RESEARCH ARTICLE

Life cycle assessment of an industrial-scale vanadium flow battery

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Editor Managing Review: Lynette Cheah

Funding information
German Federal Ministry for Economic Affairs and Climate Action, Grant/Award Number: 03ET6156E

Abstract

In the course of the energy transition, storage technologies are required for the fluctuating and intermittently occurring electrical energy. The vanadium flow battery (VFB) is an especially promising electrochemical battery type for megawatt applications due to its unique characteristics. This work is intended as a benchmark for the evaluation of environmental impacts of a VFB, providing transparency and traceability. It considers the requirements for an industrial VFB from the technical and electrochemical point of view. The system design is based on a net capacity of 8 MWh and a net power of 1 MW. This ex ante study is a cradle-to-grave life cycle assessment (LCA) for a VFB to identify, analyze, and evaluate the environmental impacts for a lifetime of 20 years. Moreover, potential environmental impacts of several subsequent life cycles of the emission-intensive and long-lasting vanadium electrolyte are evaluated. With a focus on the electrolyte, the extraction process of vanadium pentoxide is studied in detail for the first time. Consequently, recommendations for the design of the life cycle of VFBs and for comparative LCAs with other energy storage technologies can be derived. Based on this work, more detailed work can follow, which helps to estimate the recycling potentials and emissions more precisely. This article met the requirements for a gold-gold *JIE* data openness badge described at https://jie.click/badges

KEYWORDS
climate change, energy storage, industrial ecology, life cycle assessment, vanadium flow battery, vanadium pentoxide

1 | INTRODUCTION

Storage systems are of ever-increasing importance for the fluctuating and intermittently occurring renewable electrical energy. The vanadium flow battery (VFB) can make a significant contribution to energy system transformation, as this type of battery is very well suited for stationary energy storage on an industrial scale (Arenas et al., 2017). The concept of the VFB allows conver electrical energy into chemical energy at high efficiencies. The energy conversion takes place in electrochemical cells and the energy is stored in aqueous electrolytes in external tanks.
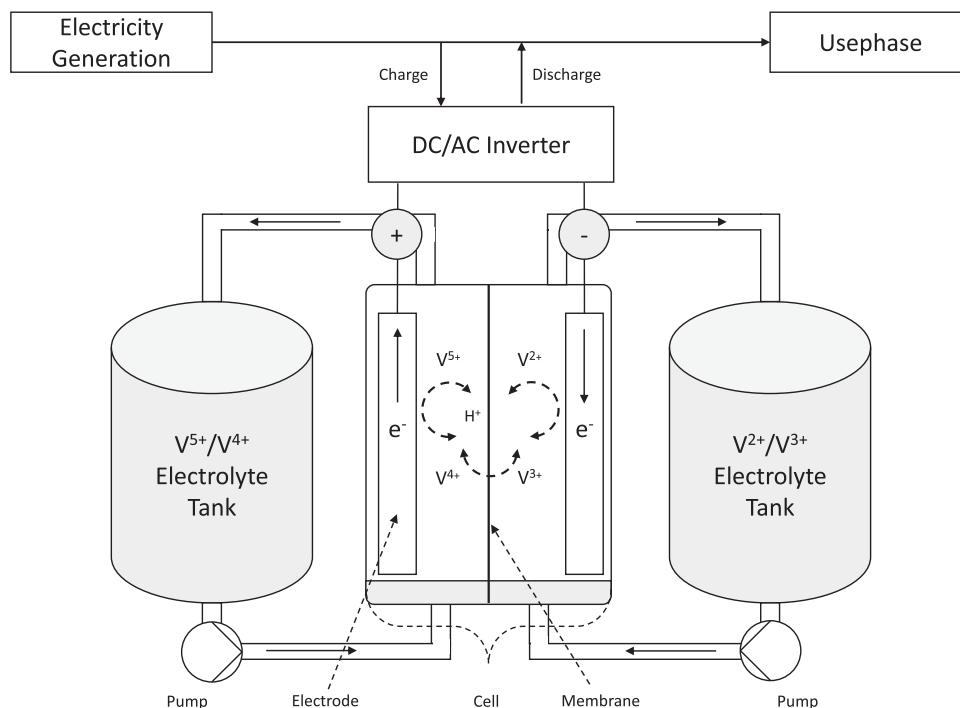
FIGURE 1 Schematic structure of a vanadium flow battery

The resulting independent scalability of power and energy capacity allows an adaptation to a wide variety of requirements (Minke et al., 2017). A further advantage is the high cycle life, which is ensured by a very low electrolyte contamination (Rydh, 2003). The high amount of cycles is possible mainly due to the use of the same chemical element on both half-sides and the separation of the positive and negative electrolytes. The positive electrolyte and the negative electrolyte stored in external tanks are pumped through the cells. The VFB electrolyte is a solution of vanadium ions in sulfuric acid, where the vanadium (V) is the active material in the electrolyte. The redox couple V^{5+}/V^{4+} operates in the positive electrolyte and the redox couple V^{2+}/V^{3+} in the negative electrolyte. The schematic structure of a VFB is illustrated in Figure 1.

In the present life cycle assessment (LCA) study, potential environmental impacts of a VFB are evaluated. The study is based on an in-depth technical analysis and electrochemical system design of megawatt-scale VFB. This bottom-up approach allows valuable insights on state-of-the-art large-scale VFB. Through this work, we fill the gap in the literature for a detailed LCA of an MW-scale VFB. The aim of this study is to reduce any uncertainties to a minimum by using updated data. In a sensitivity analysis, both primary and secondary electrolytes are considered. Various LCAs and resulting statements about potential emissions from VFBs exist in the literature (Basosi et al., 2019; Da Silva Lima et al., 2021; Fernandez-Marchante et al., 2020; Gouveia et al., 2020; He et al., 2020; Hiremath et al., 2015; L'Abbate et al., 2019; Morales-Mora et al., 2021; Rydh, 1999; Weber et al., 2018). A detailed review of comparable literature suggests a need for further research.

The most transparent and detailed LCAs have been published by Weber et al. (2018) and He et al. (2020). The LCA by Weber et al. (2018) takes up the simplified data structure by Rydh (1999) and updates the balances based on the system design by Minke (2016). The modeling and the balance sheet of Weber et al. (2018) are designed to be highly transparent. In comparison, the most recent work by Da Silva Lima et al. (2021) can only be used to a limited extent due to the lack of supporting information. In Weber et al. (2018) and Da Silva Lima et al. (2021) the electrolyte is responsible for the majority of the emissions. However, in Da Silva Lima et al. (2021) it remains unclear how the electrolyte is balanced.

