CHALMERS
UNIVERSITY OF TECHNOLOGY

SCIENTIFIC REPORT

Prospective screening life cycle assessment of a sodium-ion hybrid supercapacitor

FRIDA HERMANSSON, RICKARD ARVIDSSON, ANDERS NORDELÖF & MAGDALENA SVANSTRÖM

DEPARTMENT OF TECHNOLOGY MANAGEMENT AND ECONOMICS
Division of Environmental Systems Analysis

CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2024
www.chalmers.se

Prospective screening life cycle assessment of a sodium-ion hybrid supercapacitor

Frida Hermansson, Rickard Arvidsson,
Anders Nordelöf & Magdalena Svanström

Department of Technology Management and Economics
Division of Environmental Systems Analysis
CHALMERS UNIVERSITY OF TECHNOLOGY

Gothenburg, Sweden 2024

Prospective screening life cycle assessment of a sodium-ion hybrid supercapacitor

FRIDA HERMANSSON; RICKARD ARVIDSSON; ANDERS NORDELÖF and MAGDALENA SVANSTRÖM

Cover photo: "Cadogan Tate 12 Tonne Electric Truck" by Tony Hall is licensed under CC BY 2.0. To view a copy of this license, visit https://creativecommons.org/licenses/by/2.0/

The work in this report is licensed under Attribution-ShareAlike 4.0 International. To view a copy of this license, visit http://creativecommons.org/licenses/by-sa/4.0/

Report no. E2024:003
Department of Technology Management and Economics
Division of Environmental Systems Analysis
Chalmers University of Technology
SE-412 96 Gothenburg
Sweden
Telephone + 46 (0)31-772 1000

Summary

Hybrid supercapacitors combine batteries' energy density with capacitors' power density. They can extend the lifetime of an electrical vehicle battery by reducing the number and depth of the charge/discharge cycles and by enhancing the battery's power capacity. Traditionally, hybrid supercapacitors contain lithium, a geochemically scarce metal. To mitigate a future lithium shortage, measures could be taken to substitute lithium with more abundant materials. One option is sodium-ion hybrid supercapacitors.

In this report, we assess the climate and mineral resource scarcity impacts of manufacturing a sodium hybrid supercapacitor by means of life cycle assessment. The goal is to identify hotspots to aid researchers, developers, and potential manufacturers in making environmentally benign design choices.

The considered sodium-ion hybrid supercapacitor is not yet produced at large scale but only in laboratories. To address this, we scale up the production process to an industrial scale using frameworks available in the literature. Results show that the activated carbon electrode is responsible for most of the environmental impact due to the use of nitric acid in processing the activated carbon. If nitric acid could be replaced, recycled, or reduced, this would lower the environmental impact considerably. Additionally, we provide guidance on how to scale up the mass of the sodium-ion hybrid supercapacitor to meet the requirement of a vehicle. This upscaling also means that the results can be used in screening assessments by vehicle developers interested in how the sodium-ion hybrid supercapacitor could influence the environmental impact of their vehicle.

Content

1. Introduction

Hybrid supercapacitors (HSC) combine the high energy density of traditional batteries with the high power density of traditional capacitors (Liu et al., 2021). Using HSCs can extend a battery's lifetime by reducing the number and depth of the charge/discharge cycles by extending the battery's power load (Conte, Genovese, Ortenzi, & Vellucci, 2014). Traditionally, HSC contains lithium as an important anode material. Typically, the HSC uses a high-capacity battery-type electrode and a high-rate capacitor-type electrode (Lamb & Burheim, 2021).

Lithium is a geochemically scarce metal, and the global demand is expected to increase (Prior, Wäger, Stamp, Widmer, & Giurco, 2013). Measures could be taken to develop HSCs based on more abundant materials to mitigate a potentially upcoming resource shortage. One such HSC is the all-organic aqueous sodium-ion HSC developed by Karlsmo and Johansson (2022), with electrodes consisting of perylene tetracarboxylic dianhydride (PTCD, an organic dye molecule) and activated carbon. The electrolyte consists of a combination of sodium and magnesium sulphate salts and water, and a cellulose film separates the two halves of the cell. Compared to lithium-ion HSCs, this HSC has a lower energy density but a relatively high-power density. In theory, this sodium-ion HSC should be preferable from a mineral resource scarcity perspective compared to conventional HSCs considering its content of abundant materials – for example, cellulose is the most abundant biopolymer on Earth (Dessbesell, Paleologou, Leitch, Pulkki, & Xu, 2020) and both sodium and magnesium belong to the most abundant metals in the Earth's crust (Rudnick & Gao, 2003). However, whether the sodium-ion HSCs have lower mineral resource scarcity impacts also in a broader life-cycle perspective remains to be quantitatively investigated.

2. Goal definition

To investigate the environmental and resource impacts of a sodium-ion HSC, life cycle assessment (LCA) can be applied (International Organization of Standardization, 2006). The goal of this LCA study is to identify hotspots in the HSCs' cradle-to-gate life cycle for further improvements of its environmental and resource performance. The intended audience of the study is researchers, developers, and potential manufacturers of this HSC. They can use the results of this study to make impactful environmental improvements in the design of the HSC. There is also a wider potential audience interested in energy and power storage devices in general, which might be interested in the environmental impacts of the sodium-ion HSC studied. Additionally, we provide a basis for a rough scaling of the sodium-ion HSC, so that vehicle developers can use the results as a building block to assess what influence a transition to a sodium-ion HSC could have on their vehicle. This study is intended as an initial, screening LCA of the technology. There are no comparative assertions in the study.

The sodium-ion HSC considered in this study has no large-scale manufacturing yet. It is the potential impacts of this technology at future large scale that we are interested in studying from an environmental and resource point of view. This means that a prospective LCA approach is needed, in which the product system of the HSC is placed at a future time (Arvidsson et al., 2023), specifically,

a time at which it has reached large-scale production. This report thus assesses the impacts of the sodium-ion HSC at an upscaled level using prospective LCA. The report structure follows the main phases of an LCA: goal and scope definition, life cycle inventory analysis, life cycle impact assessment and interpretation.

3. Scope definition

The function of the studied sodium-ion HSC is two-fold: To provide energy and to provide power. The developers of the studied HSC have estimated the energy and power densities of the sodium-ion HSC at approximately 0.5 Wh/kg and 140 W/kg, respectively. Considering this dual function, and since no comparative assertion is made in this study, a simplified assumption was made that the functional unit is the manufacturing of a cell with a mass of 1 kg. However, the basis for the initial calculations is the production of a small coin cell, as this is what the data is collected for. The HSCs' cradle-to-gate life cycle is shown in Figure 1 (see next page).

