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Flow battery production: Materials selection and environmental impact

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ABSTRACT

Energy storage systems, such as flow batteries, are essential for integrating variable renewable energy sources into the electricity grid. While a primary goal of increased renewable energy use on the grid is to mitigate environmental impact, the production of enabling technologies like energy storage systems causes environmental impact. Thus, understanding the impact of producing energy storage systems is crucial for determining the overall environmental performance of renewable energy from a systems perspective. In this study, the environmental impact associated with the production of emerging flow battery technologies is evaluated in an effort to inform materials selection and component design decisions. The production of three commercially available flow battery technologies is evaluated and compared on the basis of eight environmental impact categories, using primary data collected from battery manufacturers on the battery production phase including raw materials extraction, materials processing, manufacturing and assembly. In the baseline scenario, production of all-iron flow batteries led to the lowest impact scores in six of the eight impact categories such as global warming potential, 73 kg CO_2 eq/kWh; and cumulative energy demand, 1090 MJ/kWh. While the production of vanadium redox flow batteries led to the highest impact values for six categories including global warming potential, 184 kg CO_2 eq/kWh; and cumulative energy demand, 5200 MJ/kWh. Production of zinc-bromine flow batteries had the lowest values for ozone depletion, and freshwater ecotoxicity, and the highest value for abiotic resource depletion. The analysis highlight that the relative environmental impact of producing the three flow battery technologies varies with different system designs and materials selection choices. For example, harmonization of the battery system boundary led to freshwater eutrophication and freshwater ecotoxicity values for vanadium redox flow batteries lower than the values for zinc-bromine flow batteries. Regarding alternative material use strategies, we conclude that vanadium redox flow batteries exhibit the lowest potential in four of the eight impact categories including global warming potential at 61 kg CO_2 eq/kWh. In zinc-bromine flow batteries, the titanium-based bipolar plate contributes higher environmental impact compared to carbon-based materials, and the polymer resins used in all-iron flow batteries could be replaced with material with lower potential for ecotoxicity. Overall, the analysis reveals the sources of potential environmental impact, due to the production of flow battery materials, components and systems. The findings from this study are urgently needed before these batteries become widely deployed in the renewable energy sector. Furthermore, our results indicate that materials options change the relative environmental impact of producing the three flow batteries and provide the potential to significantly reduce the environmental impact associated with flow battery production and deployment.

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1. Introduction

Reducing dependency on fossil fuels by introducing renewable energy such as wind and solar is fundamental to achieving climate mitigation goals (Chu and Majumdar, 2012; Sáez-Martínez et al., 2016). For example, the State of California expects to mitigate climate change through a comprehensive policy-driven initiative that requires 100% conversion of the electricity supply grid to low-carbon sources by the year 2045 with the goal to achieve an 80% decrease in economy-wide greenhouse gas (GHG) emissions by the year 2050 compared to 1990 levels (CA Senate Bill No.32, 2016; CA Senate Bill No.100, 2018). To maximize the utility and increase the penetration of renewable energy, utility-scale energy storage is required. In recent years, several advanced energy storage technologies have been developed with battery storage systems seen as one of the most researched and successfully commercialized (Liu et al., 2018; Luo et al., 2015; Mehrjerdi and Hemmati, 2019). Among the various types of battery storage systems, flow batteries represent a promising technology for stationary energy storage due to scalability and flexibility, separation of power and energy, and long durability and considerable safety in battery management (Alotto et al., 2014; Leung et al., 2012; Wang et al., 2013).

As an emerging battery storage technology, several different types of flow batteries with different redox reactions have been developed for industrial applications (Noack et al., 2015; Park et al., 2017; Ulaganathan et al., 2016). With extensive research carried out in recent years, several studies have explored flow batteries with higher performance and novel structural design (Davies and Tummino, 2018; Yin et al., 2014; Yuan et al., 2016). Further, studies focused on the cost perspective have explored the economic feasibility of flow battery production (Dmello et al., 2016; Ha and Gallagher, 2015; Viswanathan et al., 2014) In contrast, little to no assessment of the environmental impact due to flow battery production has been undertaken (L'Abbate et al., 2019; Weber et al., 2018). Thus, environmental benefit associated with only the use phase of flow batteries in the electric grid could be inaccurately estimated, because detailed data on flow battery production, and corresponding environmental impact, are not available (Hiremath et al., 2015; Park et al., 2017; Schmidt et al., 2019). We know from the extensive literature that environmental impact assessment of lithium-ion battery production has been well documented (Ellingsen et al., 2014; Majeau-Bettez et al., 2011; Notter et al., 2010). These early studies established the foundation for future assessments and provided important guidance for both the design of future lithium-ion battery technologies and the evaluation of alternative chemistries (Dunn et al., 2015; Olivetti et al., 2017; Peters and Weil, 2018).

Early evaluation of novel flow battery technologies and chemistries could likewise inform better materials selection and system designs before the market becomes well-established. To fill this gap in established knowledge, the present study focuses on using life cycle assessment to evaluate the environmental impact associated with the industrial-scale production of emerging flow battery energy storage technologies and the corresponding sensitivity to materials selection decisions. As such, this study contributes to the concept of cleaner production in two key ways. First, by providing the environmental impact data necessary to inform sustainability assessments, the development and deployment of flow battery technologies in the energy grid can be guided by data-supported metrics. Second, by providing an understanding of the materials and production methods that contribute disproportionately to high environmental impact, manufacturers can identify the need for selecting alternative material sets or production pathways to improve the environmental impact profile of their technology.

2. Material and methods

The goal of this study is to understand the environmental impact associated with the production of flow batteries. We have systematically evaluated three different state-of-the-art flow battery technologies: vanadium redox flow batteries (VRFB), zinc-bromine flow batteries (ZBFB) and all-iron flow batteries (IFB). Eight impact categories are considered, and the contribution by battery component is evaluated. To more deeply evaluate the environmental impact of the materials, energy, and resources used for each component, we investigated the upstream unit processes required for battery production. Sensitivity analysis is included in an effort to inform materials selection decisions and system design.

2.1. Flow battery technologies

Flow batteries have three major components: cell stack (CS), electrolyte storage (ES), and auxiliary parts or 'balance-of-plant' (BOP) (see Fig. 1) (Chalamala et al., 2014). The cell stack determines the power rating for the system and is assembled from several single cells stacked together. The stack is supported by accessories such as current collectors, gaskets and stack shells or end plates (Cunha et al., 2015; Dinesh et al., 2018; Leung et al., 2012). A single cell usually consists of a bipolar plate, electrode, membrane and cell frame (Cunha et al., 2015; Chalamala et al., 2014; Leung et al., 2012). Liquid electrolytes, stored in tanks, determine the energy capacity of the flow battery. The balance of plant includes several peripheral components that support the operation of the battery including recirculation loops consisting of pump and pipes, a battery management system (BMS) for operational control, a power conditioning system (PCS) for current conversion, and other structural supporting accessories (Chalamala et al., 2014). The accessories used in the cell stack and peripheral components included in the balance of plant can vary for different flow batteries.

In the current study, we investigated three types of flow batteries: VRFB, ZBFB, and IFB. Their design configurations are presented in Fig. 2, and the corresponding chemical reactions are provided below.

Vanadium Redox Flow Battery (VFRB):

Cathode: $VO^{2+} + H_2O - e^- \rightleftharpoons VO_2^+ + 2H^+$

Anode: $V^{3+} + e^- \rightleftharpoons V^{2+}$

Cell: $VO^{2+} + H_2O + V^{3+} \rightleftharpoons VO_2^+ + V^{2+} + 2H^+$

Zinc-bromine Flow Battery (ZBFB):

Cathode: $2Br^- - 2e^- \rightleftharpoons Br_2$

Anode: $Zn^{2+} + 2e^- \rightleftharpoons Zn$

Cell: $2Br^- + Zn^2 \rightleftharpoons Zn + Br_2$

All-iron Flow Battery (IFB):

Cathode: $2Fe^{2+} - 2e^- \rightleftharpoons 2Fe^{3+}$

Anode: $Fe^{2+} + 2e^- \rightleftharpoons Fe$

Cell: $3Fe^{2+} \rightleftharpoons Fe + 2Fe^{3+}$

The design of VRFB can be categorized as a full-flow system in which all the reacting chemicals are dissolved in a liquid phase, while the ZBFB and IFB are hybrid systems since metal forms as a

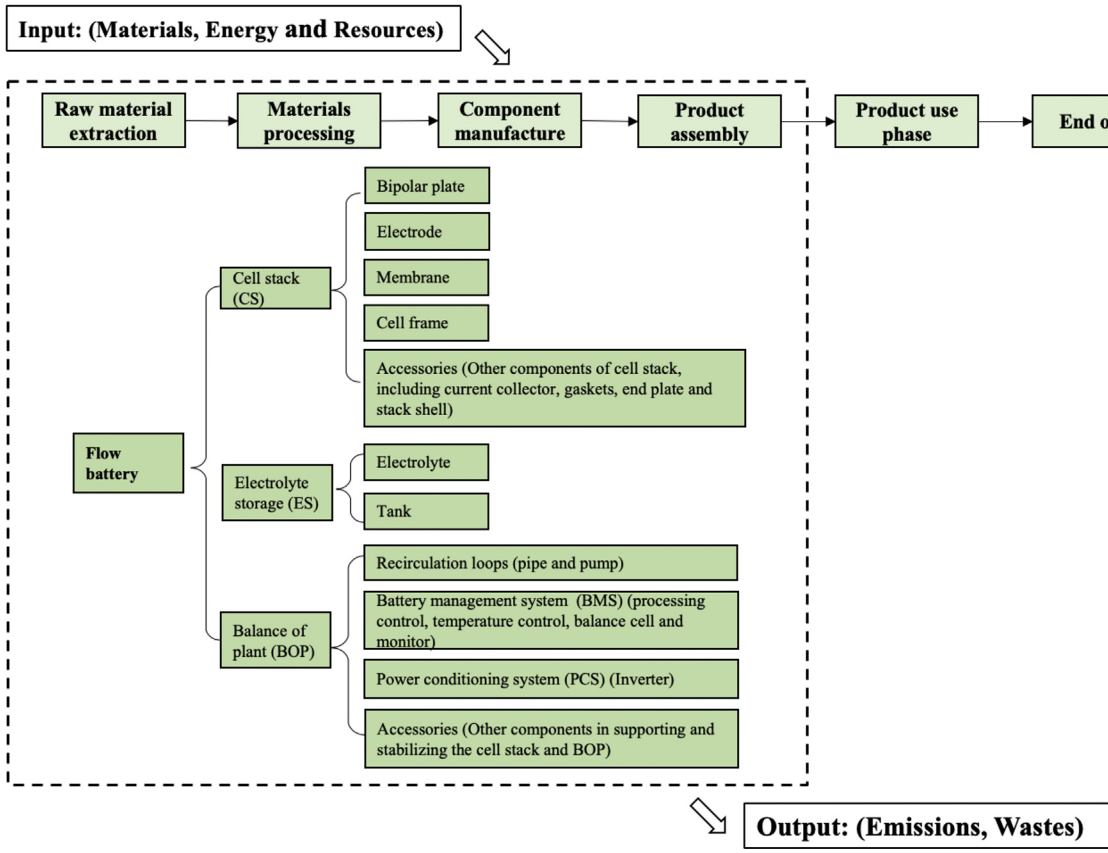

Fig. 1. The system boundary and classification of flow battery components used in this study are shown schematically. Note that the use phase and end-of-life phase are beyond the scope.