Following the key finding, that vanadium pentoxide (V_2O_5), and with it the electrolyte, accounts for a significant proportion of the emissions a validation of these processes and the overall system is intended in the present work. The foci of the paper are primarily the emission-intensive electrolyte and, consequently, the accounting and modeling of the V_2O_5. For V_2O_5 there is only one transparent data set, the one in the GaBi (2018) database that is not freely available. In addition, in this data set a magnetic separation process is considered, whereas a blast furnace process should be appropriate for common V_2O_5 production routes.

For balances of V_2O_5, the works by Weber et al. (2018) and He et al. (2020) should be mentioned in particular. The balances by Weber et al. are often used as a basis in other works. He et al. compare different balances for the V_2O_5, in particular the data from Weber et al. (2018), Jungbluth and Eggenberger (2018), and Chen et al. (2015). Our approach highlights itself especially through the use of primary data, transparency, technical data, and the type of steel processing considered. It is important for the steel process and the following steps to use the primary data of the same ore, because the losses during extraction and the energy balances are strongly dependent on the ore. Furthermore, assumptions and superficial considerations must be avoided. The LCA is based on V_2O_5 from the Mapochs mine in South Africa (Goso et al., 2016). For the first time, the

potentially high-emission electrolyte production process is completely and transparently analyzed and quantified by means of energy and mass balances. The system design of the VFB is based on current industrial standard. Thus, a special focus is put on an electrochemical and technical design as relevant aspects are not covered in the literature.

2 | ENVIRONMENTAL LIFE CYCLE ASSESSMENT

The environmental LCA method framework is based on the international standard ISO 14040 (2006) or ISO 14044 (2006). The standard includes four important steps: goal and scope definition, inventory analysis, impact assessment, and interpretation. In the present section, the LCA methodology is presented briefly. Detailed technical facts are presented in Supporting Information S1. In addition, life cycle inventory (LCI) data are provided in Supporting Information S2, as well as in a separate Microsoft Excel file. Therefore, the model can be reconstructed and understood in a transparent and user-friendly way.

2.1 | Goal and scope

The fundamental objective of this work is to quantify emissions resulting from storage in a VFB and the creation of a solid and transparent database. In this study, an LCA based on a cradle-to-grave approach is prepared and analyzed. The cradle-to-grave life cycle consists of the phases: raw material extraction, production, use, and end-of-life (EOL), whereas the focus of this study is put on the production phase of the battery. An extended cradle-to-cradle approach would be of interest, but due to the young age of VFB technology in combination with its long lifetime, the recycling possibilities or second life options can only be viewed in perspective. In industrial VFB no recycled material is used for stack relevant components, therefore no assumptions with recycled materials are made. Components are stack relevant if they have a high contribution to the efficiency of the battery. These components are mainly the bipolar plate (BPP) and the membrane.

The investigated industrial VFB configuration base on a nominal power of 1 MW and a nominal energy capacity of 8 MWh. This corresponds to an energy to power (E/P) ratio of 8:1 h. The functional unit (FU) is defined as the provision of the total energy provided over the entire life cycle. The total energy is defined by the number of cycles a battery performs multiplied by the energy provided per cycle. The cycle life of the battery is 20 000, which means the total discharge capacity is 160 GWh (Jiang et al., 2020; Sánchez-Díez et al., 2021). In the use phase only the energy losses resulting from the energy supply and the efficiency of the battery are accounted for, while the stored energy (160 GWh) is neglected. By balancing the stored energy, the results would be distorted and the influence of the renewable energy technology as well as the respective location would have a significant influence on the emissions. For a comparison, the efficiency must be considered, but the sources of renewable energy have to be considered as well.

2.2 | Life cycle inventory

The VFB system can be split into the four main modules: stack, electrolyte, foundation, and support. The four groups are illustrated in Figure 2. The first group is the stack, which includes all electrochemical cell components. The module energy storage comprises the vanadium electrolyte and the storage tanks. The module support covers all components needed for the balance of plant. The last group is the foundation.

The LCI in Figure 2 (more details in SI) is based on a nominal power of 1 MW and a nominal capacity of 8 MWh. This capacity is realized by 375.4 m^3 of vanadium electrolyte with a vanadium concentration of 1.6 mol L^{-1} and a total sulfate concentration of 4 mol L^{-1}(Martin et al., 2020; Skyllas-Kazacos et al., 2016). The cycle life refers to a lifetime of 20 years and an overall system efficiency of 70% is assumed. The most important technical key parameters are shown in Table 1.

Primary data and particular information on technical and electrochemical set up of VFB originate from the joint research project Re3dOx funded by the German Federal Ministry for Economic Affairs and Climate Action (03ET6156F). Primary data on vanadium mining production are based on the Mapochs mine in South Africa. The technical system design is based on preliminary works (Minke & Ledesma, 2019; Minke & Turek, 2015; Minke et al., 2017) and described in detail in the SI.