Data for the composition and inventory is based on the journal publication by Karlsmo and Johansson (2022) and was partly adjusted based on correspondence with the authors. As the data for producing the sodium HSC is provided for lab-scale, measures have been taken to upscale the data to represent an industrial-scale production system. For simplicity, we have assumed that the material yield in all steps is 100%, meaning that any losses are assumed to be negligible.

The geographical scope of the study is global, meaning that global datasets are generally preferred, or other types of broader datasets representing larger regions, such as Europe. The temporal positioning of the product system is at a future point in time, making this a prospective LCA (Arvidsson et al., 2023). The exact time at which the studied technology is expected to reach large-scale production (if ever) is highly uncertain, but will most likely happen after 2030, perhaps around 2040 at the earliest.

Considering the screening nature of this study, a limited number of impact categories and indicators are considered. This also reflects the lack of detailed data on, for example, (eco)toxic emissions from the foreground system, making the inclusion of such impact categories of questionable value. In this study, we consider two impact categories: (i) Climate impact using the IPCC2021 methodology and (ii) mineral resource scarcity using the crustal scarcity indicator (CSI) by Arvidsson et al. (2020). The climate change indicator is based on the radiative forcing of greenhouse gas emissions accumulated over a certain time horizon (assumed 100 years), measured in kg carbon dioxide (CO_2) equivalents. The CSI considers the relative geochemical abundance of elements, minerals, rocks and ores in Earth's crust, measured in kg silicon (Si) equivalents. The modelling is performed using the OpenLCA software (GreenDelta, versions 1.11.0 and 2.1.0), and background data comes from the Ecoinvent database (version 3.9.1) as implemented in OpenLCA.

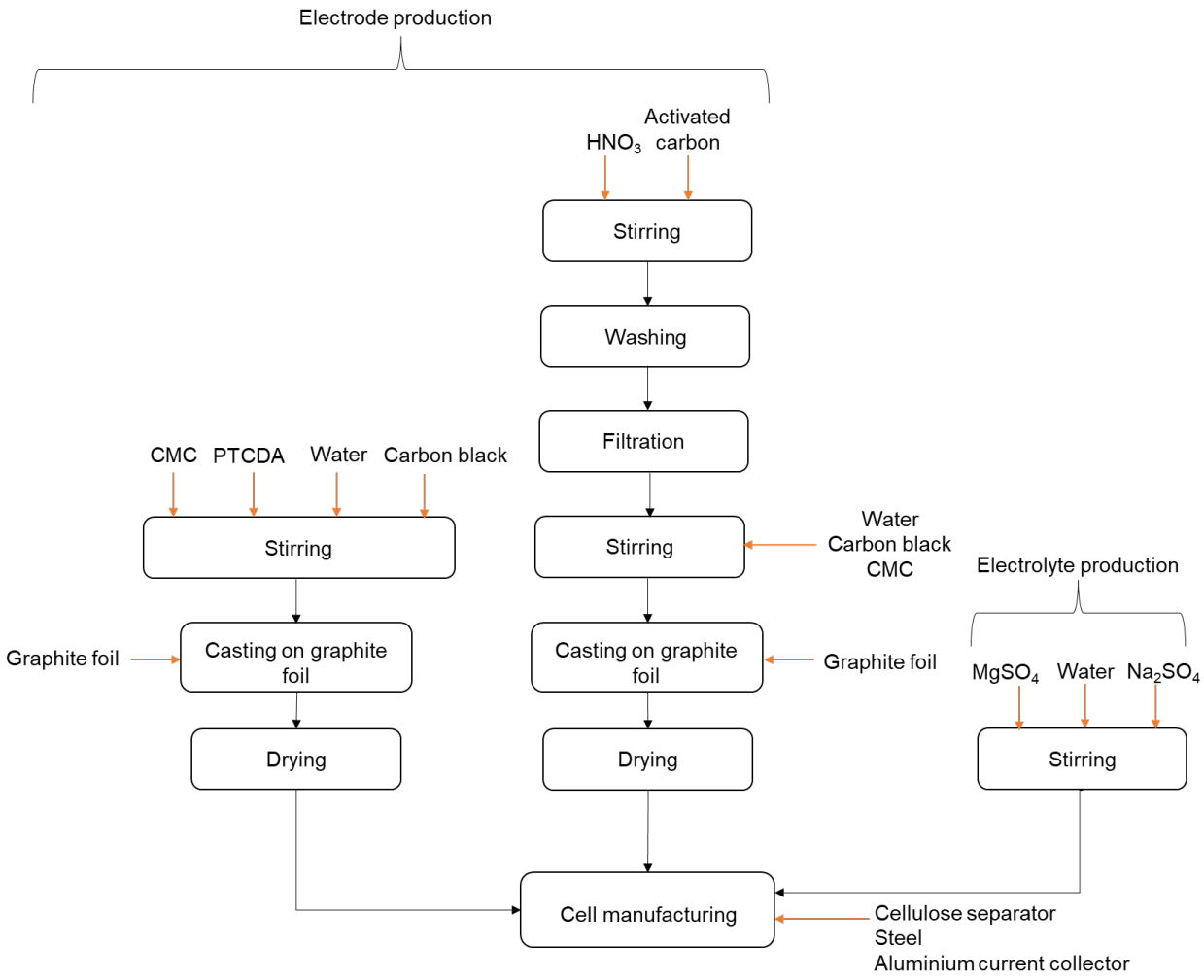

Figure 1: The cradle-to-gate life cycle of the sodium-ion hybrid supercapacitor. Orange arrows represent inputs for which production-related data was obtained from the Ecoinvent database. PTCDA is an abbreviation of perylene-tetracarboxylic dianhydride, and CMC is an abbreviation of carboxymethyl cellulose.

4. Life cycle inventory analysis

4.2 Bill of materials

The starting point of this study is a coin cell with a diameter of 10 mm (0.785 cm^2), described in the paper by Karlsmo and Johansson (2022). In the PTCDA electrode, the weight ratio for PTCDA: carbon black (CB): carboxymethyl cellulose (CMC) is 75:15:10, with a loading of 0.7-1 mg/cm^2 active material (PTCDA). We here assume an average loading of 0.85 mg/cm^2. This results in 0.85×0.785 = 0.67 mg PTCDA, 0.85×0.785×(15/75) = 0.13 mg CB, and 0.85×0.785×(10/75) = 0.089 mg CMC, with a total mass of 0.85×0.785/0.75 = 0.89 mg for a 0.785 cm^2 coin cell. The mass of the graphite foil is 19.4 mg/cm^2, resulting in 19.4×0.785 = 15.2 mg needed for the coin cell. This results in a total mass of 16.11 mg for the PTCDA electrode.