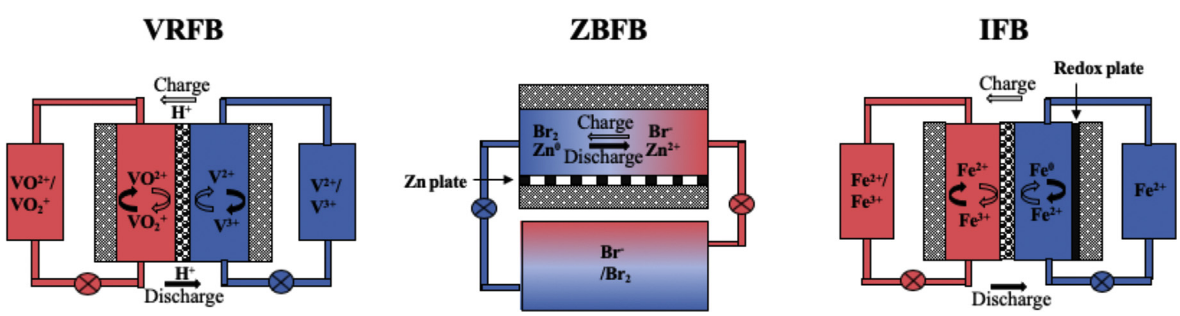

Fig. 2. The chemical reactions and system design for the three flow battery technologies are illustrated in this schematic. Flow battery types include: VRFB = vanadium redox flow battery; ZBFB = zinc-bromine flow battery; and IFB = all-iron flow battery.

solid phase deposited on the electrode surface (Chalamala et al., 2014; Leung et al., 2012). Typically, a membrane is inserted in each cell to maintain two separate flow paths, as seen in Fig. 2 for VRFB and IFB. This is not the case for ZBFB because the cell stack in this battery only requires one flow path, which avoids the use of a membrane and additional storage tanks. More specifically, as specified by the manufacturer, the bipolar plate and electrode in ZBFB is not manufactured from more traditional carbon-based materials (Park et al., 2014) but instead is produced from titanium metal. The titanium plate is processed as one integrated conductive board in ZBFB with injection molded polyethylene as the cell frame. In contrast, for VRFB and IFB, the bipolar plate, electrode, membrane and cell frame are compacted together as separate layers in VRFB and IFB with a traditional bipolar plate design. Table 1 provides further details on the battery components and the materials from which they are made.

2.2. System description and life cycle inventory

The goal of this study is to conduct a detailed environmental impact assessment of flow battery production and to evaluate the sensitivity of the results to materials selection and system design choices. The battery production phase is comprised of raw materials extraction, materials processing, component manufacturing, and product assembly, as shown in Fig. 1. As this study focuses only on battery production, the battery use and end-of-life phases are not within the scope of the study. Supply chain transportation is also excluded from the scope due to the high level of uncertainty associated with the materials and components, which can be produced in different parts of the world. The functional unit for the

Table 1
The component breakdown and materials used in the three flow batteries.

Component	Vanadium redoxflow battery	Zinc-bromine flow battery	All-iron flow battery
Cell stack			
Bipolar plate	Graphite Polyethylene	Titanium Polyethylene	Graphite Vinyl ester
Electrode	Carbon fiber felt	/	Carbon fiber felt
Membrane	Nafion®	/	Polyethylene
Cell frame	Glass fiber Polypropylene	Polyethylene	Glass fiber reinforced polymer
Accessories			
Current collector	Copper	Titanium	Aluminum
Gasket		Polyethylene	Ethylene propylene diene
Supporting shell and frame	Steel Chlorinated polyvinyl chloride	Steel Polyethylene	Steel
Electrolyte storage			
Electrolyte	Hydrochloric acid Sulfuric acid Vanadium pentoxide Water	Zinc bromide Bromide Water	Ferrous chloride Potassium chloride Manganese chloride Water
Tank	Polyethylene	Polyethylene Steel	Isophthalic polyester
Balance of plant			
Recirculation loop			
Pump	/	/	/
Pipe	Polyethylene	Polyethylene	Polyvinyl chloride
Battery management system			
Process control system	Electronics	Electronics	Electronics Carbon fiber felt
Thermal management system	Fan Heat exchanger	Fan Heat exchanger	Fan
Power conditioning system	Inverter	Inverter	Inverter
Accessories	Titanium Polyvinylidene fluoride	Polyethylene Steel Titanium Aluminum	/

production phase is one kWh energy capacity stored in one battery package.

The materials and processing methods associated with each component in the three flow batteries, which were established on the basis of primary inventory data collected from battery manufacturers, are shown in Figs. A 1 – A 3. These components are further aggregated into the three subsystems mentioned above: cell stack (CS), electrolyte storage (ES) and balance of plant (BOP). The Ecoinvent database provided the reference life cycle inventory (LCI) datasets for materials used (Wernet et al., 2016), including primary extraction (mining), refining, and fabrication. In cases where reference life cycle inventory datasets were not available in Ecoinvent, we relied on published peer-reviewed literature for materials production such as vanadium pentoxide (Chen et al., 2015; Jungbluth and Eggenberger, 2018; Weber et al., 2018), carbon fiber felt (Minke et al., 2017; Romaniw, 2013) and battery membrane materials (Mohammadi and Skyllas-Kazacos, 1995). We used 'global' (GLO) or 'rest of world' (RoW) data in Ecoinvent in the absence of regional or country-specific data. A complete constitution of the life cycle inventory is provided in detail in Section S1 of the Supplementary Material.

2.3. Impact assessment

We selected eight midpoint environmental impact categories for characterizing the environmental impact of producing the three flow battery technologies, using SimaPro software (Simapro, 2017). Global warming potential (GWP), ozone depletion potential (ODP), fine particulate matter (PM), acidification potential (AP) and freshwater eutrophication potential (EP) are calculated using the ReCiPe midpoint 2016 (ReCiPe) method (Huijbregts et al., 2017). Freshwater ecotoxicity potential is based on the USETox model (potentially affected fraction of species (PAF)) using the 'recommended' characterization factors (Hauschild et al., 2008; Henderson et al., 2011; Rosenbaum et al., 2008), the characterization factors for abiotic resource depletion potential are determined using the CML-IA method (Guineé, 2001), and fossil fuel energy use is calculated using the cumulative energy demand included in the Ecoinvent database (Frischknecht et al., 2007). To fully account for the environmental impact of the materials, energy, and resources used for each component, we also investigated the unit processes in Ecoinvent representing the upstream production activities. The contributions of the unit processes are distributed into five categories: 'materials production', 'energy consumption', 'resource use', 'waste treatment', and 'other related'. To avoid an excessive number of unit processes in the contribution analysis, those unit processes contributing less than 1% to the total impact score are not included in the contribution analysis.

2.4. Uncertain issues and sensitivity analysis

While primary data for battery manufacturing is preferable over modeled data, the collection of primary data revealed variability among manufacturers. Specifically, the level of detail in the data was not consistent from manufacturer to manufacturer, especially for the accessories and balance of plant, which provided us with the opportunity to explore the impact of component selection on environmental impact results. Also, with the goal to evaluate the impact of materials selection decisions and potentially guide future flow battery design, the production methods for three select materials are explored in greater depth. Thus, a series of scenarios are considered here to quantify these uncertainties.

To harmonize the different datasets submitted by the manufacturers, we adopted a harmonized battery system boundary with comparable sets of components, and we applied a two-step modification to the life cycle inventory (see details in Supplementary Material Section S2). For the first step, the accessories associated with the cell stack and balance of plant are subtracted from the system. These components are influenced mainly by the design choices of particular flow battery units and are not necessarily core attributes of a given battery technology. Secondly, the life cycle inventory for battery management system and power conditioning system in the balance of plant are harmonized for the three flow batteries to make sure the devices considered for comparison are equivalent. More specifically, these are modified to evaluate production of devices, including electronic systems, not just materials, as was provided by the manufacturer of ZBFB. See Supplementary Material Section S2 and Table S33 for details. Hereafter, we refer to this as the 'harmonized system boundary.' Since it is a more harmonized boundary, we use it as the basis for the materials selection based scenario analyses described below.

In an effort to look more deeply into the effect of materials selection and processing choices on the comparative environmental impact of flow battery production, various core materials, specifically vanadium pentoxide, Nafion®, and carbon fiber felt, are explored. Three sets of scenarios are applied, as outlined in Table 2 (additional details are provided in Section S3 of the Supplementary Material). For vanadium pentoxide production, different production processes are considered, as well as different data sources and different allocation methods. For membrane materials, an alternative material, Daramic®, is evaluated; and for the carbon fiber felt, different precursors are considered as well as different data sources. These three materials were selected for the scenario analysis because alternative production methods and/or materials were readily identifiable but not yet recorded in standardized life cycle inventory databases.

3. Results and discussion

With the battery technology and assessment framework specified, we begin with a baseline environmental impact assessment of flow battery production using the original data provided by manufacturers. This analysis is followed by the analysis of production impacts for the harmonized system boundary, and then subsequently by the sensitivity analysis relative to options for vanadium pentoxide production, membrane materials, and carbon fiber felt production methods.

3.1. Baseline environmental impact assessment

The results of the baseline environmental impact assessment for the production of the three flow batteries, distributed by component and by unit process, are presented in Fig. 3 *and 4,* respectively. The IFB system exhibits the lowest impact scores in six of the eight impact categories, except ozone depletion potential and freshwater ecotoxicity potential. The ZBFB system has the lowest impact scores for ozone depletion potential and freshwater ecotoxicity potential, but the highest for abiotic resource depletion potential. The VRFB system exhibits the highest impact scores for global warming potential, ozone depletion potential, fine particulate matter, acidification potential, freshwater eutrophication potential, and cumulative energy demand. As shown in Fig. 3, the distribution of impacts contributed by production of individual components varies among the three flow battery technologies, but consistent major contributors are the cell stack (CS) or the electrolyte storage (ES) components, except for the impact categories of freshwater eutrophication potential and abiotic resource depletion potential, which are driven by the balance of plant. The results in Fig. 4 help to clarify the reason for these distributions, since the environmental impact is generally driven by the materials and production processes associated with these components. In Fig. 4, the boundary between the gray and colored portions of the bar indicates the 1% cut-off threshold and the corresponding pie charts show the detailed distribution for unit processes included in the portion above the 1% cut-off threshold. Select materials that are major contributors to certain impact categories are separated out as independent sub-categories in the pie charts to highlight their contributions to the total. For example, production of the vanadium pentoxide (V_2O_5) used in VRFB triggers high impacts for global warming potential, acidification potential, fine particulate matter, and cumulative energy demand, and the production of the tetrafluoroethylene used as a processing material for the Nafion® membrane triggers high impact for ozone depletion potential (Banerjee and Curtin, 2004; Sayler, 2012; Weber et al., 2018). For ZBFB, production of the titanium used in the bipolar plate contributes to global warming potential, ozone depletion potential,

Table 2
Scenarios for evaluating uncertainty on select materials in the flow batteries.