In our previous work (Minke & Ledesma, 2019) on maintenance within the life cycle of VFB, we differentiate between three different possible scenarios. The present study refers to the "maintenance scenario." In this model, the pumps, the inverters, and the complete stacks need to be replaced after 10 years. The electrolyte does not have to be changed in the 20 years of the system lifetime; an internal rebalancing is sufficient for this period (Schafner et al., 2021). The mass balance of all components based on this maintenance scenario is listed in Figure 2. The total weight of the battery is 1 831 004 kg, resulting in a reference flow of 0.01144 kg (kWh)$^{-1}$.
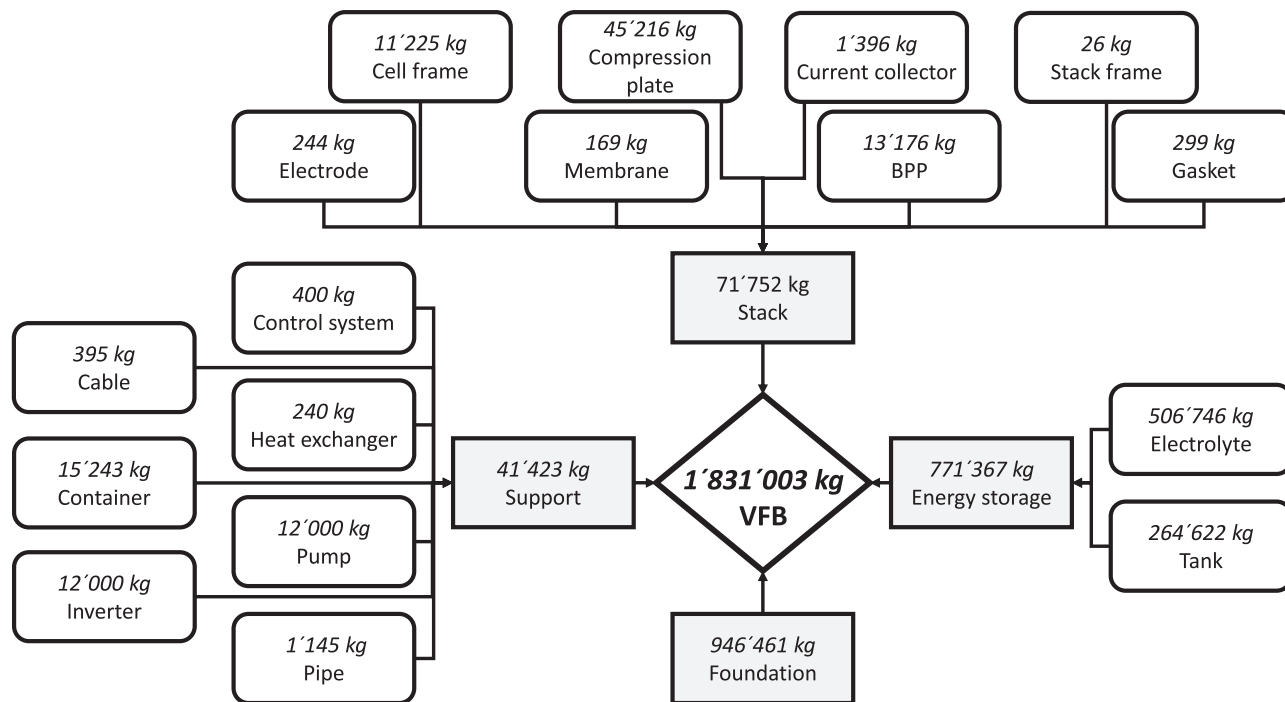
FIGURE 2 Main components of a 1 MW – 8 MWh vanadium flow battery with mass balance

TABLE 1 Technical stack data

Parameter	Quantity	Unit
Number of stacks	10	
Cells	60	Cells per stack
Active membrane area	0.72	m^2
Vanadium concentration	1.6	$mol\,L^{-1}$
Open-circuit voltage	1.42	V
System efficiency	70	%
Target current density	2.00	$kA\,m^{-2}$
Specific volume flow	466	$L\,(h^{-1}\,m^{-2})$
Total volume flow	20 148	$L\,h^{-1}$
Nominal power density	2.60	$kW\,m^{-2}$
Nominal output stack	112.32	kW

2.2.1 | Life Cycle Impact Assessment (LCIA)

The modeling software is Umberto LCA+ with ecoinvent (cut-off model) as background LCA database (Ecoinvent Centre, 2019). The CML-2001 method is used as life cycle impact assessment (LCIA) method.

The following impact indicators are selected: acidification potential (AP), eutrophication potential (EP), photochemical oxidation (PO), abiotic resource depletion potential (ADP), global warming potential (GWP), stratospheric ozone depletion potential (ODP), terrestrial ecotoxicity potential (TAETP), freshwater aquatic ecotoxicity potential (FAETP), human toxicity potential (HTP), and marine aquatic ecotoxicity potential (MAETP).
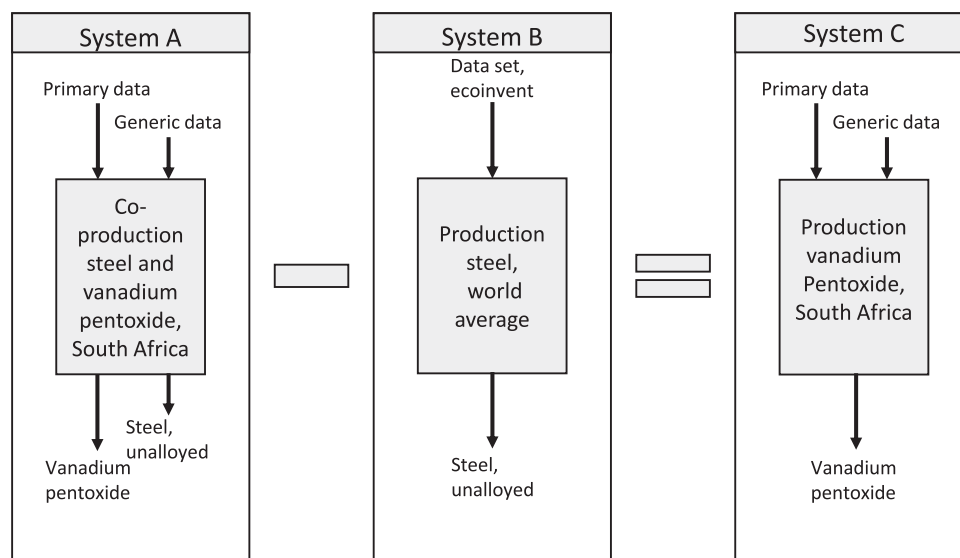
FIGURE 3 Scheme of system expansion approach for calculation of vanadium pentoxide production in South Africa

2.2.2 | System expansion

The complex and high-impact upstream processes of vanadium electrolyte manufacturing are modeled in an original approach in the present study and considers the ISO standards 14040 (2006), 14044 (2006), and 20915 (2018). The minor part is the manufacturing of the aqueous electrolytes by preparing solutions with the active material vanadium pentoxide (V_2O_5). But the major part is the V_2O_5 extraction on the basis of coupled mining and steelmaking processes.

The system expansion approach is illustrated in Figure 3. The system expansion allows an interpretation of different manufacturing ways, an allocation of emissions would undermine this fact. An allocation would also distort the result, especially an economic allocation would become a snapshot, because the prices of steel and especially of V_2O_5 are very volatile. The initial scenario is based on primary data from the Mapochs mine in South Africa, a former major supplier of V_2O_5. Under the new ownership, the mine is currently no longer in operation. In this approach, the environmental impacts of vanadium production are decoupled from those of the steelmaking process. The system expansion allows a comparison of the emissions of the modified electric arc furnace in South Africa with the standard production of steel. In general, primary steel is produced in a blast furnace, but in the case of the ore from the Mapochs mine, it is produced in an open slag bath (Steinberg & Pistorius, 2009; Taylor et al., 2006). The open slag bath is a subtype of the electric arc furnace. Due to the high titanium content in the ore, it is more efficient to use an electric arc furnace instead of a blast furnace because of the extraction rate (Taylor et al., 2006).