The activated carbon (AC) electrode has a weight ratio of AC: CB: CMC at 75:15:10, and an active material loading of 2-3.5 mg/cm^2 activated carbon is needed. Again, we use the average loading value 2.75 mg/cm^2. A 0.785 cm^2 capacitor cell thus needs 0.785×2.75 = 2.16 mg AC, 0.785×2.75×(15/75) = 0.43 mg carbon black, and 0.785×2.75×(10/75) = 0.29 mg CMC. The mass of the graphite foil is 15.2 mg also for this electrode, which results in a total mass of 18.1 mg for the AC electrode.
A cellulose film separates the electrodes. We assume the cellulose film weighs 80 g/m^2, based on the basis weight for homogenized cellulose nanofiber film as reported by Shanmugam, Chandrasekar, and Balaji (2023), which converts to 8 mg/cm^2. This means that 0.785×8 = 6.28 mg of separator is needed. The coin cell contains 40 µL electrolyte with a 1.4 g/cm^3 density, corresponding to 0.04×1.4 = 0.0560 g, or 56.0 mg. The electrolyte consists of 64 wt.% deionised water, 17 wt.% Na_2SO_4 and 19 wt.% $MgSO_4$. We assume that the casing constitutes 2 vol.% of the inside volume of the coin cell (based on numbers from Chordia, Wikner, and Nordelöf (2022)), that the cell has the density of 1.5 g/cm^3 (see Appendix for calculations), and that the tabs constitute 2 wt.% of the cell. Finally, we assume that the mass composition of the coin cell can be scaled linearly to a 1 kg cell. This results in the mass composition (bill of materials) shown in Table 1.

Table 1: The material composition (bill of materials) for the coin cell, scaled to 1 kg cell weight.

BILL OF MATERIALS for one coin cell (mg)			Mass percent in cell	**BILL OF MATERIAL for 1 kg cell (g)**
PTCDA electrode	PTCDA	0.667	0.614%	6.14
	Carbon black	0.133	0.123%	1.22
	CMC	0.0890	0.0819%	0.819
	Graphite foil	15.2	14.0%	140
AC electrode	Activated carbon	2.16	1.99%	19.9
	Carbon black	0.432	0.397%	3.97
	CMC	0.288	0.265%	2.65
	Graphite foil	15.2	14.0%	140
Electrolyte	Deonised water	35.9	33.1%	331
	Na_2SO_4	9.70	8.93%	89.3
	$MgSO_4$	10.4	9.55%	95.5
Separator	Cellulose (CMC)	6.28	5.78%	57.8
Casing	Steel	10.0	9.21%	92.1
Tabs	Aluminium	2.13	1.96%	19.6

The following sections (4.2-4.8) calculate the inputs of other materials and energy. The calculations are based on the size of the coin cell, but the processing inputs are upscaled from lab scale to industrial scale. Finally, the inputs needed to produce the cell are upscaled linearly to calculate the impacts related to the functional unit (1 kg cell).

4.3 PTCDA electrode production

The production begins by mixing 3 wt% CMC in ultrapure water. As 0.089 mg CMC is needed in the final cell, 0.089 mg pure CMC and (0.089/0.03)-0.089 = 2.9 mg ultrapure water are added. To scale up to large-scale production, we apply the solvent reduction factor of 20%, as suggested by Piccinno, Hischier, Seeger, and Som (2016), resulting in only 2.9×0.8 = 2.3 mg of water. PTCDA and carbon black are mixed and added to the CMC solution, followed by stirring for 12 h. Assuming a 1000 L tank, the electricity for stirring can be calculated in J using Equation 1 from Piccinno et al. (2016).

$$E_{Stirring} = 0.0180 m^5 s^{-3} \times \rho_{mix} \times t \qquad \text{(Eq. 1)}$$

The parameters for calculating the electricity requirement of the stirring are found in Table 2, and the result is 0.88 MJ. This amount of electricity for the stirring is then normalised to the batch of 3.2 mg by taking into account that the energy calculated using Equation 1 corresponds to a total of 1000 L with a density of 1132 kg/m^3, i.e., a total of 1132 kg. This means that a batch of 3.2 mg requires only 0.881×(0.0000032/1132) = 2.48×10^{-9} MJ.

Table 2: Parameters for calculating the electricity requirement during stirring.

Parameter	Value	Unit
$\rho_{\text{Carbon black}}$	1.95	g/cm^3
$m_{Carbon\ black}$	0.133	mg
$V_{\text{Carbon black}}$	6.84*10^{-5}	mL
ρ_{PTCDA}	1.7	g/cm^3
m_{PTCDA}	0.667	mg
V_{PTCDA}	3.92*10^{-4}	mL
ρ_{CMC}	1.6	g/cm^3
m_{CMC}	0.0890	mg
V_{CMC}	5.56*10^{-5}	mL
ρ_{DIwater}	1	g/cm^3
m_{Diwater}	2.30	mg
V_{Diwater}	2.30*10^{-3}	mL
ρ_{mix}	1132	kg/m^3
t	43 200	s
E_{stir}	0.881	MJ

The electrode slurry is cast on the graphite foil, followed by vacuum drying for 12 h. The energy requirement during drying is calculated using Equation 2 provided by Piccinno et al. (2016), where vacuum drying is scaled up as an oven-drying process. The liquid to be evaporated in this case is 23

mg of water, thus C_P = 4186 J/kg°C, m = 23×10^{-6} kg, T_{boil} = 100°C, T_0 = 25°C, ΔH = 2260 KJ/kg, and m_{vap} = 2.3×10^{-6} kg.

$$Q_{drying} = \frac{C_{P,liquid} \times m_{liquid} \times (T_{boil} - T_0) + \Delta H_{vap} \times m_{vap}}{0.8} \quad \text{(Eq. 2)}$$

This results in 7.4*10^{-6} MJ needed during the vacuum drying. Most heating processes in the chemical industry use steam as an energy source. We assume that 1 kg of steam corresponds to 2.75 MJ (in line with the unit process for steam production in the chemical industry in Ecoinvent 3.9). This means that 2.7*10^{-6} kg steam is needed in the vacuum drying. Table 3 shows the unit process for the upscaled PTCDA electrode manufacturing.

Table 3: Unit process for PTCDA electrode production. "Market process provider" refers to the datasets used in the Ecoinvent database.