Scenarios	Description
Vanadium pentoxide	
Scenario A1	The vanadium pentoxide production from blast furnace crude steel making process based on manufacturing data from PAN. Steel, Sichuan, China (Chen et al., 2015).
Scenario A2	The vanadium pentoxide production from the electric arc furnace steelmaking process based on literature data (Weber et al., 2018).
Scenario A2*	The vanadium pentoxide production plus the allocated impact from the electric arc furnace steelmaking process based on literature data. The steel manufacturing modeling is modified from Ecoinvent and monetary value is used for allocation (Weber et al., 2018).
Scenario A3	The vanadium pentoxide production based on manufacturing data from granulate generated in power plant burning crude oil (Jungbluth and Eggenberger, 2018).
Scenario A4	The vanadium pentoxide production based on stoichiometric calculation from fly ash generated in power plant burning crude oil (Jungbluth and Eggenberger, 2018).
Membrane	
Scenario B1	The Nafion® membrane production based on literature data, the manufacturing modeling is modified from Ecoinvent (Weber et al., 2018).
Scenario B2	The Daramic® membrane production based on literature data, the manufacturing modeling is modified from Ecoinvent (Mohammadi and Skyllas-Kazacos, 1995).
Carbon fiber felt	
Scenario C1	The carbon fiber felt production using polyacrylonitrile (PAN) as a precursor based on modeling data (Romaniw, 2013).
Scenario C2	The carbon fiber felt production using polyacrylonitrile (PAN) as a precursor based on manufacturing data from SGL Carbon SE (Minke et al., 2017).
Scenario C3	The carbon fiber felt production using Rayon as a precursor based on manufacturing data from SGL Carbon SE (Minke et al., 2017).

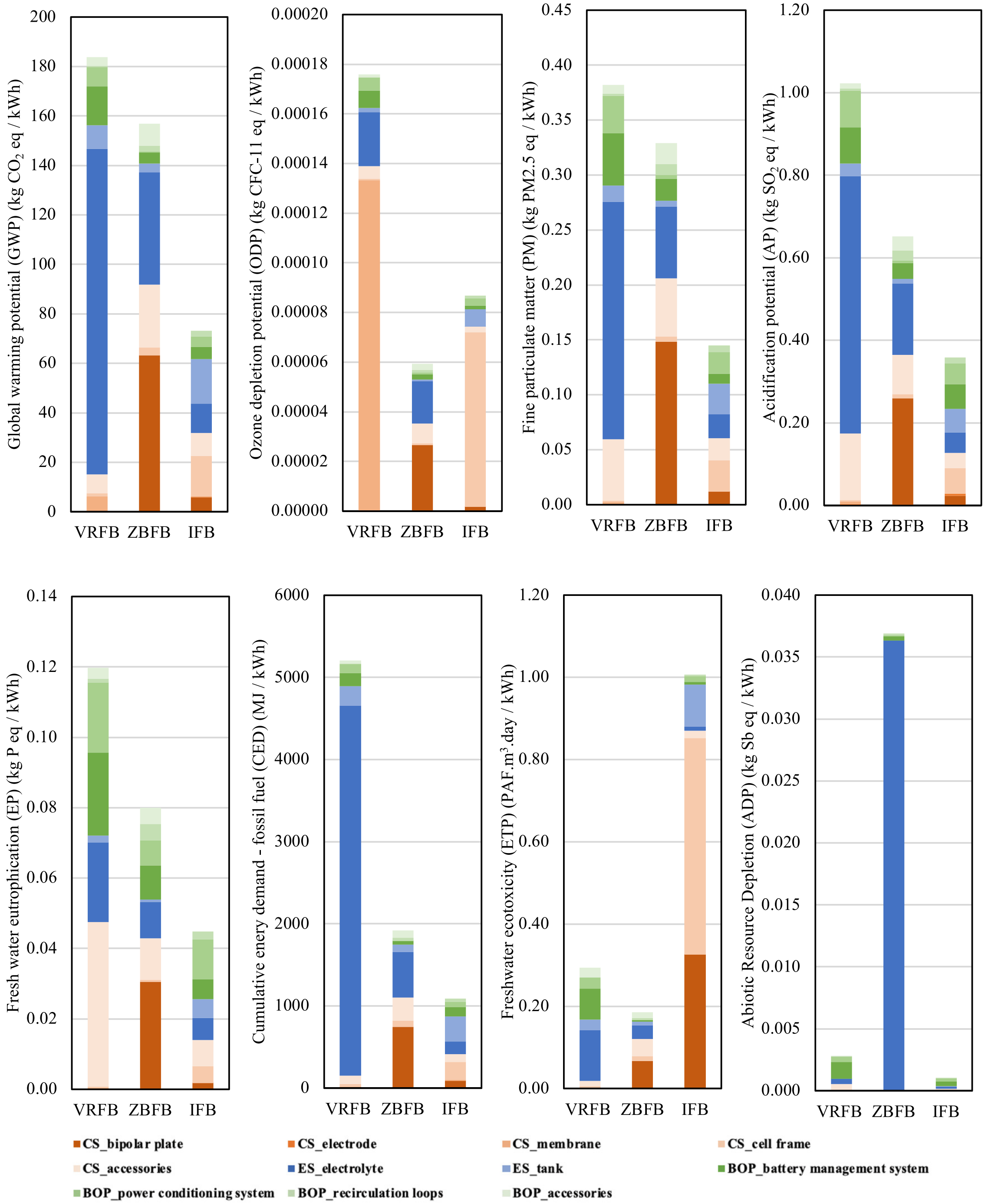

Fig. 3. The potential environmental impact of flow battery production is shown, as distributed by battery component. Flow battery types include: VRFB = vanadium redox flow battery; ZBFB = zinc-bromine flow battery; and IFB = all-iron flow battery. Flow battery components include: cell stack (CS), electrolyte storage (ES) and balance of plant (BOP).

acidification potential, fine particulate matter, cumulative energy demand, and freshwater ecotoxicity potential; and production of the bromine used as a core chemical in the electrolyte dominates the high abiotic resource depletion potential. For IFB, the production of resin used in the glass fiber reinforced polymer cell frame leads to the high freshwater ecotoxicity potential. Considering each impact category individually, the results show a few trends. For instance, ozone depletion potential and abiotic resource depletion potential are triggered primarily by raw materials production, whereas freshwater eutrophication potential is triggered primarily by waste treatment. Comparing the triggers for the different battery chemistries, for the global warming potential and acidification potential impact categories, the primary triggers for VRFB and IFB are unit processes associated with materials production, while for ZBFB energy consumption during production is more important. For fine particulate matter, energy consumption and resource use contribute more than.

We also highlight findings for global warming potential, freshwater ecotoxicity potential, and abiotic resource depletion potential. The high total impact of global warming potential for VRFB is

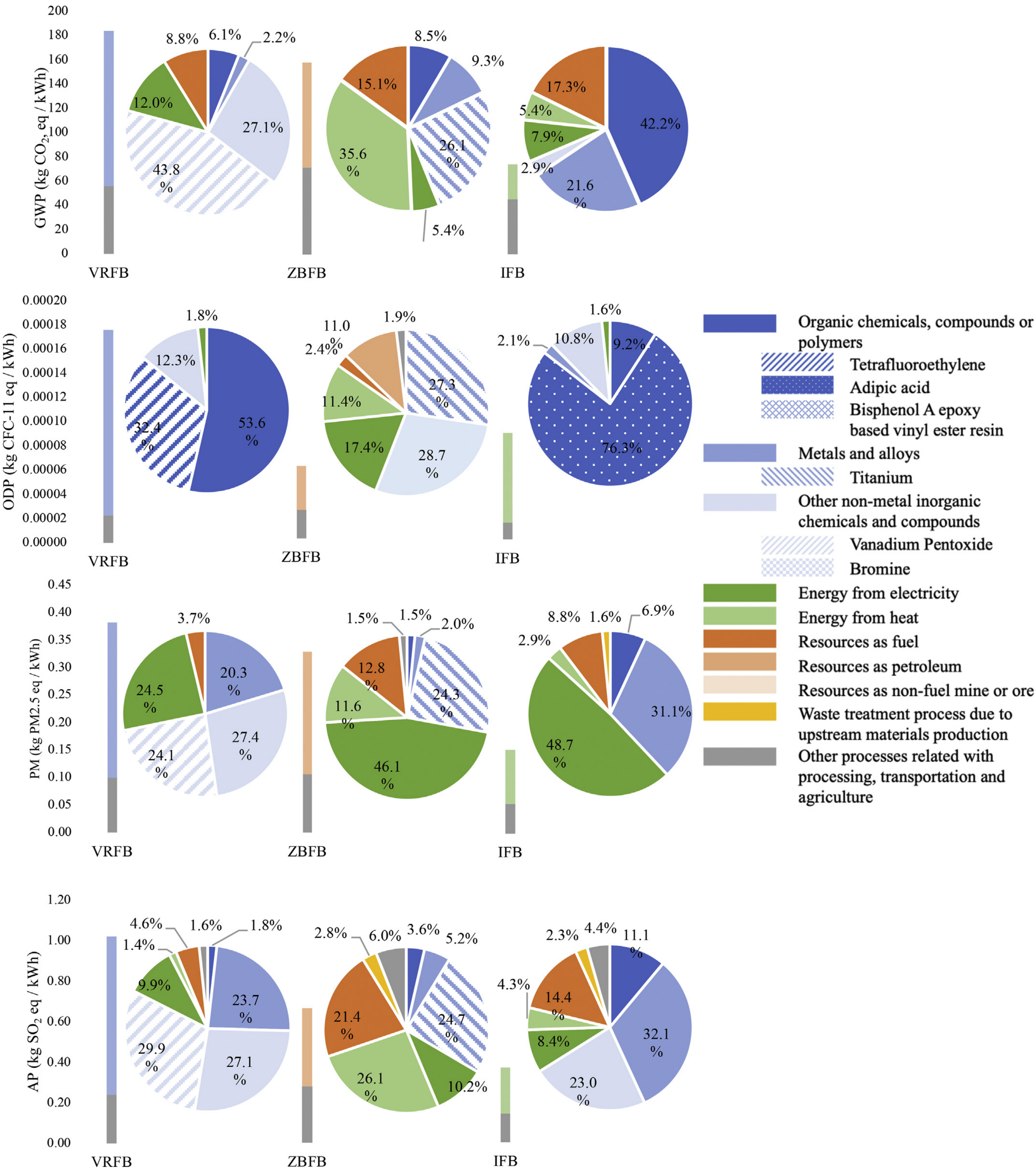

Fig. 4. The contributions to the eight impact categories are shown, distributed by materials use, energy consumption, resource use, waste treatment, and other processes, and based on the analysis of unit processes adopting a 1% cut-off value of total contribution for production of the three flow batteries, with tetrafluoroethylene, adipic acid, bisphenol A epoxy-based vinyl ester resins, titanium, vanadium pentoxide, and bromine, highlighted separately as major triggers for at least one or more impact categories.

primarily due to production of the electrolyte, which accounts for 72% of the total score. For ZBFB, production of the bipolar plate is the highest contributor at 40%, followed by production of the electrolyte (29%). For the IFB, the impact is largely due to production of the storage tank (39%) and the cell frame (22%). Looking closely at the unit process analysis for global warming potential, for