For system A in Figure 3 the mass and energy balance of the electrolyte process and the extraction of vanadium are created using primary data. The magnetite is mined in South Africa and has a V_2O_5 concentration of 1.65 wt% (Nkosi et al., 2017; Steinberg & Pistorius, 2009). Besides China and Russia, South Africa is considered one of the largest vanadium producers, which ensures the representativeness of the result (Petranikova et al., 2020). About 80% of the vanadium extracted worldwide results from the processing of magnetite (Song et al., 2013). Thus, V_2O_5 is a by-product in steel production.

The process flow chart with the mass balance for the production of 1 kg V_2O_5 as by-product from steel production is illustrated in Figure 4. The steelmaking process starts with 170.43 kg of iron ore from mining production. After the pretreatment of the ore, 102.78 kg titanium magnetite remains. The pretreated magnetite passes through a pre-reduction kiln with pulverized coal, dolomite and silica, a maximum temperature of 1140°C is reached (Evraz Highveld Steel & Vanadium Limited, 2018; Goso et al., 2016). In this work, these components are referred to as additions for the kiln process.

The considered titanium magnetite from South Africa is produced in an open slag bath. An LCA of this local process is not described in the literature yet. The emission values based on the primary data used here are validated with the use of the literature data for different manufacturing processes of steel (Das & Kandpal, 1997; Hu et al., 2006; Renzulli et al., 2016; Sakamoto & Tonooka, 2000). The high amount of steel (62.58 kg per 1 kg of V_2O_5) is related to the poor extraction rate of the magnetite. The ore contains 1.65 wt% V_2O_5, but only 0.973 wt% can be extracted technically and, more importantly, economically. The discard titanium slag contains about 0.9 wt% V_2O_5 (Lekobotja et al., 2017). At a quantity of 0.448 kg titanium slag per kg ore, 0.00403 kg V_2O_5 per 1 kg ore cannot be extracted due to the high titanium content in the ore. Furthermore, the ore cannot be used for other purposes (Goso et al., 2016). A higher extraction rate regarding the titanium slag would technically be possible, but is not increased for economic reasons at this time. Therefore, the titanium slag can be neglected when calculating the emissions, the same applies
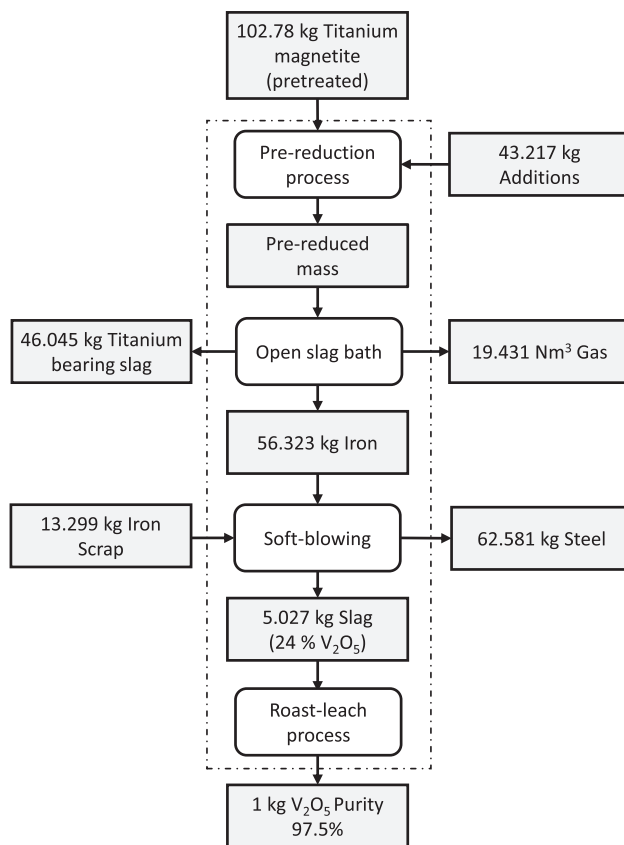
FIGURE 4 Process flow chart with mass balance for the production of 1 kg vanadium pentoxide (V_2O_5) as by-product from steel production

to the produced gas, because the extent to which the gas is used in the system or otherwise is not clearly defined. The vanadium slag contains 24 wt% V_2O_5 after the soft-blowing process. The slag technically contains V_2O_3, but the proportion was converted to V_2O_5 (Steinberg et al.). The subsequent roast–leach process with the vanadium slag is based on a laboratory analysis of the magnetite from Mapochs mine (Goso et al., 2016). For the calculation of further losses incurred during extraction, it is mandatory to use data on the ore under study. As explained for the titanium slag, the losses depend strongly on the composition of the ore or the vanadium slag. After the roast–leach process, only 0.973 wt% V_2O_5 with a purity of 97.5 wt% is extracted. The corresponding extraction rate of the roast–leach process is 82 wt% but it only refers to the vanadium content (Goso et al., 2016). The purity of 97.5 wt% corresponds not to the standard of state-of-the-art GfE Vanadium Electrolyte Solution 1.6 M (GfE Metalle und Materialien GmbH, 2012; Martin et al., 2020). No balances for a purity of 99.6% of the V_2O_5, which would correspond to the GfE standard, can be found in the literature (Martin et al., 2020). However, a significant increase in effort can be expected based on the significantly higher price for purer V_2O_5 (Cao et al., 2018). In the previous LCAs, purity of the V_2O_5 was not sufficiently discussed. The purity of the V_2O_5 not only has a significant impact on the performance of the battery but also on the price. Especially because of the price, less pure electrolyte is currently being researched, but the impact on the performance of the battery is still unclear. In particular, the long-term cell performance and the potential detrimental effects of impurities in the electrolyte have not yet been sufficiently researched (Skyllas-Kazacos et al., 2016). On the market, there is generally no standard for the composition of the electrolyte. However, an electrolyte with high purity is explicitly desired by the customer (Cao et al., 2018).

The extraction of vanadium can be done in several ways; due to clarity, only one strategy is analyzed (Nkosi et al., 2017). A total of 62.58 kg of steel is produced in order to reach the manufacturing of 1 kg V_2O_5 as by-product. The mass and energy balances of the relatively simple electrolyte manufacturing process using sulfuric acid, water, and electric energy are explained in detail in the SI of this article.

System B in the system expansion (Figure 3) is modeled with a global average quality steel data set from ecoinvent database (Ecoinvent Centre, 2019). Due to the cost-intensive production in electric arc furnace, it is mainly used for the production of quality and stainless steels, but about the quality of the steel there are no reliable sources, so the choice of an average steel in system B is a conservative approach. The proportion of vanadium resulting from steel production in this data set is very small and therefore it is negligible. The intention behind this accounting is that the steel produced in system A reduces the amount of steel to be produced in global average processes. Accordingly, the emissions from system B are accounted as savings or credits, because the production of steel from system B is prevented by system A.