Input	**Value**	**Unit**	**Market process provider**
CMC	0.0889	mg	carboxymethyl cellulose production, powder | carboxymethyl cellulose, powder | Cutoff, U – RER
Deionised water	2.30	mg	market for water, deionized | water, deionized | Cutoff, U – Europe without Switzerland
PTCDA	0.667	mg	market for chemical, organic | chemical, organic | Cutoff, U – GLO
Carbon black	0.133	mg	market for carbon black | carbon black | Cutoff, U – GLO
Graphite foil	15.2	mg	graphite production | graphite | Cutoff, U market for graphite | graphite | Cutoff, U – RER
Electricity	2.48×10^{-9}	MJ	market group for electricity, medium voltage | electricity, medium voltage | Cutoff, U – RER
Steam	2.69*10^{-6}	kg	steam production, in chemical industry | steam, in chemical industry | Cutoff, U – RER
Output	**Value**	**Unit**	**Market process provider**
PTCDA electrode	16.1	mg	n/a

4.4 Activated carbon electrode production

The production of the AC electrode starts by mixing activated carbon (2.16 mg) in an aqueous solution of 50 mL 1 M nitric acid (HNO_3). After reducing the solvent use by 20% to account for upscaling (in line with the suggestion by Piccinno et al. (2016)), the resulting volume is 40 mL. The corresponding amount of substance (n) can be calculated by multiplying the concentration (c) of 1 M (or 1 mol/L) by the volume (V) of 40 mL:

$$n = c \times V = \frac{1mol}{litre} * 40\ mL = 0.04\ \text{mol} \qquad \text{(Eq. 3)}$$

The mass of HNO_3 in the solution is then calculated by multiplying with the molar mass (*M*) of HNO_3:

$$m = n * M = 0.04\ mol * 63.01 \frac{g}{mol} = 2.52\ g \qquad \text{(Eq. 4)}$$

The density of 1 M HNO_3 is approximately 1.0 g/cm^3, or 1 kg/L, meaning that for the 40 mL, a mass of 40 g (1 M) HNO_3 is added in total. To achieve the right concentration, 37.48 g of deionized water must also be added in addition to the 2.52 g HNO_3. The solution is then stirred for 12 h, and the electricity needed for this is calculated using Equation 1 and the values in Table 4. Again, the electricity required for stirring is scaled based on a 1000 L batch volume, corresponding to 1000 kg. The electricity requirement per kg of stirred electrolyte is thus $0.778\times(40*10^{-3}/1000) = 3.11*10^{-5}$ MJ.

Table 4: Parameters for calculating the electricity requirement during stirring.

Parameter	**Value**	**Unit**
$\rho_{Activated\ carbon}$	2.05	g/cm^3
$m_{Activated\ carbon}$	2.16	mg
$V_{Activated\ carbon}$	$1.05*10^{-3}$	cm^3
ρ_{HNO3}	1	g/cm^3
m_{HNO3}	40	g
V_{HNO3}	40	mL
ρ_{mix}	1000	kg/m^3
t	43 200	s
E_{stir}	0.778	MJ

The mix is then washed with deionized water. The developers of the studied HSC estimate the volume of the washing water at 80 mL. The washing water and HNO_3 are removed by filtration, assumed to require 10 kWh/tonne (0.01 kWh/kg) of dry material (Piccinno et al., 2016), resulting in $0.01\times2.16*10^{-6} = 2.16\times10^{-8}$ kWh, which corresponds to 7.77×10^{-8} MJ.

Then follows some steps that are the same as for the PTCDA electrode manufacturing. The washed AC, CB, and CMC are added to water, and we assume that the same amount is added as for the PTCDA electrodes, i.e., CMC corresponds to 3 wt.% of the solution compared to water. This results in (0.288/0.03)-0.288 = 9.31 mg added water, corresponding to 7.45 mg after being upscaled in line with the -20% rule of thumb for solvents, as per Piccinno et al. (2016). The solution is then stirred for 12 h. The parameters used to calculate the stirring energy are found in Table 5. We again normalise

the electricity requirements to 10.3 mg from the total batch of 1000 L using a density of 1157 kg/m^3, meaning that 10.3 mg requires 0.899×(0.0000103/1157) = 8.03*10^{-6} MJ.

Table 5: Parameters used to calculate the stirring electricity for the AC electrodes.

Parameter	Value	Unit
$\rho_{\text{Carbon black}}$	1.95	g/cm^3
$m_{Carbon\ black}$	0.431	mg
$V_{\text{Carbon black}}$	2.21*10^{-4}	mL
ρ_{AC}	2.0	g/cm^3
m_{AC}	2.16	mg
V_{AC}	1.11*10^{-3}	mL
ρ_{CMC}	1.6	g/cm^3
m_{CMC}	0.288	mg
V_{CMC}	0.18*10^{-4}	mL
ρ_{DIwater}	1	g/cm^3
m_{Diwater}	7.45	mg
V_{Diwater}	7.45*10^{-3}	mL
ρ_{mix}	1157	kg/m^3
t	43 200	s
E_{stir}	0.899	MJ

The slurry is then cast on a graphite foil (same amount as for the PTCDA electrode), followed by vacuum drying for 12 h. Using Eq. 2 and the values C_P = 4186 J/kg°C, m = 7.4×10^{-6} kg, T_{boil} = 100°C, T_0 = 25°C, ΔH = 2260 KJ/kg, and m_{vap} = 7.4×10^{-6} kg results in 23.8 J needed. This energy corresponds to 8.66*10^{-6} kg of steam used for heating, assuming 2.75 MJ/kg steam. The unit process for the AC electrode is found in Table 6.

Table 6: Unit process for the AC electrode production. "Market process provider" refers to the datasets used in the Ecoinvent database.

Input	Value	Unit	Market process provider
CMC	0.288	mg	carboxymethyl cellulose production, powder | carboxymethyl cellulose, powder | Cutoff, U – RER
Deionised water	117	g	market for water, deionized | water, deionized | Cutoff, U – Europe without Switzerland
HNO_3	2.52	g	market for nitric acid, without water, in 50% solution state | nitric acid, without water, in 50% solution state | Cutoff, U - RER w/o RU
Activated carbon	2.16	mg	activated carbon production, granular from hard coal | activated carbon, granular | Cutoff, U – RER
Carbon black	0.431	mg	carbon black production | carbon black | Cutoff, U – GLO
Graphite foil	15.2	mg	graphite production | graphite | Cutoff, U – RER
Electricity	$3.92*10^{-5}$	MJ	market group for electricity, medium voltage | electricity, medium voltage | Cutoff, U – RER
Steam	$8.66*10^{-6}$	kg	steam production, in chemical industry | steam, in chemical industry | Cutoff, U - RER
Output	**Value**	**Unit**	**Market process provider**
AC electrode	18.1	mg	n/a
Polluted water, e.g. with HNO_3	117	cm^3	treatment of wastewater, average, wastewater treatment | wastewater, average | Cutoff, U - Europe without Switzerland

4.5 Electrolyte

Na_2SO_4 and $MgSO_4$ are used to produce the electrolyte. This is done by dissolving Na_2SO_4 in ultra-pure water before adding $MgSO_4$ and stirring for 1 hour (3600 s). The mixture has a density of 1.4 g/cm^3 according to an estimation by the developers of the studied HSC. Using Eq. 1, the energy required for stirring is 0.0907 MJ. In our case, we normalise this number to the amount used to stir one batch of electrolyte as produced in the lab (corresponding to 3.12 g), resulting in only $0.0907\times(0.00312/1400) = 2.02\times10^{-7}$ MJ being used. The unit process for the electrolyte production is found in Table 7.