VRFB and ZBFB, the products derived from metallurgical processes contribute more to the higher global warming potential than do other materials used in the flow battery system. For example, the high global warming potential of electrolyte production in VRFB is due to the use of V_2O_5, which is a by-product of steel manufacturing (Mohammadi and Skyllas-Kazacos, 1995; Moskalyk and Alfantazi,

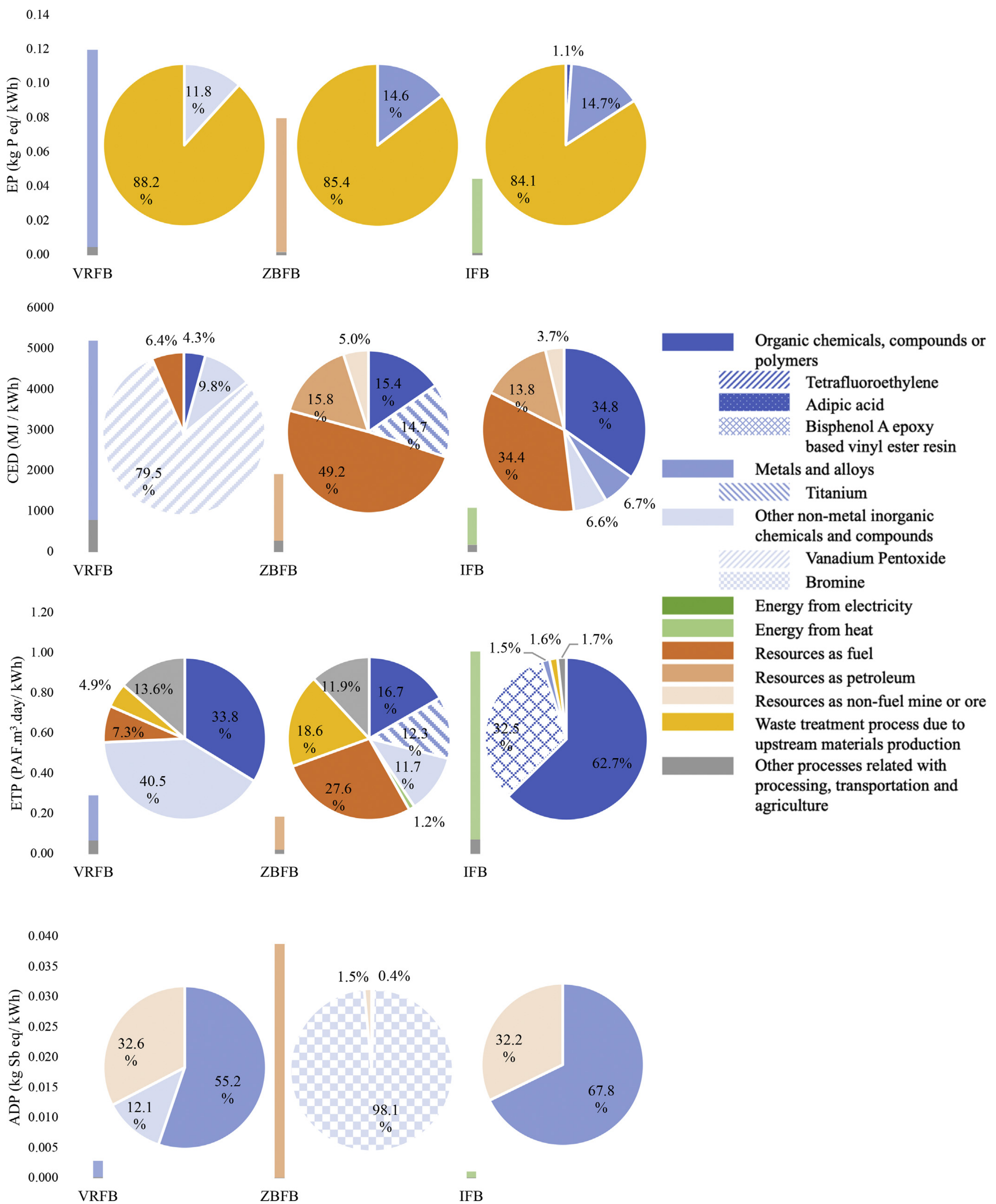

Fig. 4. (*continued*).

2003). The bipolar plate for ZBFB contains titanium, the production of which generates a higher global warming potential than that of the graphite-based materials used in the other two flow batteries. For IFB, production of several organic substances used as processing materials for the storage tank and cell frame correspond to high global warming potential scores causing these two components to be the highest contributors to global warming potential. Results on fine particulate matter and acidification potential follow similar trends.

For freshwater ecotoxicity potential, the IFB system has the highest impact score due to production of the cell frame (52%) and the bipolar plate (32%), and the unit process analysis from Fig. 4 indicates that this is primarily due to the production of organic compounds especially the bisphenol-A epoxy-based vinyl ester resin. In contrast, for VRFB and ZBFB, their bipolar plates are made of graphite and titanium, respectively, and the cell frames are made of polyethylene - both of which do not require production of materials with high freshwater ecotoxicity potential. Instead, the relatively low freshwater ecotoxicity potential value for VRFB is caused primarily by the production of non-metal inorganic materials. For ZBFB, which has the lowest freshwater ecotoxicity potential value, the titanium bipolar plate is the component generating the highest freshwater ecotoxicity potential due to the production of titanium. Interestingly, the ZBFB system has a significantly larger abiotic resource depletion potential than VRFB and IFB. From the results in Fig. 4 we find the production of bromine contributes to a much higher resource depletion potential than any of the other materials. The remainder is then due to the production of metals such as copper and gold contained in electronic devices, which is consistent with the results for VRFB and IFB.

3.2. Harmonized battery system boundary environmental impact assessment

The modifications to the battery system boundary are intended to harmonize the different datasets provided by the battery manufacturers. The previously defined battery system boundary for the baseline results was modified to a harmonized battery system by eliminating the accessories and modifying the battery management system and power conditioning system components. Further details are provided in Section 2.4. The results from the harmonized battery system boundary analysis are compared to the baseline results in Fig. 5 (detailed distributions by component, which are analogous to those in Fig. 3, are presented in Fig. B1 in Appendix B). Due to the nature of this harmonization, the impact values for VRFB and IFB are reduced in all cases because the system boundary has been curtailed for these two battery systems. The subtraction of the accessories has the greatest effect on these impact reductions, compared to the effect of modifying the balance of plant components, suggesting that these components could perhaps be better designed to minimize the impact caused by the production of these accessories. The most significant effect of subtracting the accessories is seen for the freshwater eutrophication potential value for VRFB; fine particulate matter and acidification potential values for VRFB are also noticeably changed. The changes for IFB are consistently small.

For ZBFB, the potential environmental impacts are mixed. Subtracting the accessories reduces the impact, especially for global warming potential, fine particulate matter, acidification potential, and freshwater eutrophication potential. However, the modification of the balance of plant leads to increased impact values for all impact categories, because the battery system boundary has been expanded in this case to include production of electronic devices, not just materials, suggesting that the role of the electronic devices should not be neglected for these battery systems. When the two modifications are combined, the results for ZBFB lead to net increases in ozone depletion potential, freshwater eutrophication potential, freshwater ecotoxicity potential and abiotic resource depletion potential, and net decreases in the other categories (global warming potential, fine particulate matter, and acidification potential). Importantly, this harmonization lead to changes in the relative rankings of the three flow battery technologies for a few of the impact categories: ZBFB is now the worst for freshwater eutrophication potential, second for freshwater ecotoxicity potential and essentially equal to VRFB for fine particulate matter; which highlights the importance of this sensitivity analysis in comparing the production of the three flow battery systems. The exclusion of the accessories and the modifications to the balance of plant represent a battery system boundary that highlights the core functional components in the flow batteries, therefore, we used the results after this harmonization for the remaining sensitivity analyses (noted by the yellow bars in Fig. 5 and detailed in Fig. B1 in Appendix B).

3.3. Sensitivity analysis on materials selection and processing

In this section, the relative environmental impact associated with production of different materials selection options was investigated in an effort to highlight that the use of alternative materials may reduce overall environmental impact of flow battery production.

3.3.1. Vanadium pentoxide

The results shown in Figs. 3–5, support the conclusion that V_2O_5 production plays an important role in several impact categories including global warming potential, fine particulate matter, acidification potential and especially cumulative energy demand for the VRFB system. Of the four processing routes investigated in this scenario analysis, the V_2O_5 produced in Scenarios A1 and A2 (and A2*) is a by-product of steel production, but for Scenarios A3 and A4, it is produced from crude oil burning residues. Fig. 6 presents the environmental impact results for V_2O_5 production normalized to per kg for each of the five scenarios listed in Table 2. Significant variations are observed. In general, the V_2O_5 produced from crude oil corresponds to less environmental impact than the V_2O_5 produced from steel production. Also, the differences between the two crude oil scenarios are relatively small, whereas there are substantial differences seen for the various scenarios based on steel production. Scenario A1 is based on actual production data, whereas Scenario A2 uses simulated data, and the process conditions are different. The large differences in global warming potential and cumulative energy demand values for these two scenarios correspond to the different production methods, as the steel in Scenario A1 is made using a blast furnace which consumes large amounts of hard coals (see Table S14 in SI section S1), while in Scenario A2, the steel is made using an electric arc furnace. The higher fine particulate matter and freshwater eutrophication potential values for Scenario A2 are due to the emission of sulfur dioxide calculated based on the stoichiometric calculation, while for Scenario A1, there is a desulphurization process reported as a pretreatment which reduces the sulfur dioxide emissions. Also, comparing the results of Scenario A2 and Scenario A2*, the allocated impacts from the steel production contribute to a rather high impact score, especially for global warming potential, ozone depletion potential, freshwater eutrophication potential, and cumulative energy demand. Overall, the results for Scenario A2* are the highest, except for the impact category of cumulative energy demand, for which Scenario A1 is highest. These wide variations in estimated potential environmental impact associated with V_2O_5 production are influenced by multiple factors such as extraction