For this accounting, the system boundaries have to be considered. In the last step of the soft-blowing steelmaking process in system A, vanadium slag is produced as a by-product, which has to pass through further steps as shown in Figure 4. For the calculation of system C from Figure 3, mining
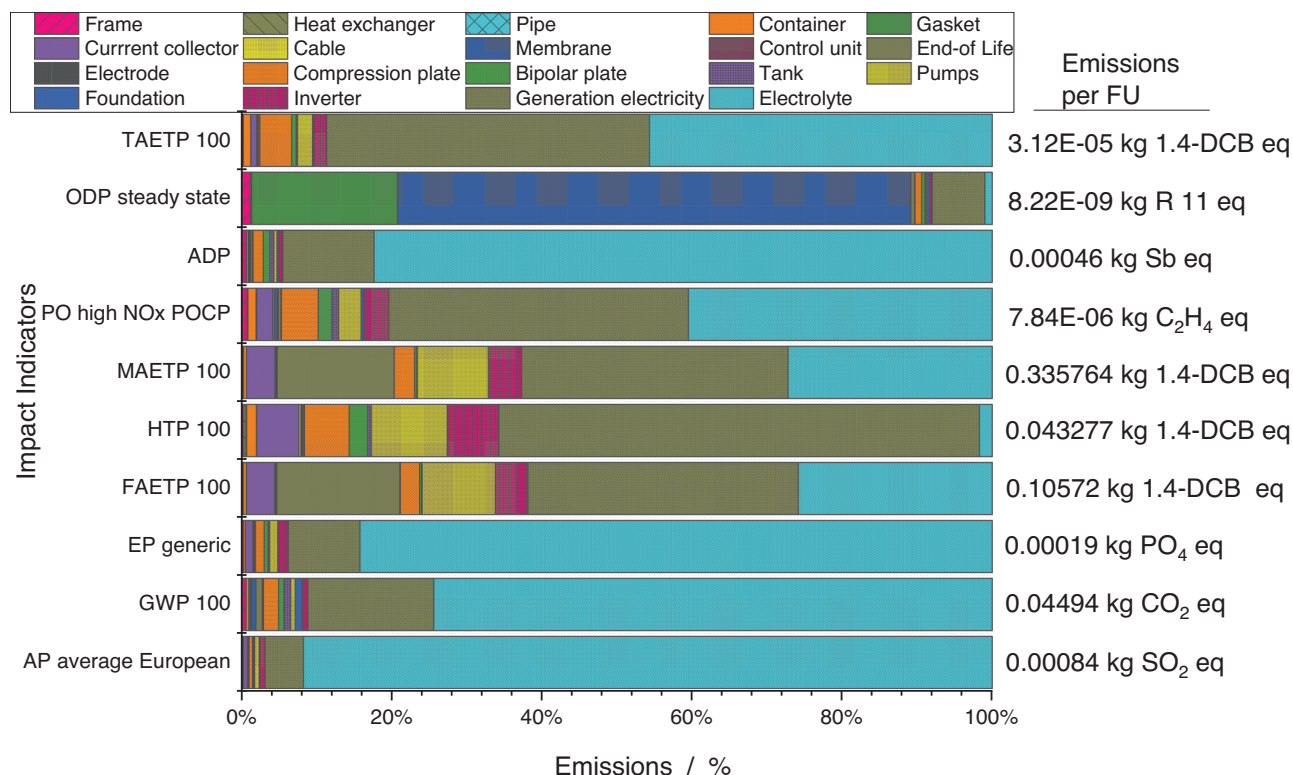
FIGURE 5 A breakdown in percentage of the emissions of the different impact indicators. The emissions are based on a cradle-to-grave approach. Impact categories: AP (acidification potential), EP (eutrophication potential), PO (photochemical oxidation), ADP (abiotic resource depletion potential), GWP (global warming potential), ODP (stratospheric ozone depletion potential), TAETP (terrestrial ecotoxicity potential), FAETP (freshwater aquatic ecotoxicity potential), HTP (human toxicity potential), MAETP (marine aquatic ecotoxicity potential). Underlying data for Figure 5 are available in tab "Data plotted in Figure 5" in Supporting Information S2

to soft blowing is defined as the system boundary; accordingly, further processing of the vanadium slag is not accounted for. In addition, to ensure a certain degree of comparability, credits may only be awarded within the system boundary, thus no negative emissions can result for the V_2O_5.

3 | RESULTS AND DISCUSSION

In this section, the LCIA results are presented and discussed. First, the percentage shares of the individual components are analyzed. Second, a spotlight is put on GWP in terms of CO_2 equivalents. In addition, the study examines how potential emissions evolve over an extended time horizon by considering multiple subsequent life cycles of the emission-intensive and long-lasting vanadium electrolyte.

3.1 | LCIA results

LCIA results are illustrated in Figure 5, which shows the relative contribution of battery components to the various environmental impact indicators. Additionally, absolute emissions per FU are stated for all indicators.

The electrolyte as well as the electric energy supply dominates almost all indicators. Since the electrolyte has a high non-quantifiable value after 20 000 cycles, this effect must be investigated in a sensitivity analysis. In the considered period of 20 years, the generation of electricity with a share of 16.8% of CO_2 eq is only dominated by the electrolyte (74.4%) in the GWP indicator. The provision of electricity causes high percentages of emissions, especially for the indicators TAETP (43%) and HTP (64%). In the model, the term "generation of electricity" refers only to the losses caused by system efficiency of the battery and energy provision of the battery is accounted for. Thus, battery efficiency has a significant impact on the emissions. Likewise, reduced efficiency would result in higher electrolyte demand. However, the assumed total system efficiency of 70% is a very conservative estimation; in the literature, figures of 75–90% for the system efficiency are provided (Hu et al., 2017).

The electrolyte clearly dominates the acidification potential (AP) at 91.8%. Whereas the electrolyte has the lowest impact on the ODP with 0.9%, which is dominated by the membrane (68.3%). The reason lies in the perfluorinated Nafion membrane material with an elaborate synthesis, including a polymerization reaction of tetrafluoroethylene and perfluoro sulfonyl fluoride ethyl-propyl-vinyl ether and losses in the upstream processes (Gebert, 2004; Minke, 2016; Minke & Turek, 2015).

Besides the impact of the Nafion membrane on ODP, the stack components have a significantly lower share of the emissions. It has to be noted that this result corresponds to the specific design and maintenance assumptions used in this study. In general, influencing factors are the E/P ratio, the current density, and the lifetime or cycle life of the stacks. For example, halving the current density would lead to an almost doubling of the required stacks. The E/P ration must always be considered as the power and the capacity can be scaled independently. A strong relationship between the E/P ratio and the resulting emissions of the electrolyte and the stacks can be demonstrated.