Table 7: Unit process to produce electrolyte for the electrolyte. "Market process provider" refers to the datasets used in the Ecoinvent database.

Inputs	Amount	Unit	Market process provider
Magnesium sulfate	0.578	g	magnesium sulfate production | magnesium sulfate | Cutoff, U - RER
Sodium sulfate	0.540	g	sodium sulfate production, from natural sources | sodium sulfate, anhydrite | Cutoff, U - RER
Deionized water	2	g	market for water, deionised | water, deionised | Cutoff, U - Europe without Switzerland
Electricity	$2.02*10^{-7}$	MJ	market group for electricity, medium voltage | electricity, medium voltage | Cutoff, U - RER
Outputs	**Amount**	**Unit**	**Market process provider**
Electrolyte	3.12	g	n/a

4.6 Separator

The separator is made from a cellulose film. Data for the separator is obtained from a cellulose battery cell separator dataset developed by Wickerts, Arvidsson, Nordelöf, Svanström, and Johansson (2024), as shown in Table 8.

Table 8: Unit process for producing 1 kg cellulose separator, adapted from Wickerts et al. (2024). "Market process provider" refers to the datasets used in the Ecoinvent database.

Inputs	Value	Unit	Market process provider
Cellulose	0.79	kg	market for cellulose fibre - CH
Epichlorohydrin	0.45	kg	market for epichlorohydrin - RER
Sodium hydroxide	1.1	kg	market for sodium hydroxide, without water, in 50% solution state - GLO
Urea	1.9	kg	market for urea - RER
Water	13	kg	market for water, deionized – Europe without Switzerland
Electricity	5.3×10^{-4}	kWh	market group for electricity, medium voltage - RER
Steam	18	kg	market for steam, in chemical industry - RER
Injection moulding	1.0	kg	market for injection moulding - RER
Chemical factory	4.0×10^{-10}	item	chemical factory construction, organics | chemical factory, organics | Cutoff, U - RER
Outputs	**Amount**	**Unit**	**Market process provider**
Cellulose separator	1.0	kg	n/a
Wastewater	$1.6*10^{-2}$	m^3	market for wastewater, average – Europe without Switzerland
Hydrogen	9.3×10^{-3}	kg	Emission to air

4.7 Casing

The manufacturing of the steel casing is assumed to be similar in processing to that of car parts described by Hermansson et al. (2023). This means the steel is processed by sheet rolling and deep drawing, and we assume no material losses. We assume that the coin cell casing weighs 10.0 mg.

4.8 Tabs

We assume that the tabs needed correspond to 2 wt.% of the cell, in line with suggestions by Chordia et al. (2022). We assume that the tabs are made from aluminium. This results in a total of 2.13 mg of aluminium needed.

4.9 Manufacturing of capacitor cell

Unlike the conventional HSC, the sodium-ion HSC does not need an energy-demanding clean and dry environment for assembly (Karlsmo & Johansson, 2022). Therefore, energy requirements for the assembly are assumed to be negligible. The unit process for the HSC is found in Table 9.

Table 9: Unit process for the sodium-ion HSC production. "Market process provider" refers to the datasets used in the Ecoinvent database.

Input	**Value**	**Unit**	**Market process provider**
Activated carbon electrode	18.1	mg	Table 6
PTCDA electrode	16.1	mg	Table 3
Electrolyte	0.0560	g	Table 7
Separator	0.00628	g	Table 8
Casing	10.0	mg	deep drawing, steel, 650 kN press, automode | deep drawing, steel, 650 kN press, automode | Cutoff, U - RER
	10.0	mg	sheet rolling, steel | sheet rolling, steel | Cutoff, U - RER
	10.0	mg	market for steel, low-alloyed | steel, low-alloyed | Cutoff, U - GLO
Tabs	2.13	mg	market for aluminium collector foil, for Li-ion battery | aluminium collector foil, for Li-ion battery | Cutoff, U - GLO
Output	**Value**	**Unit**	**Market process provider**
Sodium-ion hybrid supercapacitor cell	1	1 coin cell (weighting 109 mg)	n/a

5. Life cycle impact assessment and interpretation

Normalised results for the climate impact and CSI for a coin cell weighing 109 mg are shown in Figure 2. The absolute values for a cell weighing 1 kg (upscaled linearly from the inputs needed for the coin cell) are shown in Table 10. Results show that the AC electrode contributes the most to climate impact (96%) and CSI (88%). This is mainly due to the HNO_3 input (90% and 74%, respectively). Another hotspot for the activated carbon electrode is the deionised water used to process the AC electrode (2% and 11%, respectively).