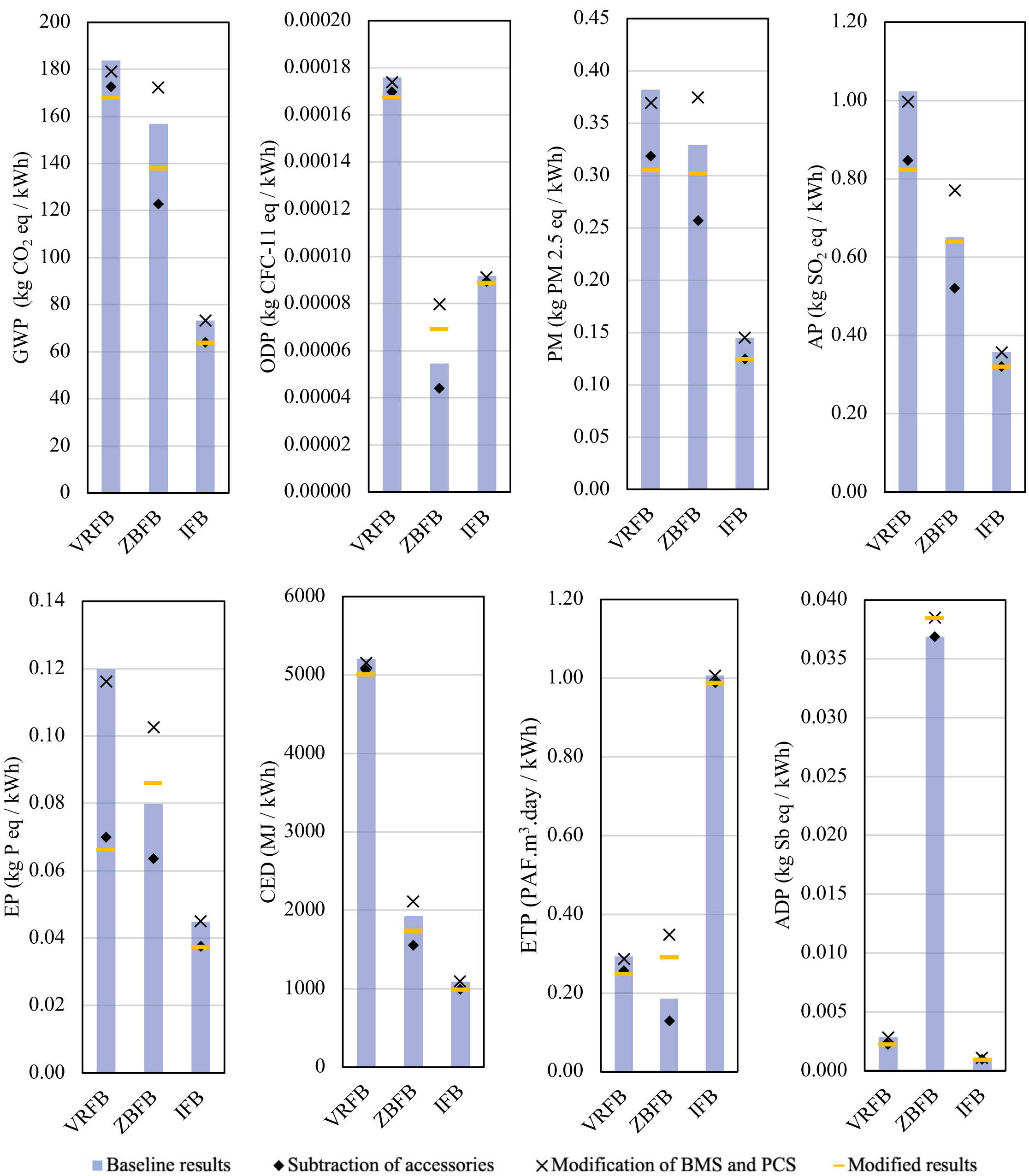

Fig. 5. The change in environmental impact results are shown for production of the three flow batteries given the modifications to the battery system boundary to harmonize across the three battery types, which includes subtracting the accessories and modifying the battery management system and power conditioning system components.

sources, processing routes and allocation rules. Given the variations described here, there is clearly a need for a unified and systematic life cycle inventory data set for V_2O_5 production.

The effect of these changes in V_2O_5 production not only affect the environmental impact categories directly, as described above, but they also translate to corresponding effects on the environmental impact associated with producing the VRFB flow battery system, as shown in Fig. 7; the earlier results for ZBFB and IFB (taken from Fig. 5) are included for comparison. For many of the impact categories, the different scenarios lead to changes in the relative ranking among the three flow battery technologies. For instance, if V_2O_5 produced from crude oil burning residue is assumed (Scenarios A3 or A4), production of VRFB no longer corresponds to the highest global warming potential, fine particulate matter, acidification potential, and cumulative energy demand values, and actually ranks lowest for global warming potential and cumulative energy demand under Scenario A3. If Scenario A2 is used, production of VRFB no longer corresponds to the highest values for global warming potential and cumulative energy demand, but presents increased values for fine particulate matter and acidification potential. For the impact categories of ozone depletion and abiotic resource depletion potential, however, the flow battery rankings are independent of the scenarios. When adopting Scenario A2*, which is the only scenario that considers the allocated

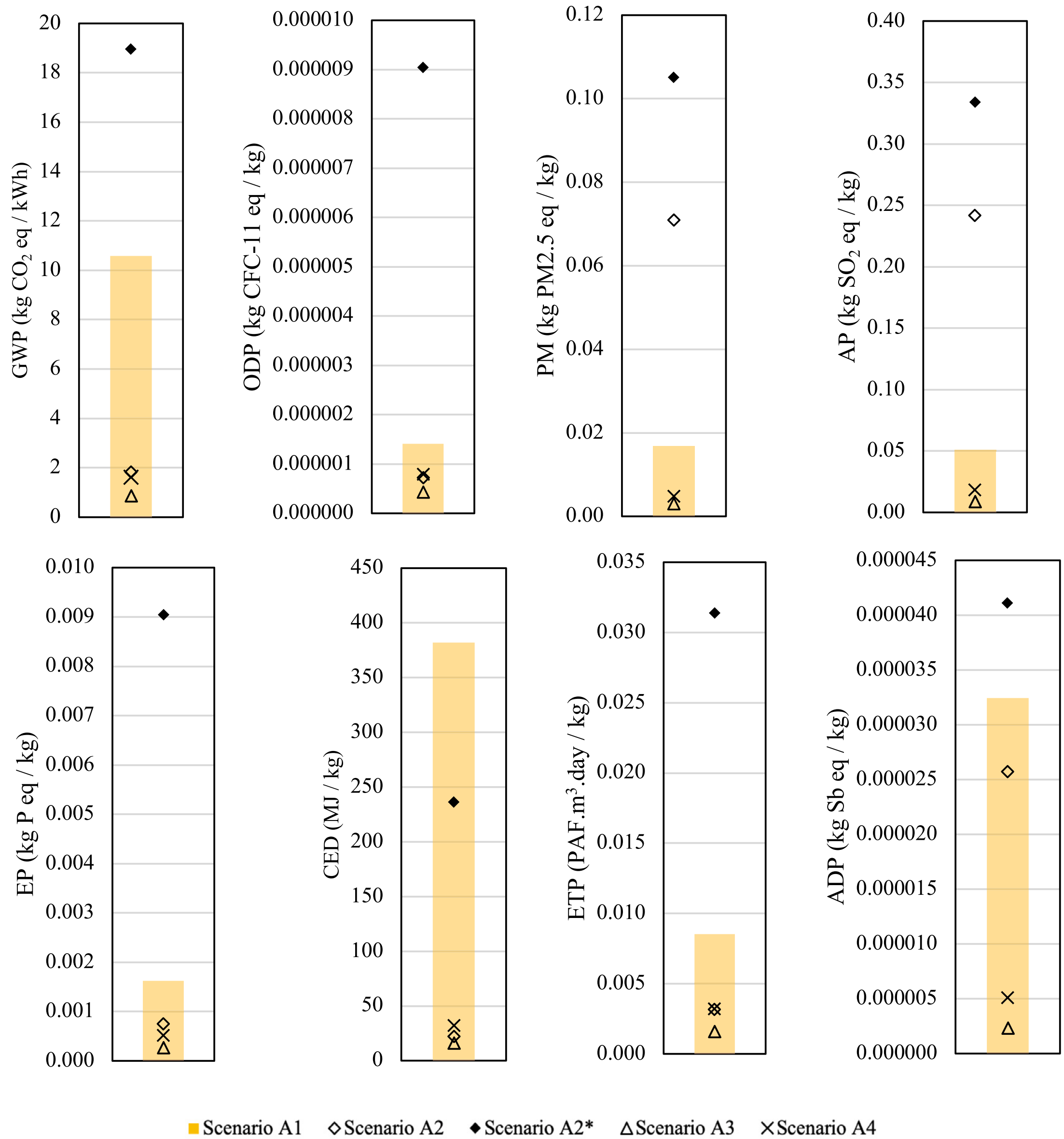

Fig. 6. Variations in environmental impact per kg of vanadium pentoxide production are shown, assuming different scenarios for extraction sources and processing routes.

emissions from the steel production, the impact values increase for global warming potential, ozone depletion potential, fine particulate matter, acidification potential, freshwater eutrophication potential, and freshwater ecotoxicity potential, but decrease for cumulative energy demand; these changes do not, however, result in changes in rank.

3.3.2. Membrane materials

The second scenario analysis focuses on the membrane materials used for the flow batteries. Although Nafion® is commonly used as the membrane material in flow batteries, various alternative membrane materials have also been developed for battery use. As described in a recent publication by Shi et al. (2019), newly developed membrane materials have been tested with higher ion conductivity and stability that could improve the battery performance, however, the associated production data are not yet complete for a comprehensive impact assessment. Nafion®, a sulfonated fluorocarbon polymer, is currently the most widely applied membrane material in VRFB (Prifti et al., 2012; Schwenzer et al., 2011). From the results shown in Fig. 3, the major contributor to ozone depletion potential for VRFB production is the Nafion® membrane, which corresponds to 76% of the total ozone depletion potential. A recent life cycle assessment study on VRFB compared the Nafion® membrane with sPEEK, another sulfonated membrane, the results of which indicate that production of Nafion® would trigger a much higher environmental impact than sPEEK (Weber et al., 2018). Here, with Scenario B2, we consider production of a non-sulfonated alkane-based alternative membrane material, Daramic®, the data for which are derived from a literature review (see details provided in Section S3 of Supplementary Material). The results presented in Fig. C1 (in Appendix C) show that the environmental impact associated with production of a Nafion®