3.2 | GWP results

The GWP per FU equals 0.045 kg CO_2 $(kWh)^{-1}$ (see Figure 5). In the previous section, the importance of accounting for the use phase on the basis of battery efficiency has already been emphasized. The 16.8% of CO_2 eq emissions are caused by the energy losses during the use phase of the VFB.

This figure is strongly dependent on the renewable energy chosen. In the model a 1–3 MW onshore wind power located in Germany is assumed, which is a preferable energy generation technology in terms of GWP. For comparison, the GWP per kWh of supplied renewable energy for a 570 kWp open ground photovoltaic system located in Germany is five times higher (Ecoinvent Centre, 2019).

The major contributor to the total GWP is the vanadium electrolyte with a share of 74.4% of CO_2 eq (Figure 5). In this light, a correct elaboration of the production process and corresponding emissions of vanadium pentoxide (V_2O_5) is crucial. The production of primary V_2O_5 is coupled to the steelmaking process in South Africa. In particular, the poor extraction ratio of V_2O_5 from ore has a major impact on emissions. Despite the unfavorable electricity mix in South Africa, the production of steel is not significantly more CO_2 intensive than the usual European production. The electricity mix from South Africa emits 71% (1.06 kg CO_2 eq $(kWh)^{-1}$) more CO_2 eq than the German electricity mix. This effect is enhanced by the use of an electric arc furnace, which requires mainly electricity and no coke.

The CO_2 eq emissions from the steelmaking and V_2O_5 production process (see process flow chart in Figure 4) are shown in a Sankey diagram in Figure 6. It shows that most of the emissions result from energy demand for the furnace as well as the preparation of the ore with coal in the pre-kiln. Up to the "soft-blowing" step, all necessary processes for the production of vanadium and steel are identical. Starting with the resulting vanadium slag all emissions can be fully attributed to the V_2O_5. For the production of 1 kg of V_2O_5 62.58 kg of steel are produced. Most of the electrolyte emissions, 47.8%, result from the provision of electricity for the furnace. The pretreatment of the ore by burning the coal in the pre-kiln also causes a significant share of the CO_2 for the electrolyte production with 38.6%. However, this pre-kiln treatment is necessary due to the ore composition and is not addressed in the previous LCAs. The roast–leach process with a resulting purity of 97.5 wt% of the V_2O_5 has a very low impact on the GWP at 1%. Consequently, the purity of the V_2O_5 is only relevant from an economic but not from an environmental point of view, whereas the roast–leach processes are always strongly dependent on the ore. In the future, steelmaking will generate significantly reduced emissions, especially through renewable energies and the use of hydrogen as a reduction agent in electrical arc furnaces. Compared to 1990, technological advances are expected to reduce CO_2 emissions by 47–95% (Otto et al., 2017). Accordingly, the electrolyte will only cause a fraction of the emissions. In the next chapter, a very important point will be considered for a potential reduction of the emissions, the reuse of electrolytes.

3.3 | Sensitivity analysis

Since an assessment of the electrolyte at the end of the period is difficult for many reasons, this aspect is examined by means of a sensitivity analysis. The statement that the electrolyte can be used for another 20 years without further treatment is just as wrong as considering the electrolyte as waste at the end of the operation phase. The residual value of the electrolyte cannot be quantified at this point based on the literature, but its consideration has a significant impact on battery emissions. There are various irreversible contaminants that cannot be remedied by rebalancing. For example, long-term oxygen diffusion through tubes, hoses, and electrolyte vessels may lead to electrolyte oxidation to some extent. If the BPP is broken, the electrolyte may be contaminated with copper from the current collector. Furthermore, the critical concentrations of various substances are not clearly defined (Skyllas-Kazacos et al., 2016). However, further use of the electrolyte after 20 years is very likely, and measures exist to recycle and rebalance the electrolyte. The worst-case scenario would be the precipitation of the vanadium, but it would still cause significantly less emissions than the primary electrolyte. Since there are no estimates and scenarios for the reprocessing of the electrolyte up to this point, in the reuse scenarios in this study zero emissions for the electrolyte are accounted for.

Figure 7a shows the direct comparison of the potential environmental impacts of the VFB with primary electrolyte and a reuse scenario. In the reuse scenario, the reprocessed electrolyte has zero emissions. Thus, only emissions by the new VFB are accounted for. The figure shows the percentage savings due to the continued use of the electrolyte. Any emissions for the reprocessing are not considered due to insufficient data.
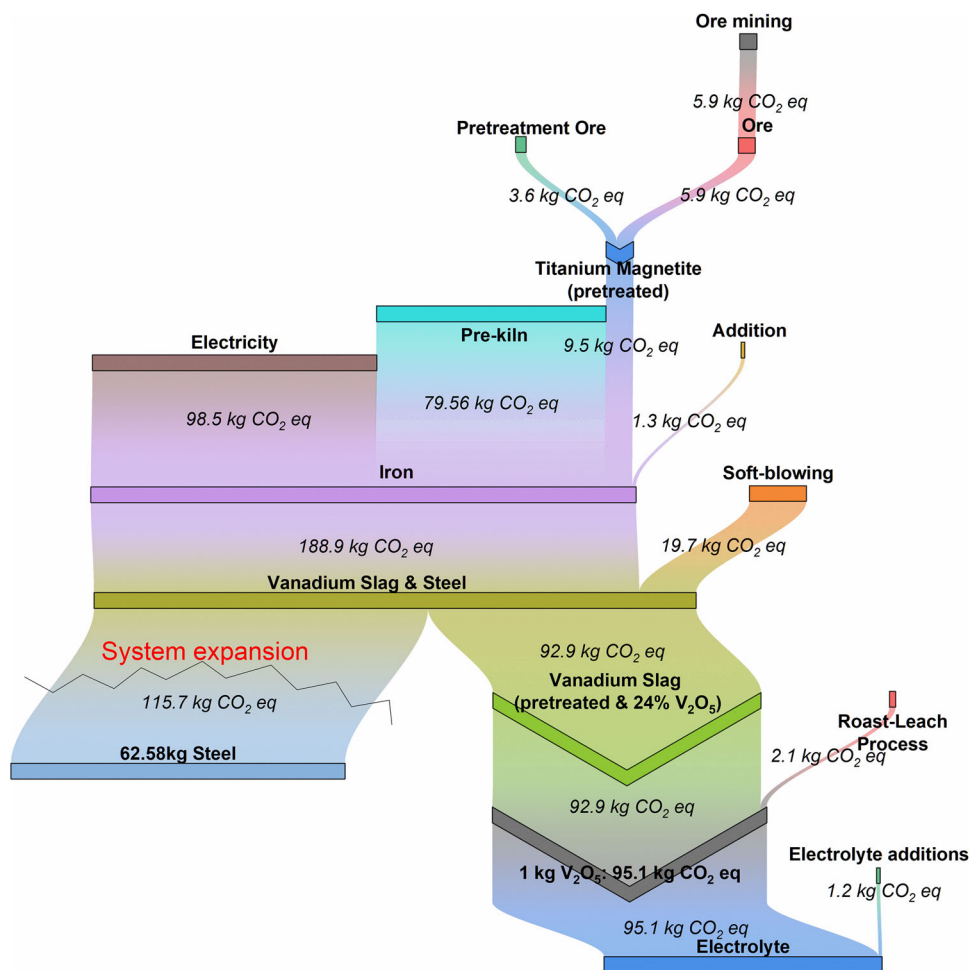
FIGURE 6 The CO_2 eq caused in the production of steel and vanadium pentoxide (V_2O_5) from raw material extraction to the finished 1 kg of V_2O_5 with a purity of 97.5 wt%. On the basis of the manufacturing steps, the allocation of emissions and the designation of the system boundaries become clear. Underlying data for Figure 6 are available in tab "Data plotted in Figure 6" in Supporting Information S2