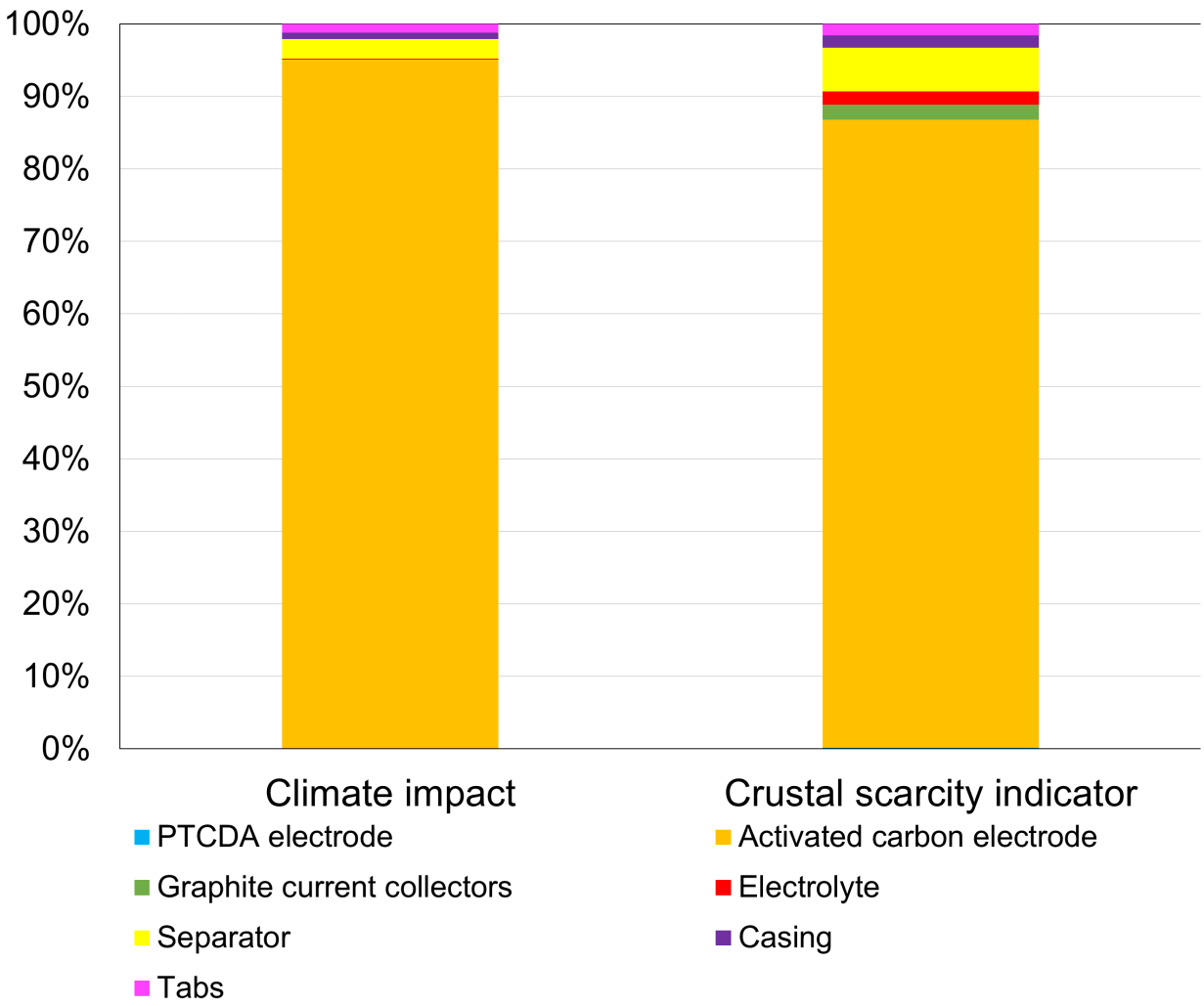

Figure 2: Climate impact and crustal scarcity indicator, normalized to 100%, showing the contributions from the main components of the sodium-ion hybrid supercapacitor.

Table 10: The climate impact and crustal scarcity indicator (CSI) results for one hybrid supercapacitor weighing 1 kg.

Component		Climate impact (kg CO_2 eq.)	CSI (kg Si eq.)
PTCDA electrode	PTCDA	1.3E-2	1.7
	Carbon black	2.8E-3	0.5
	CMC	2.8E-3	0.5
	Graphite foil	2.9E-3	21
	Deionised water	9.2E-6	0.004
	Electricity	2.2E-6	0.0002
	Steam	7.6E-3	0.3
Activated carbon electrode	Activated carbon	1.5E-1	17
	Carbon black	9.2E-3	1.5
	CMC	9.0E-3	1.7
	Graphite foil	2.9E-3	21
	Steam	2.4E-2	0.9
	Electricity	3.5E-2	4
	Deionised water	4.7E-1	213
	HNO_3	24	1481
	Waste water treatment	3.5E-1	26
Electrolyte	Deionised water	1.4E-4	0.07
	Sodium sulfate	9.0E-3	18
	Magnesium sulfate	1.9E-2	19
	Electricity	3.2E-3	0.3
Separator		6.9E-1	121
Casing		2.4E-1	34
Tabs		3.0E-1	33
Total		**26**	**2015**

To decrease the contribution of HNO_3, the input could be reduced. In fact, treating 19.9 g of AC (needed for the 1 kg cell when linearly scaled up from coin cell) requires almost 370 liters, corresponding to about two normal size bath-tubs filled with HNO_3, even when the amount has been reduced by 20% in line with the suggestion by Piccinno et al. (2016). As an example, Soudani, Souissi-najar, and Ouederni (2013) treat 5 g of activated carbon using 50 mL HNO_3 (concentrations varying from 2-6 N[1]). If we assume that we can use the same ratio between AC and HNO_3 (1M) in our production process, the resulting upscaled amount is (50/5)×0.8 = 8 mL per g AC. The resulting amount of HNO_3 needed to treat 2.16 mg AC is 8×10^{-3}L/g×2.16×10^{-3}g AC = 0.0173mL HNO_3 (consisting of 1 Mol/L×0.0173 mL×63.01 g/Mol = 0.00107 g HNO_3 and 0.0173-0.00107 = 0.0159 g

[1] N stands for Normality, a measure of concentration with the unit equivalents per litre.

deionized water to reach the right concentration, see Eq. 3 and 4. Figure 3 shows the results when adjusting the amount of HNO_3 needed in the production.