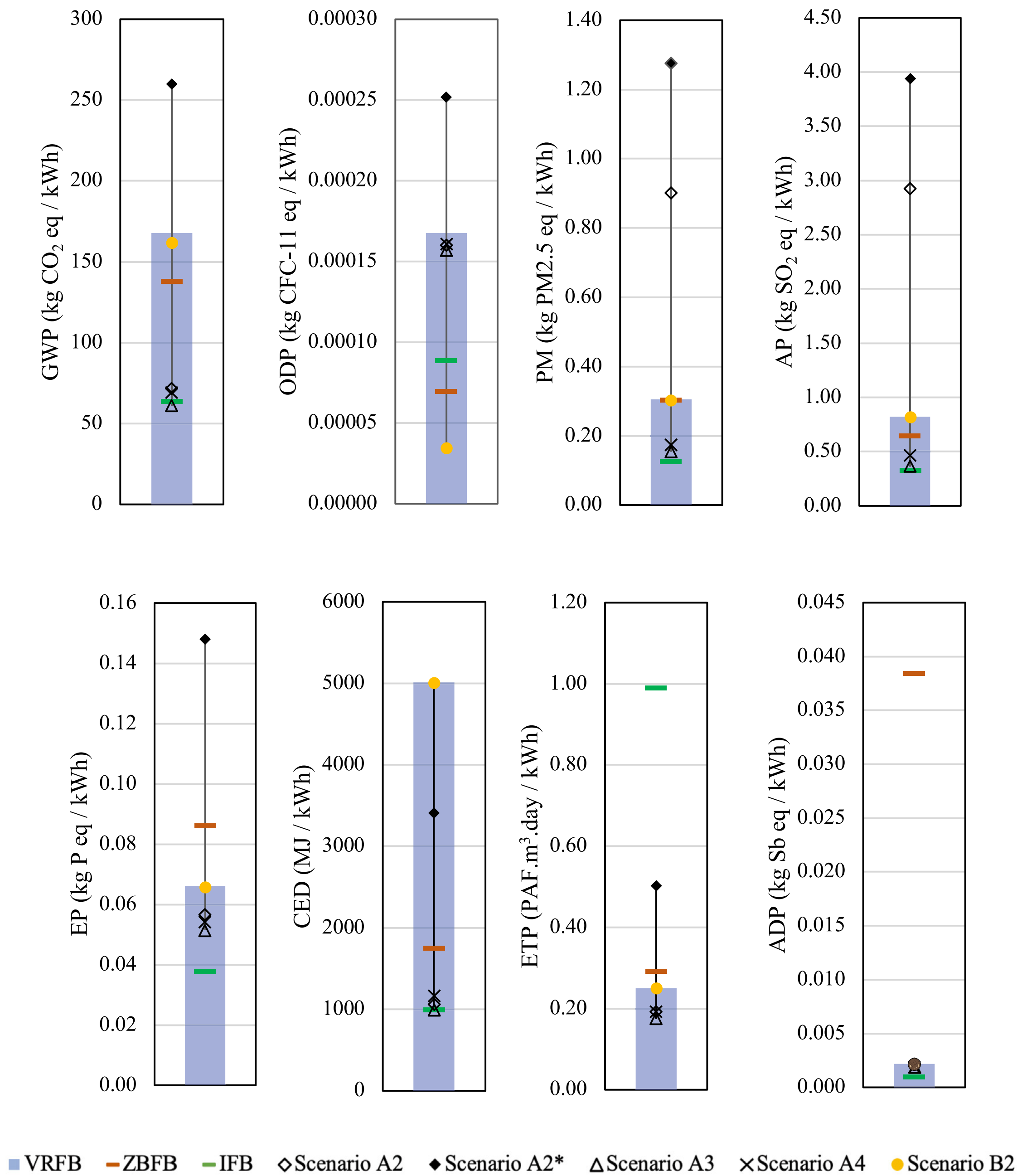

Fig. 7. The environmental impact results for flow battery production are compared, given the various scenarios for vanadium pentoxide produced from electric arc furnace (Scenario A2 and Scenarios A2*) and crude oil (Scenarios A3 and A4). The results corresponding to production of alternative membrane materials are also investigated (Scenario B2).

membrane is substantially larger than that for a Daramic® membrane. Whereas the Daramic® membrane consists primarily of polyethylene and silica, the higher impact for Nafion® are caused by the complex synthesis processes including fluorination and sulfonation with the use of several high impact polymers such as tetrafluoroethylene (TEF) (Banerjee and Curtin, 2004; Sayler, 2012; Weber et al., 2018). The results for Scenario B2 are translated into impacts values for VRFB production, as shown by the yellow circles in Fig. 7. Notably, the ozone depletion potential value is significantly reduced, to the point that VRFB is now ranked lowest for this impact category.

3.3.3. Carbon fiber felt

The use of carbon fiber felt as electrodes in flow batteries is becoming increasingly popular due to good electrical conductivity, light weight and high electrochemical stability (Meng et al., 2017). Although the amount of carbon fiber felt used in a flow battery system is small and does not significantly influence the total environmental impact, the relatively high energy consumption for carbon fiber felt production is considered here as the high-temperature pyrolysis may trigger high environmental impact (Minke et al., 2017; Romaniw, 2013). In our battery systems, the carbon fiber felt is used as electrodes for VRFB and IFB. The scenario analysis considers three different carbon fiber felt production methods (see Table 2, as well as more detailed information provided in Supplementary Material Section S4). The results per kg felt, shown in Fig. C2 (in Appendix C), indicate that production of the rayon-based carbon felt results in higher impact than that for the PAN-based carbon felt. However, there are still uncertainties associated with the PAN-based carbon felt, especially for fine particulate matter, acidification potential and freshwater eutrophication potential, as seen when comparing Scenarios C1 and C2, which are based on modeling data and manufacturing data, respectively. Despite the significant variations seen in Fig. C2 (in Appendix C), when translated to the impact assessment for producing the flow battery systems, as shown in Fig. C3 (in Appendix C), the effect becomes negligible due to the small overall impact of the carbon fiber felt electrodes. In addition, it is noted that another electrode material - graphite felt, can be prepared from carbon fiber felt with one more step − graphitization (Castañeda et al., 2017). However, the impact of graphite felt production is not considered because this material was not specified by the manufacturers that provided data for this assessment, and choosing graphite felt instead of carbon felt is unlikely to significantly change the total impact results given the small amount and minor impact of carbon fiber felt used in the battery system.

4. Conclusions

The investigation into the production of three flow batteries provides important guidance on potential environmental impact associated with battery component manufacturing, upstream production activities, battery system designs, and materials selection choices, given state-of-the-art commercial technologies. In particular, the findings and conclusions of this study are as follows: While the environmental impact clearly depends on the flow battery chemistry, especially the selection of electrolyte and cell stack materials, it also depends on the balance of plant design and production methods. Furthermore, for VRFB, because the vanadium pentoxide is the primary driver for five impact categories, alternative production routes can significantly reduce the potential impact. Also, the high ozone depletion associated with production of the Nafion® membrane can be avoided if alternative materials such as Daramic® can be used while achieving equivalent performance. In ZBFB, production of the titanium-based bipolar plate corresponds to higher environmental impact compared to production of carbon-based materials, and the polymer resins used in IFB could potentially be replaced with lower ecotoxicity materials. The results of this study also highlight that some of the environmental impact is associated with materials selection and production options that could be difficult to modify. For example, the bromine used in ZBFB electrolytes triggers a much higher abiotic resource depletion value compared to the electrolytes used in VRFB and IFB. Also, although the integrated titanium bipolar plate installed in ZBFB avoids the use of additional membranes and electrodes, which avoids potential impacts such as the high ozone depletion triggered by the Nafion® in the VRFB, the processes used for titanium production lead to higher values for global warming potential, fine particulate matter, acidification potential, and freshwater eutrophication potential. In the current landscape, the materials used to produce IFB exhibit better environmental impact performance due to the use of low impact iron-based electrolyte and carbon-based cell stack. While flow batteries do offer some use-phase advantages such as long cycle life and separation of power and energy when compared to alternatives such as lithium-ion systems, the IFB, ZBFB, and VRFB systems considered here all exhibit similar use-phase efficiencies. Thus, the differences in the environmental impact profile between these flow battery technologies are due to the materials selection and battery production aspects. Tradeoffs between the use-phase benefits and production phase impacts are, however, not yet well understood and are the topic of an ongoing study investigating the net environmental benefits of flow batteries as a technology class for grid applications by considering various temporal and geographical characteristics and dynamic renewable resource profiles.

More broadly, this study highlights 1) that materials selection choices, even within the same technology, can significantly affect the environmental impact of production, 2) that significant uncertainty exists in the environmental impact data for the materials and production processes used to fabricate energy storage systems. Further, this study contributes new data on the life cycle environmental impacts of emerging flow battery production and their distribution across material choices and production pathways. This enables 1) flow battery manufacturers to make informed decisions about the selection of materials and methods used to fabricate their products and 2) environmental impact assessments to account for uncertainty associated with materials selection and production pathways. Conventionally, environmental impact is only one of many factors influencing materials selection decisions. Considerations such as material cost and level of performance are often prioritized above environmental impact considerations, yet trade-offs may exist between these criteria. Therefore, further research into developing materials and production methods that simultaneously yield improvements relative to all criteria, e.g., low-cost, high-performance, and low environmental impact options, is needed. With evolving technologies, batteries with newly developed materials, designs and production methods, which correspond to lower environmental impact, should be pursued.

CRediT authorship contribution statement

Haoyang He: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing - original draft, Visualization. **Shan Tian:** Investigation, Writing - original draft. **Brian Tarroja:** Conceptualization, Writing - review & editing, Supervision, Project administration, Funding acquisition. **Oladele A. Ogunseitan:** Writing - review & editing. **Scott Samuelsen:** Supervision, Funding acquisition. **Julie M. Schoenung:** Conceptualization, Writing - review & editing, Visualization, Supervision, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Process Flow for Flow Battery Production

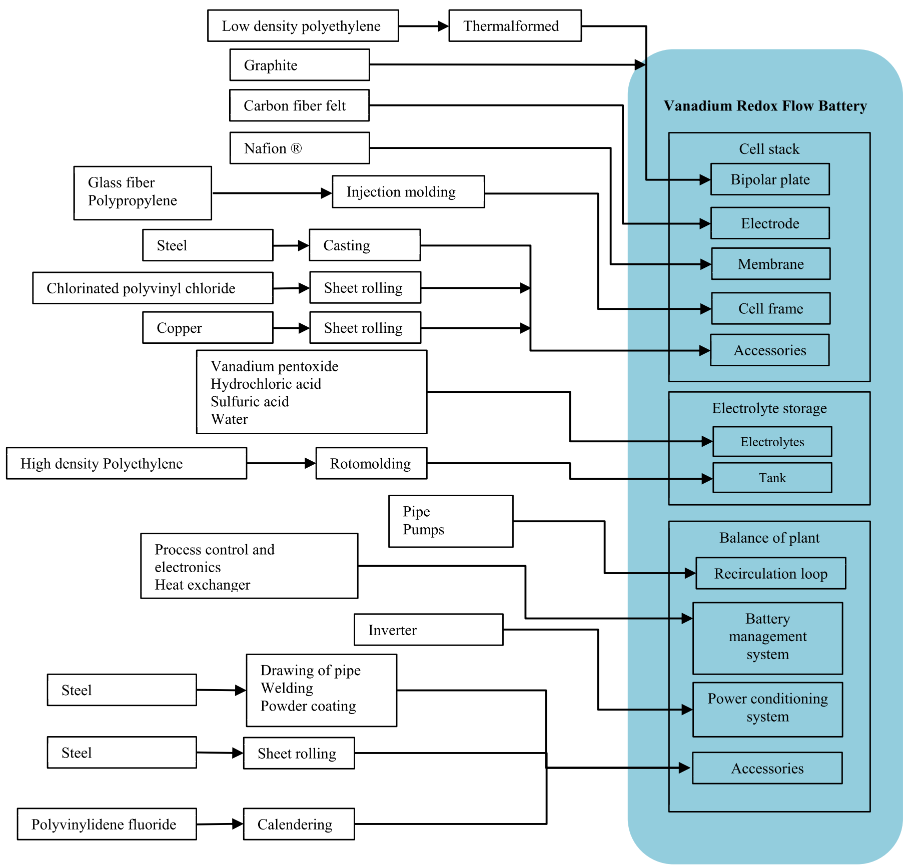

Fig. A 1. The process flow diagram for producing a vanadium redox flow battery.