These emissions are assumed to be relatively small compared to the production of the electrolyte. In addition, the foundation is not considered again. The influence of the foundation is marginal compared to the electrolyte. In the 10 considered impact indicators, this leads to a reduction of emission between 0.97% (ODP) and 91.8% (AP). On average, a VFB using reprocessed vanadium electrolyte instead of primary electrolyte has only 53% of potential environmental impacts.

It is widely anticipated that the vanadium electrolyte may be reused in several life cycles. Thus, a fair allocation of the primary electrolyte's emissions over the life cycles is desirable. In this work, emissions of primary vanadium electrolyte are equally divided over the primary and subsequent reuse life cycles. In Figure 7b the influence of up to four reuse scenarios on AP, GWP, and HTP are illustrated. The curves are flattening significantly after the first reuse scenario, but GWP and AP show strong decreases in the following product life cycles. In contrast, emissions can only be slightly reduced in the HTP, because its main emissions result from the stack and the electricity generation.

The indicator values decrease to a varying extent over the 100 years considered. This is intended as a model proposal for the differentiated consideration of electrolyte and battery with their very different lifetimes.

3.4 | Discussion

In the discussion we refer to the criteria outlined in Section 1. For comparison of LCA results, two requirements have to be met: an appropriate FU for the cradle-to-gate approach and a high level of transparency in the LCI usually provided in extensive Supporting Information S2. For a valid comparison of the results with Weber et al. (2018) we first need to fit the model. The model is changed to a cradle-to-gate approach, accordingly the use phase and the EOL are not considered.
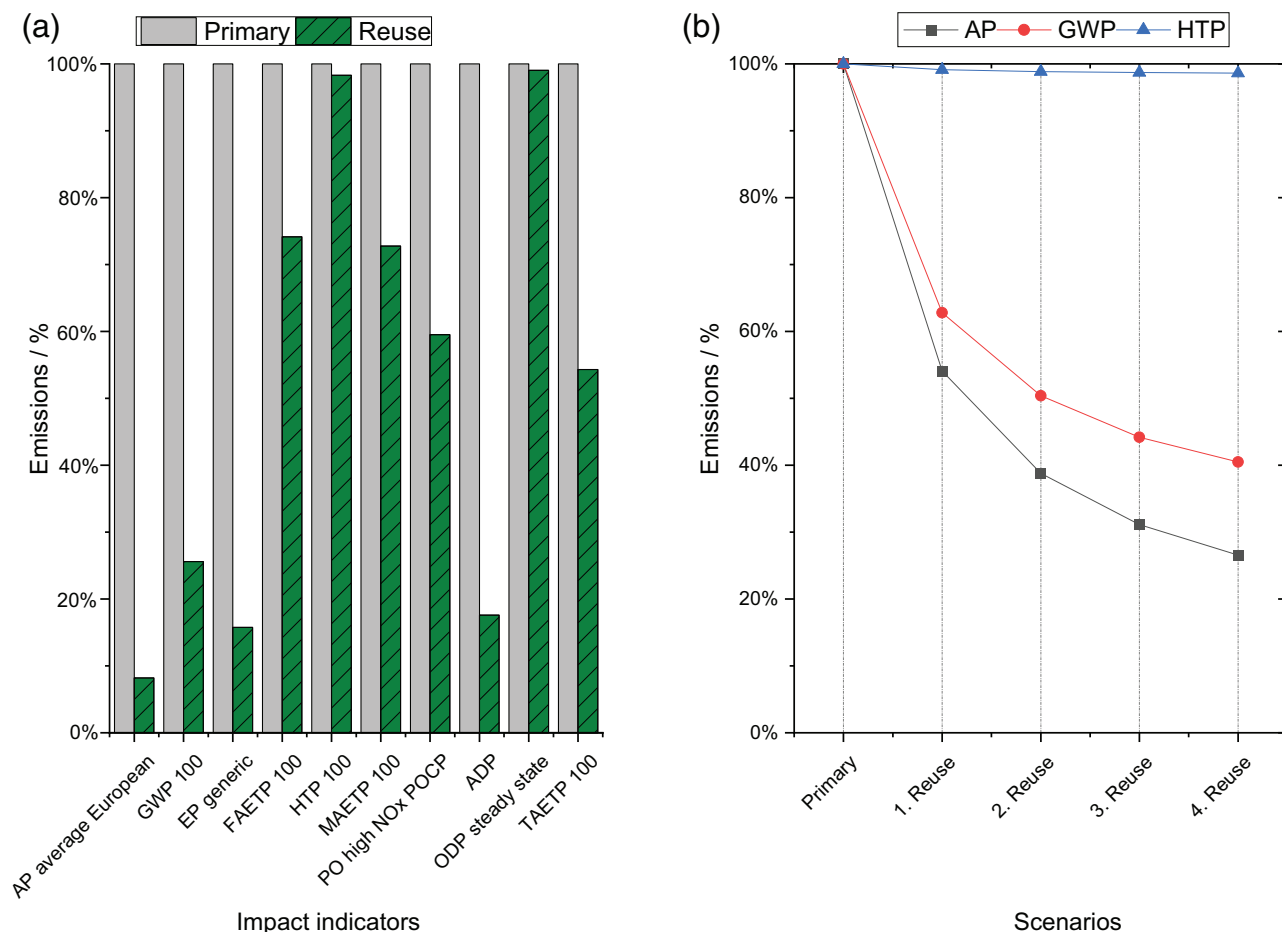
FIGURE 7 (a) Comparison of potential environmental impacts of a 1 MW/8 MWh vanadium flow battery (VFB) with primary vanadium electrolyte and reuse of electrolyte (zero emissions for second life cycle of electrolyte). (b) Development of potential environmental impacts of VFB over up to four reuse cycles of electrolyte in new VFB (emissions of primary electrolyte equally divided over life cycles). Underlying data for Figure 7 are available in tab "Data plotted in Figure 7" in Supporting Information S2