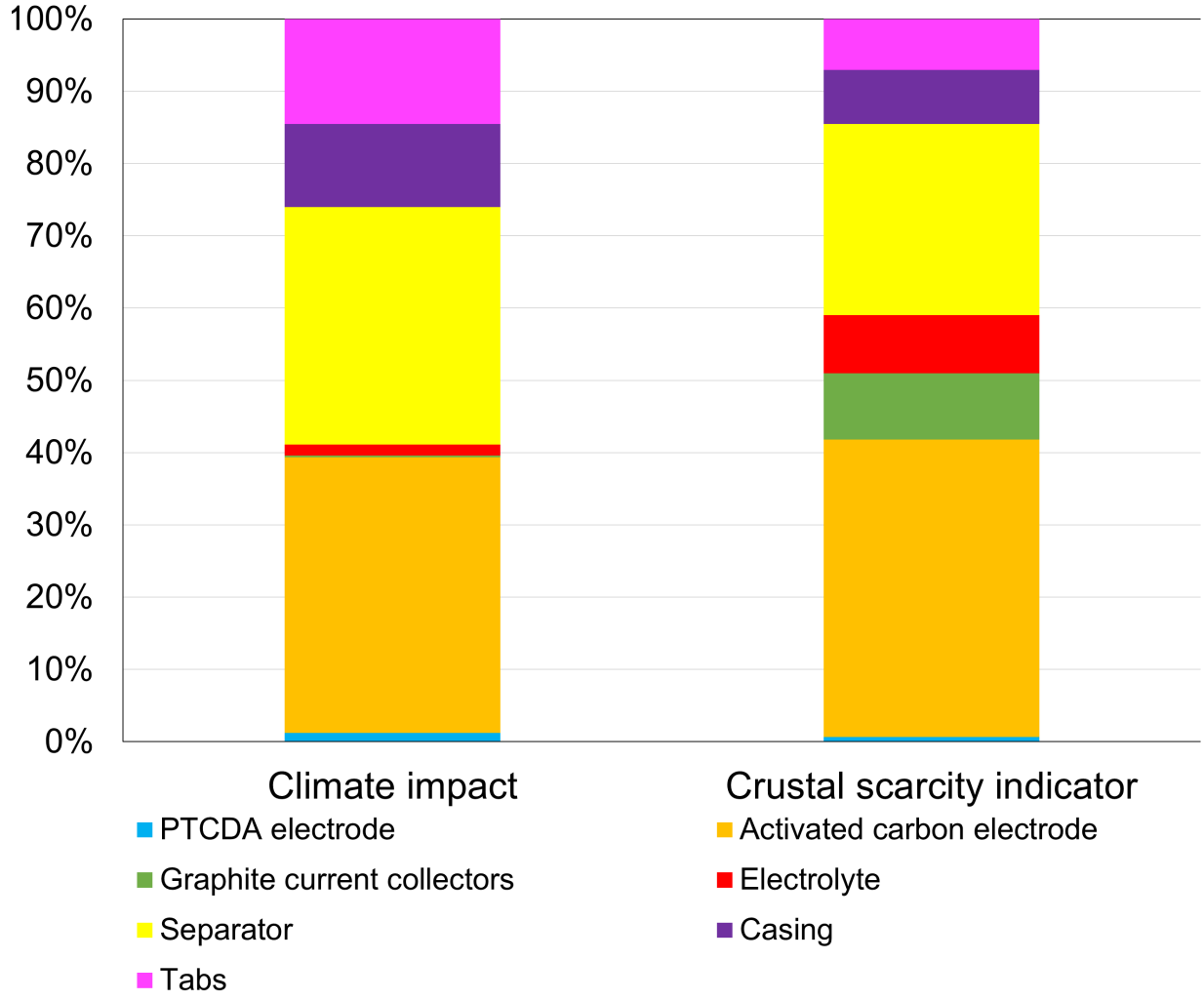

Figure 3: Climate impact and crustal scarcity indicator, normalized to 100%, showing the contributions from the main components of the sodium-ion hybrid supercapacitor when decreasing the use of HNO_3.

Figure 3 shows that when decreasing the amount of HNO_3, the activated carbon electrode is still a main contributor. This is now primarily related to the use of deionized water (climate impact and CSI) and the treatment of polluted water (climate impact). Another main contributor is now the cellulose separator due to the use of steam and urea (for climate impact) and sodium hydroxide and epichlorohydrin (for the CSI) in the production process. Notably, using less HNO_3 increases the relative impacts related to casing and tabs.

Table 11 shows the linearly upscaled impacts from producing a 1 kg cell.

Table 11: The climate impact and crustal scarcity indicator (CSI) results for one hybrid supercapacitor weighing 1 kg, when using less HNO_3.

Component		Climate impact (kg CO_2 eq.)	CSI (kg Si eq.)
PTCDA electrode	PTCDA	1.3E-2	1.7
	Carbon black	2.8E-3	0.5
	CMC	2.8E-3	0.5
	Graphite foil	2.9E-3	21
	Deionised water	9.2E-6	0.004
	Electricity	2.2E-6	0.0002
	Steam	7.6E-3	0.3
Activated carbon electrode	Activated carbon	1.5E-1	17
	Carbon black	9.2E-3	1.5
	CMC	9.0E-3	1.7
	Graphite foil	2.9E-3	21
	Steam	2.4E-2	0.9
	Electricity	3.5E-2	4
	Deionised water	3.0E-1	145
	HNO_3	1.0E-3	0.7
	Waste water treatment	1.8E-1	18
Electrolyte	Deionised water	1.4E-4	0.07
	Sodium sulfate	9.0E-3	18
	Magnesium sulfate	1.9E-2	19
	Electricity	3.2E-3	0.3
Separator		6.9E-1	121
Casing		2.4E-1	34
Tabs		3.0E-1	33
Total		**2**	**459**

As it is assumed that the production of the hybrid supercapacitor is to take place in the future, we also assess the influence of changes to the energy system. We therefore change the European energy mix to a Swedish energy mix, assuming that the energy system in Europe will be significantly decarbonized in the future. The procedure for changing the electricity mix in the foreground system, and parts of the background system is described in the Appendix. Figure 4 shows the climate impact and CSI in a future where less nitric acid is used, and the electricity system is significantly decarbonized.

