	Na_2FeSiO_4	47	45	44
5	0.710	44	$Na_2MnFe(CN)_6$	44	44	15
6	0.647	43	$Na_3MnPO_4CO_3$	43	43	47
7	0.638	15	P2-Na0.67Mn0.5Fe0.5O_2	15	15	43
8	0.593	39	Na_2MnPO_4F	39	39	39
9	0.492	36	$NaFePO_4$	36	48	36
10	0.473	38	$Na_4Fe_3(PO_4)P_2O_7$	38	36	38
11	0.443	37	Na1.702$Fe_3(PO_4)_3$	37	38	37
12	0.399	48	Na_2MnSiO_4	42	28	9
13	0.365	9	a-$NaMnO_2$	48	29	12
14	0.294	42	$Na_2Fe(PO_4)F$	9	37	48
15	0.276	28	P2-Na0.6Fe0.2 Mn0.65Ni0.15O_2	35	9	13

[a]Prussian blue analogs

18.7 Discussion

As the intention of this exercise is to reflect on the application of MCDA on sustainability assessment for emerging technologies, only a brief analysis on the results will be presented, and the main attention relies on the process. For a deeper analysis about the results (although using a different MCDA method), the original publication can be consulted [6].

18.7.1 Meaning of Results

The results presented provide insights into the process of CAM selection for SIBs according to MCDA-assisted sustainability assessment. The ranking of CAMs can be understood only as indicative for research and development trends on the material level and cannot be extrapolated into the cell level. Having this in mind, it can be said that the ranking suggests that considering the criteria CF, criticality, and costs, the most promising CAMs for SIBs could be Prussian blue analogs and Si- and

Mn-based chemistries. Some of these CAMs perform even better than commercial LIB CAMs used as benchmark here.

18.7.2 MCDA Procedure

The challenges of conducting MCDA sustainability assessment (see Chap. 2) sharpen when dealing with early-stage technologies. The following paragraphs elaborate on them.

Selection of Criteria The experience with existing energy technologies facilitates the identification of the sustainability issues associated with this decision problem, e.g., high CO_2 emissions, social acceptance, and resources availability. In this use case, this task is limited by the availability of data to compare the impacts of the energy technologies shrinking the potential set of criteria to the mentioned three. Values taken from literature were used to perform calculations, e.g., specific energy values and CAM production costs taken from the literature and estimation of precursor price via stoichiometric calculations. High effort was required for this task, and yet the uncertainty of the results is still very high due to the low TRL of the technologies and lack of robust primary data. Non-existing LCA, unknown social impacts, and volatile market prices challenge the application of MCDA for emerging technologies. Existing methods like prospective LCA could play an important role in this task [26, 47, 53], providing a systematic methodology for obtaining data.

MCDA Method Selection The use case demonstrates that the application of low-compensatory methods such as PROMETHEE II can be facilitated through the use of software and existing approaches to (initially) determine threshold values (preference parameters, p and q). In this type of problem, uncertainty analysis should be conducted carefully. The approach used here represents a deterministic MCDA with sensitivity analysis. However, sustainability assessment of emerging materials/ technologies might require stochastic MCDA methods ([42]; [55]). When searching MCDA methods that fit to the sustainability assessment requirements and account for the uncertainty in the performance data (using Cinelli, Kadziński, Miebs, Gonzalez, and Słowiński [14]), the following candidates result: fuzzy PROMETHEE II [20], PANSEM II [2], SMAA III (stochastic multicriteria acceptability analysis) [52], and SMAA-PROMETHEE [15]. Van Schoubroeck et al. [55] present an example of application of SMAA-PROMETHEE for sustainability assessment of emerging biotechnologies.

Stakeholder Integration The integration of material researchers (experts) within the MCDA process was very important for the identification of alternatives and accessing the laboratory data. However, the low diversity within the group of stakeholders hinders deeper reflections on sustainability. Integration of a diverse group of stakeholders is not only relevant for sustainability but also for technology development [40]. To the best of the author's knowledge, there are not so many studies on applications of MCDA approaches to emerging technologies. Some examples found show the integration of stakeholders from academia, government, and industry [5, 55]. Further research should be conducted on determining how diverse the group of stakeholders within sustainability assessment of emerging technologies could be.

18.8 Conclusion

In this chapter, we have presented the general requirements for MCDA sustainability assessment and an overview of their application in the field of batteries. Some recent applications of MCDA in the field of batteries show diverse approaches with a trend for deterministic, compensatory MCDA methods and inclusion of stakeholders. Available data from a use case of early-stage cathode material screening for sodium ion batteries was selected to illustrate and analyze the suitability of MCDA for assessing emerging battery technologies. In this type of decision problems, identifying the sustainability criteria is not as challenging as evaluating the performance of the alternatives. The lack and/or the high uncertainty of the performance data, e.g., laboratory data, calculations based on literature values, makes it difficult not only to evaluate but to derive concrete conclusions after conducting MCDA. However, the results obtained can be used as indicative to identify promising materials/technologies that could potentially be taken forward in their TRL.

Further development or improvement of the presented model would include exploring different alternatives to address uncertainty in weights and values, such as evaluation of ensembles, probability distributions, or using suitable stochastic MCDA methods (e.g., SMAA- and fuzzy PROMETHEE). Expanding the categories of stakeholders and its participation on the MCDA sustainability assessment is needed to improve the task of preference modeling.

In the context of sustainability assessment, it is very important to understand MCDA as an iterative process in which information, priorities, and stakeholders (categories) are constantly changing. The use of systematic approaches and specialized MCDA software is very important to keep pace with this task.

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