In our analysis we find 37 kg CO_2 eq $(MWh)^{-1}$ for a cradle-to-gate approach. A similar value is provided by Weber et al. (2018) with 38.2 kg CO_2 eq $(MWh)^{-1}$. However, for a valid comparison, the three most significant differences of the Weber et al. LCA also need to be addressed. First, in Weber et al. (2018) only about half of the required electrolyte is accounted for (272 t $\neq$ 507 t), but this is compensated by the assumptions for the composition of 1 L electrolyte (0.148 kg V_2O_5 $\neq$ 0.286 kg V_2O_5). In addition, the assumption of 8176 cycles is very detrimental to the battery, since the electrolyte must be assumed to have a minimum of 20 000 cycles, after which it still has a high unquantifiable value. However, our more detailed consideration also results in significantly more emissions for the electrolyte in our LCA.

The next interesting aspect would be a comparison of GWP from V_2O_5 production, unfortunately no explicit data is found in the literature. We therefore use the approach of validation by GWP results for the upstream steelmaking process in which V_2O_5 is a co-product. Chen et al. calculate a GWP of 2.84 kg CO_2 eq $(kg\ steel)^{-1}$ considering a vanadium titano-magnetite from South Africa. In our LCA, the result is 3.3 kg CO_2 eq $(kg\ steel)^{-1}$ based on our conservative approach (Figure 6). For the validation, the total steel production emissions are accounted for without the allocation due to the system expansion approach. Further quantitative validation of emissions is included in the SI of this article. At this point, further qualitative statements are discussed.

When considering the ore with the V_2O_5 from South Africa, two significant disadvantages were highlighted for the first time in the literature despite the high percentage. First, a high loss of V_2O_5 is generated during extraction, which cannot be further processed economically. Second, due to its composition, the ore has to be pretreated at great expense, which also causes high emissions. However, these factors are partially compensated by the use of an electric arc furnace. The data only refer to the V_2O_5 from one site in South Africa, in order to make general statements on V_2O_5 different processes and sites also need to be examined in detail. In the long term, a data set for primary V_2O_5 is needed so that the results in the literature no longer vary greatly and thus prevent the sustainability analysis of the battery. In perspective, a switch to hydrogen as a reducing agent in a more sustainable steel process would also need to be analyzed along with the consequences (Axelson et al., 2021; Gielen et al., 2020).

In our previous work, a cost advantage of large cell areas was calculated on the basis of mathematical models, which is why large cell areas were analyzed in this work (Minke et al., 2017). Due to the complex manufacturing process, there is still a high manufacturing loss, for example, 40–50% for BPP. In the future, there may be other manufacturing strategies such as injection molding or 3D printing, making also entirely new cell characteristics possible (Arenas et al., 2019).

Conservative assumptions were initially made throughout the balance sheet in order to gain further important insights based on these results. This concerns both the quality of the steel in the system expansion, recycling and, in particular, the consideration of the electrolyte after 20 years. In the model, the electrolyte is considered neutral after 20 years; this assumption is not correct and questionable. However, the value of the electrolyte cannot be quantified at that point. Equally speculative would be the accounting of failures within the operating time. In the model, an optimal course of the battery was assumed. In the literature, no in-depth understanding failures of the battery in the long term exist. In practice, stack components may fail partially or completely, or an oxidation of the electrolyte is also possible (Gundlapalli & Jayanti, 2021). Also, the importance of balancing the foundation must be put into perspective for a longer time period, but nonetheless this factor must be considered. The weight of different flow batteries and especially other storage systems can vary greatly.

Similarly, more attention needs to be paid to circular economy and material circularity in LCA (Saidani et al., 2017). The use of a flow battery offers many advantages, especially the use of modular stacks. The stacks are divided into different components which are often available in pure form with respect to the material. Accordingly, the current collector or the compression plates, for example, can possibly be recycled very efficiently. Likewise, in a further analysis, both the open-loop and the closed-loop recycling process should be analyzed with a corresponding data quality. Another point is independence from materials from critical countries of origin; this aspect must also be considered for a comprehensive sustainability analysis.

4 | CONCLUSIONS AND OUTLOOK

In this study, we present a highly transparent LCA for VFB providing detailed LCI data, accurate process analyses and detailed LCIA results. The focus of this study is to develop a new LCI data set considering state-of-the-art technical parameters of the battery. Thus, we aimed at improving the depth and level of detail for all the VFB system components: the cell stacks, balance of plant, and the electrolyte.

One highlight is the complete analysis of the V_2O_5 production process, which is the key ingredient of the battery electrolyte. Here, the upstream processing steps, mass balances, and energy balances refer to a specific ore, this balancing is unique in the literature. This allows new insights into the emissions of the electrolyte, which is responsible for a significant share of the total battery emissions. Furthermore, we provide a quantitative analysis of potential environmental impact reduction in reuse scenarios for the vanadium electrolyte; in the literature it is widely anticipated that it may be reused in several life cycles.

The following recommendations can be derived from our work. The performance parameters and lifetime of the battery and especially the electrolyte need to be further investigated. Finally, an estimation of emissions based on possible reuse scenarios of the electrolyte become increasingly important in the context of circular economy. An estimation of the best-case and worst-case scenarios would be essential for an LCA of the battery for this purpose, as possibly the emissions of both scenarios are significantly lower than the emissions of the primary electrolyte. Overall, the potential of battery recycling must also be analyzed and implemented in the model. Based on the transparent LCI provided in this work, further aspect of a potential recycling of all VFB components may be analyzed.

CONFLICT OF INTEREST
The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT
The data that supports the findings of this study are available in the supporting information of this article. The data that support the findings of this study are available from ecoinvent Centre. Restrictions apply to the availability of these data, which were used under license for this study. Data are available from the supporting information from this article with the permission of ecoinvent Centre or directly from the third party. The Attribution 4.0 International (CC BY 4.0) license from Creative Commons has been selected.

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