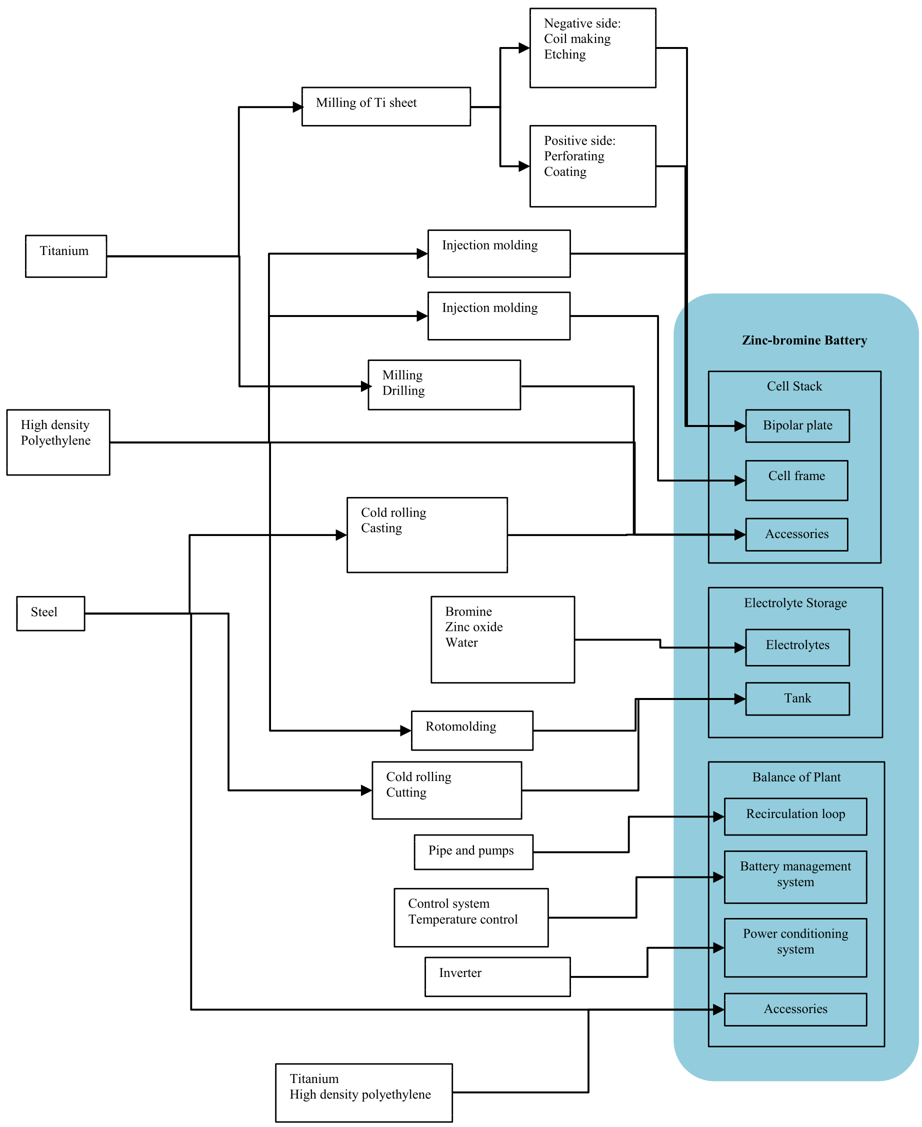

Fig. A 2. The process flow diagram for producing a zinc-bromine flow battery.

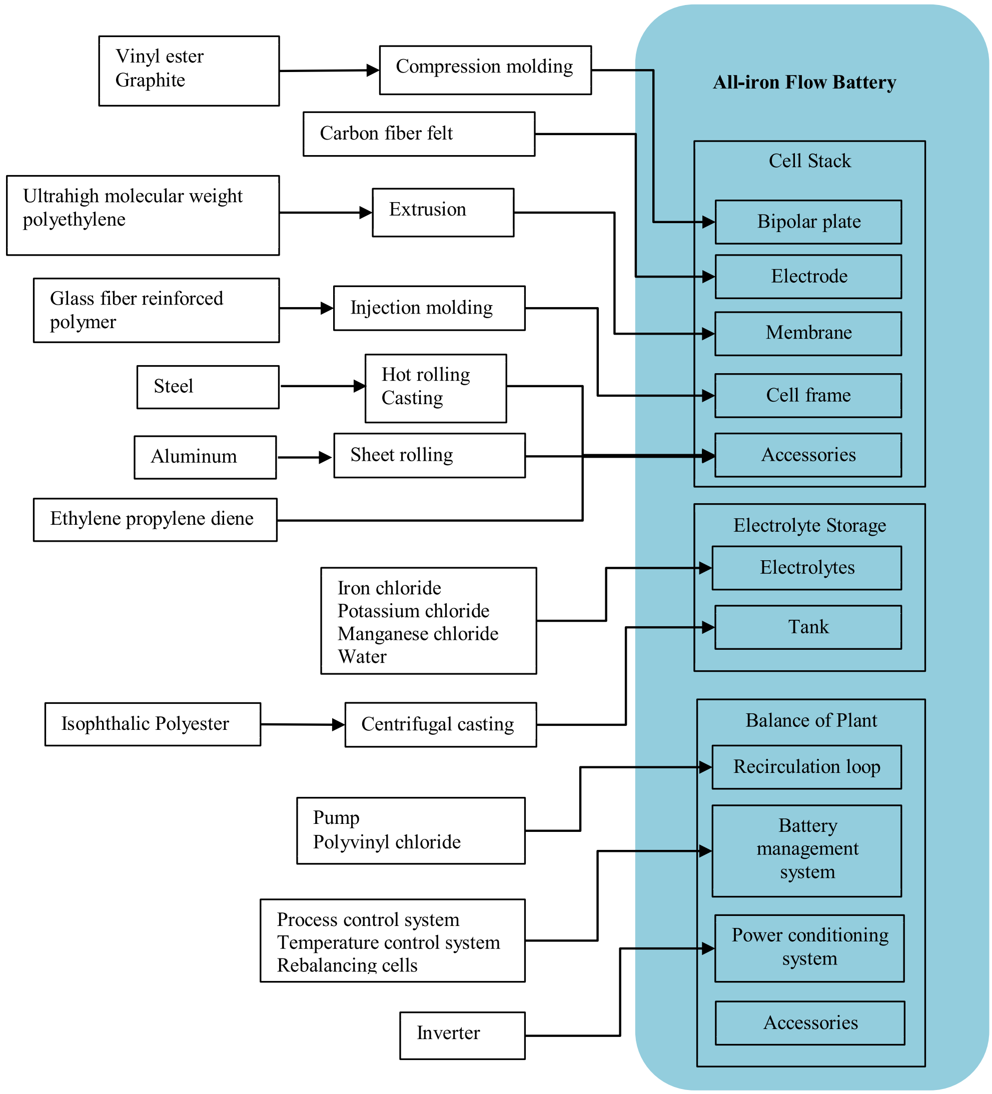

Fig. A 3. The process flow diagram for producing an all-iron flow battery.

Appendix B. Environmental Impact Assuming the Harmonized System Boundary

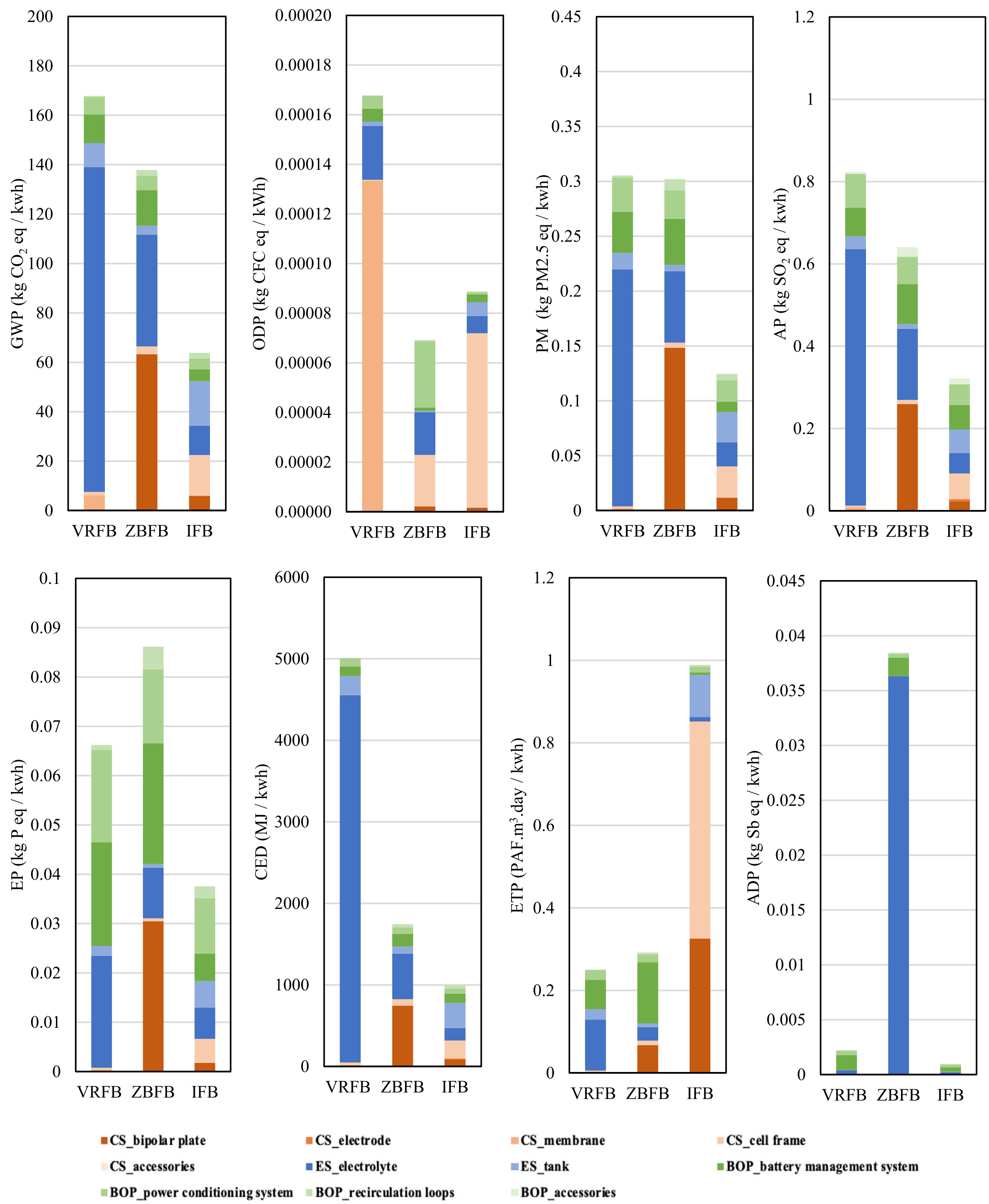

Fig. B 1. The environmental impact of flow battery production, assuming the harmonized system boundary. Flow battery types include: VRFB = vanadium redox flow battery; ZBFB = zinc-bromine flow battery; and IFB = all-iron flow battery. Flow battery components include: cell stack (CS), electrolyte storage (ES) and balance of plant (BOP).

Appendix C. Sensitivity Analysis on Membrane and Carbon Fiber Felt Production

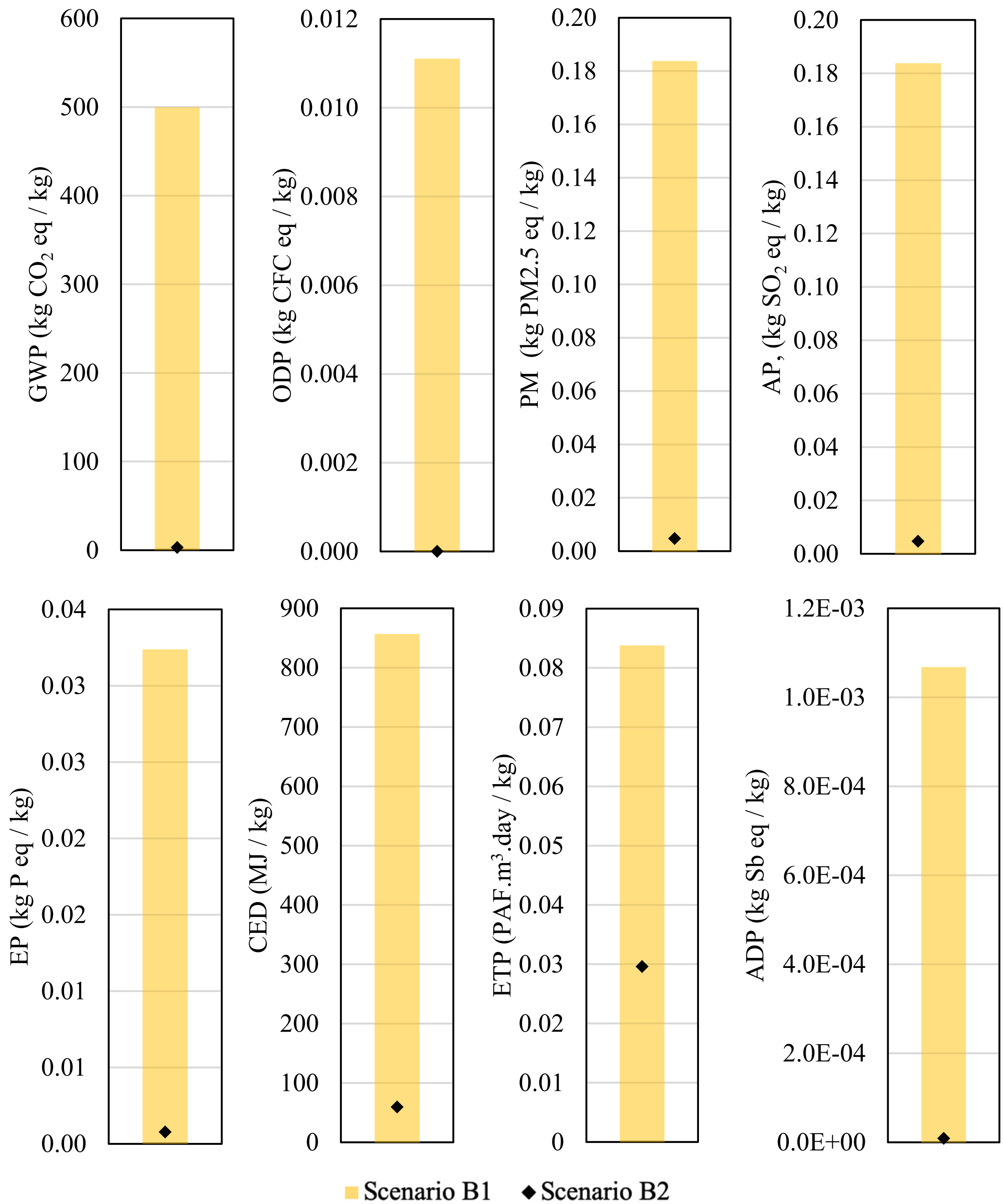

Fig. C 1. The environmental impact per kg of material, for Nafion® and Daramic® membrane production.

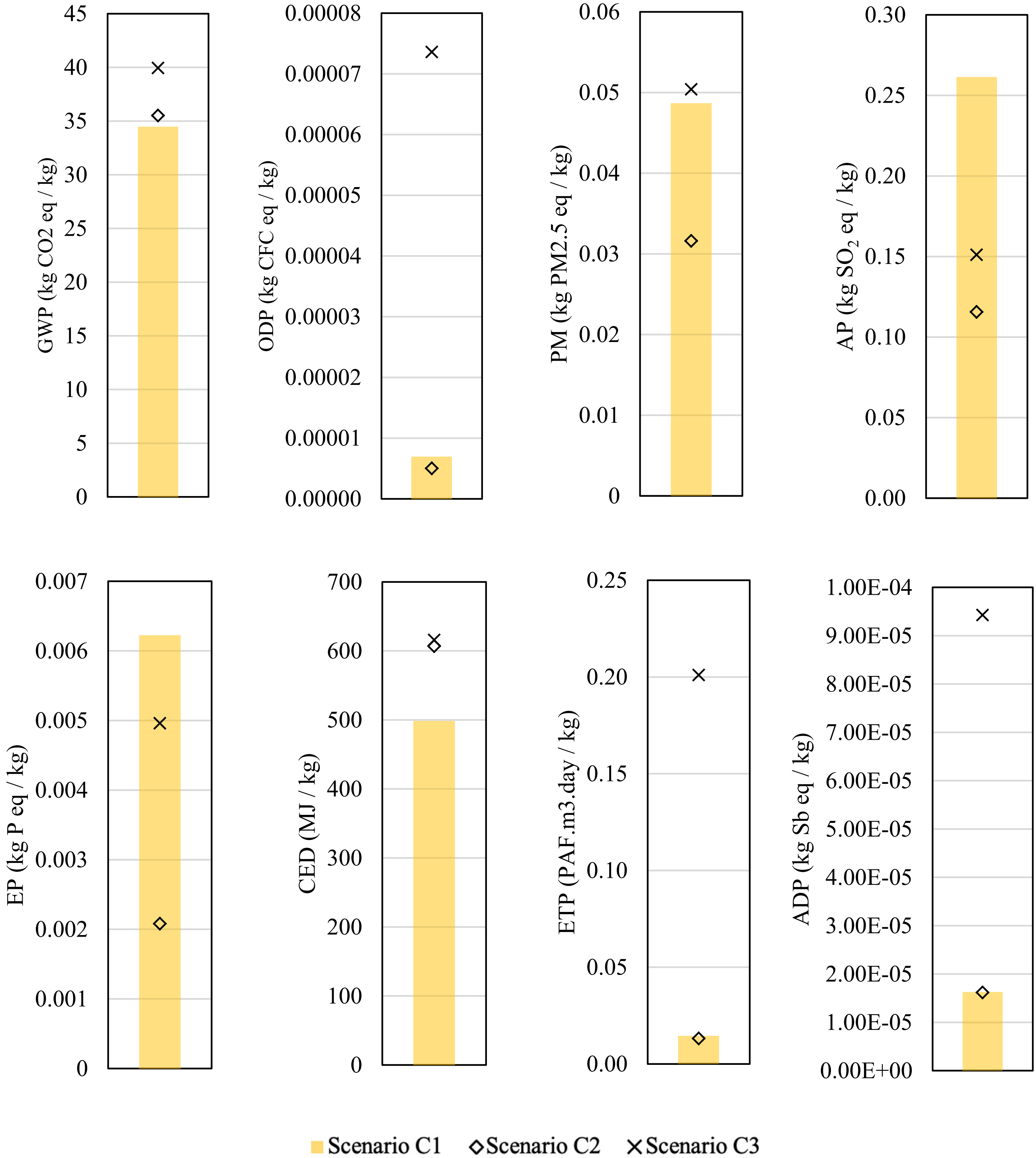

Fig. C 2. The environmental impact per kg of material, for carbon fiber felt production assuming various production scenarios.

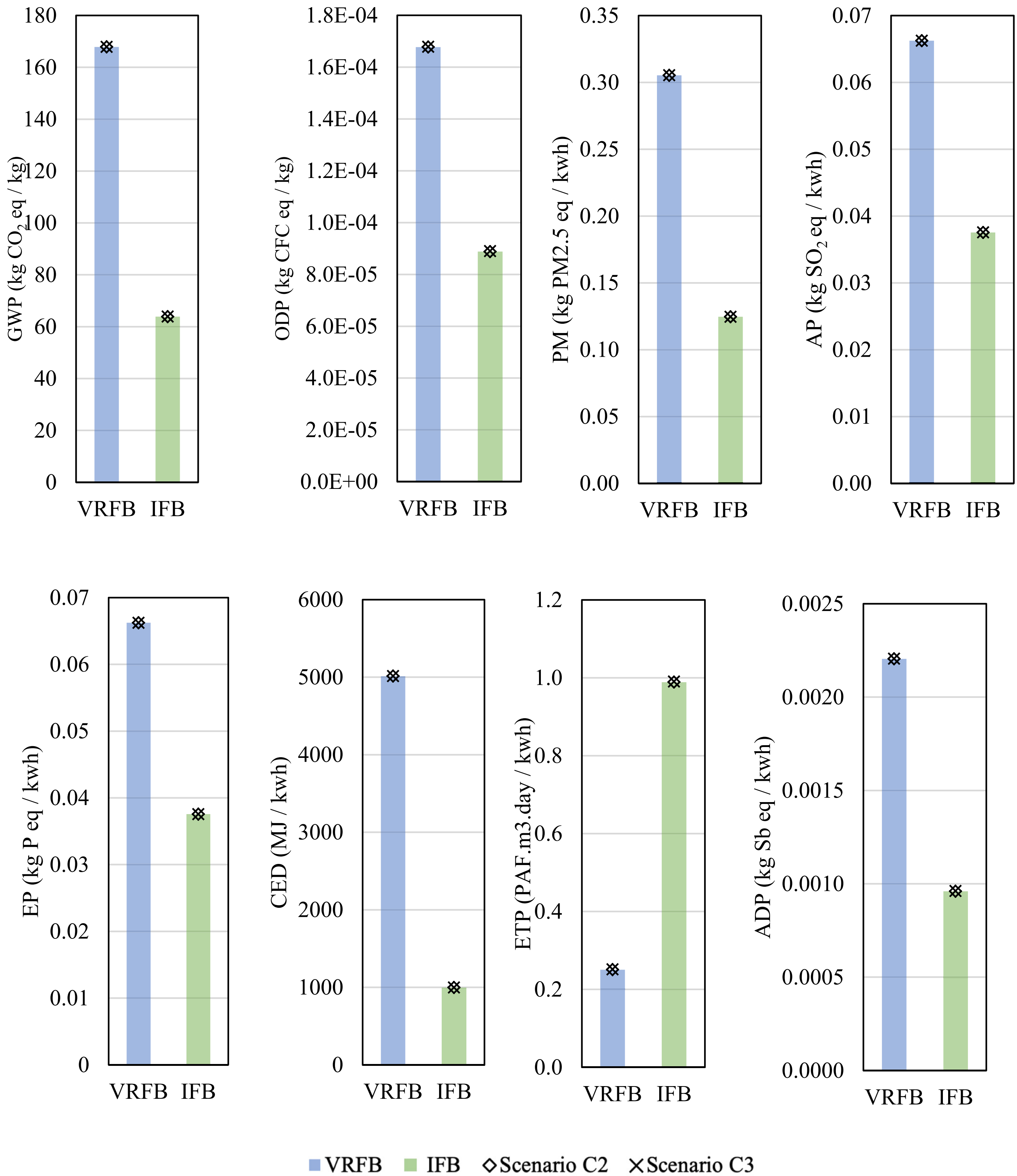

Fig. C 3. The environmental impact associated with VRFB and IFB production, assuming various scenarios for carbon fiber felt production.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2020.121740.

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