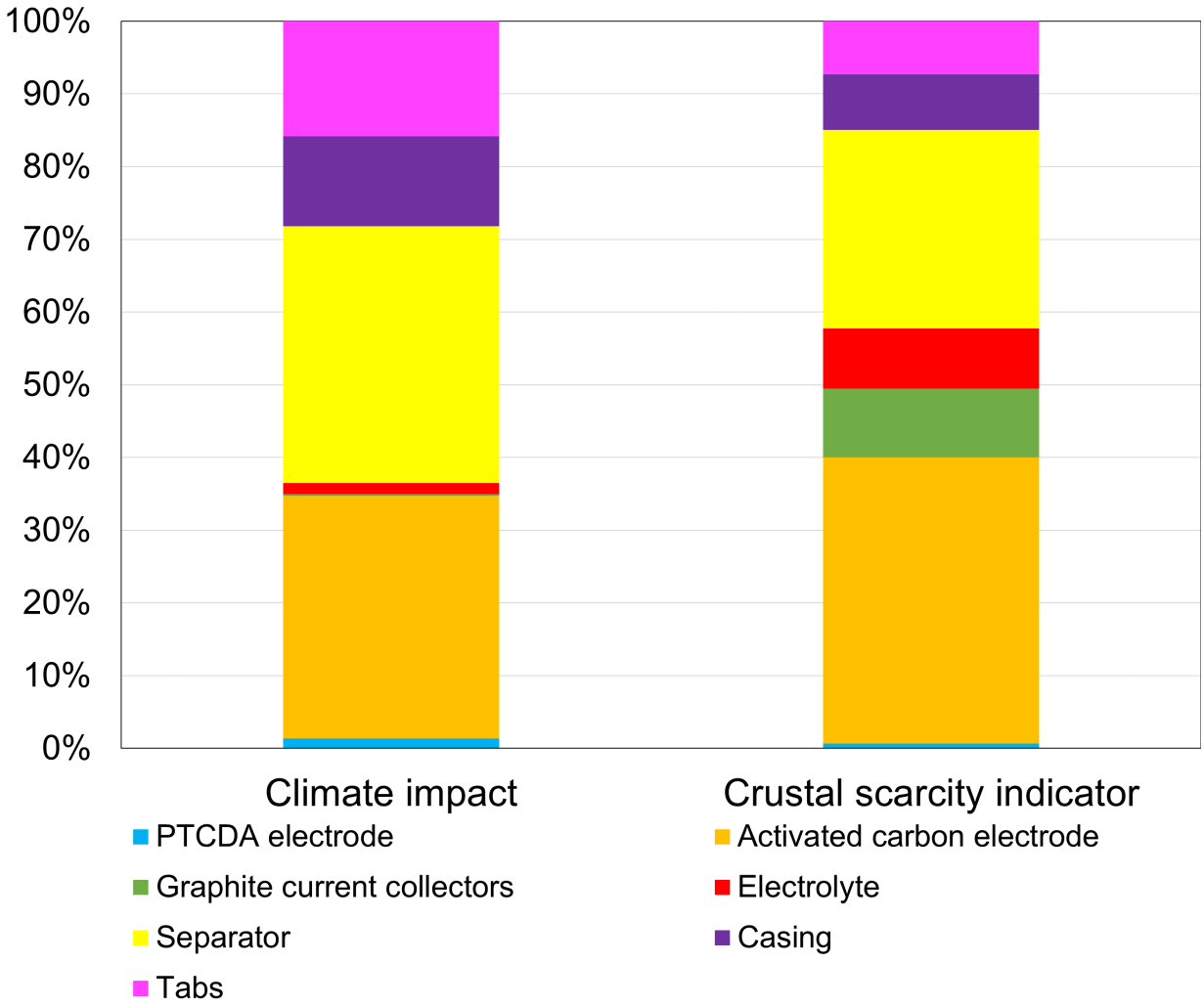

Figure 4: Climate impact and crustal scarcity indicator, normalized to 100%, showing the contributions from the main components of the sodium-ion hybrid supercapacitor when decreasing the use of HNO_3 and transitioning to a decarbonized electricity system.

Results in Figure 4 show that changing the electricity mix has little influence on the normalized environmental impacts. This is primarily due to the relatively low electricity inputs in the system compared to direct emissions of CO_2 from processes (for example the activated carbon production).

The linearly upscaled results needed to produce 1 kg of HSC cell are shown in Table 12.

Table 12: The climate impact and crustal scarcity indicator (CSI) results for one hybrid super-capacitor weighing 1 kg, when using less HNO_3 and the electricity system is decarbonized.

Component		Climate impact (kg CO_2 eq.)	CSI (kg Si eq.)
PTCDA electrode	PTCDA	1.3E-2	1.7
	Carbon black	2.8E-3	0.5
	CMC	2.8E-3	0.5
	Graphite foil	2.9E-3	21
	Deionised water	7.6E-6	0.004
	Electricity	2.3E-7	4E-5
	Steam	7.4E-3	0.3
Activated carbon electrode	Activated carbon	1.4E-1	16
	Carbon black	9.2E-3	1.5
	CMC	9.0E-3	1.7
	Graphite foil	2.9E-3	21
	Steam	2.4E-2	0.8
	Electricity	3.6E-3	0.7
	Deionised water	2.7E-1	141
	HNO_3	1.0E-3	0.7
	Waste water treatment	1.8E-1	12
Electrolyte	Deionised water	1.2E-4	0.06
	Sodium sulfate	9.0E-3	18
	Magnesium sulfate	1.9E-2	19
	Electricity	3.4E-4	0.06
Separator		6.8E-1	120
Casing		2.2E-1	34
Tabs		3.0E-1	32
Total		**1.9**	**443**

6. Scaling up data for other contexts

We assume that the data generated in this report can be upscaled and used in different screening contexts for assessing the transition to sodium-ion HSC in electric vehicles. Note that while we suggest performance can be scaled roughly linearly, reality is more complex. Therefore, the upscaled data should be seen as an indication of the environmental impact or a "building block" to be used in a compiled larger study to gain preliminary insights into the impacts of product systems involving sodium-ion HSCs.

For example, we can assume that the required function in a vehicle is 1 kW of power provided. As the power density of the studied HSC is 4500 W/kg active material, 1000W/4500 W/kg = 0.22 kg active material in the HSC is needed to achieve this function. The active materials (PTCDA and AC) constitute 2.9% of the cell (excluding casing and tabs), meaning that 0.22/0.029 = 7.6 kg total cell weight is needed. In addition, 0.79 kg steel (10% of cell without casing and tabs weight) for the casing and 0.17 kg aluminium (2.2% of cell without casing and tabs weight) for the tabs are needed. This corresponds to a total of 8.5 kg total sodium-ion HSC weight. When using the fully upscaled results (with less nitric acid and a decarbonized electricity system), this results in a climate impact of 16 kg CO_2 eq. and CSI result of 3800 kg Si eq per kW.

7. Conclusions

Results show that the use of HNO_3 in the AC electrode production process when upscaling the lab process is the main hotspot, responsible for a considerable share of the climate impact (91%) and CSI (74%) along the life cycle. Measures should be taken to decrease this use and we show that using less nitric acid could significantly decrease these impacts. This also highlights an issue with upscaling laboratory processes, even when following established frameworks. This is because at lab scale, a larger amount of solvent than is needed for the required reaction can be used. This can be either for practical reasons (size of pipettes, difficulties stirring small amounts) or because of the small scale of operations making monetary or environmental impacts from using a slightly larger amount than actually needed justifiable. However, when using frameworks to upscale, this could lead to skewed LCA results. Future research should include an investigation of the minimum amount of HNO_3 needed in the activated carbon electrode production in the lab process, as we have now used a value from literature as a proxy. This would increase the accuracy of the LCA results and could feed into future upscaling of similar lab-processes to industrial scale.

8. Acknowledgement

Funding for this study was kindly provided by the Area of Advance Energy's Sustainable Vehicle Technologies profile area, through the project "Less environmentally unfriendly and more performance next generation electric powertrains: Part III. LCA and material recyclability assessment". The authors also acknowledge helpful input from Patrik Johansson and Martin Karlsmo.

9. References

Arvidsson, R., Svanström, M., Sandén, B. A., Thonemann, N., Steubing, B., & Cucurachi, S. (2023). Terminology for future-oriented life cycle assessment: review and recommendations. *The International Journal of Life Cycle Assessment*. doi:https://doi.org/10.1007/s11367-023-02265-8

Arvidsson, R., Söderman, M. L., Sandén, B. A., Nordelöf, A., André, H., & Tillman, A.-M. (2020). A crustal scarcity indicator for long-term global elemental resource assessment in LCA. *The International Journal of Life Cycle Assessment, 25*(9), 1805-1817. doi:10.1007/s11367-020-01781-1

Chordia, M., Wikner, E., & Nordelöf, A. (2022). *A model platform for solving lithium-ion battery cell data gaps in life cycle assessment*. Paper presented at the Electric Vehicle Symposium 35, Olso, Norway. https://research.chalmers.se/publication/531922/file/531922_Fulltext.pdf

Conte, M., Genovese, A., Ortenzi, F., & Vellucci, F. (2014). Hybrid battery-supercapacitor storage for an electric forklift: a life-cycle cost assessment. *Journal of applied electrochemistry, 44*, 523-532. doi:https://doi.org/10.1007/s10800-014-0669-z

Dessbesell, L., Paleologou, M., Leitch, M., Pulkki, R., & Xu, C. (2020). Global lignin supply overview and kraft lignin potential as an alternative for petroleum-based polymers. *Renewable and Sustainable Energy Reviews, 123*, 109768. doi:https://doi.org/10.1016/j.rser.2020.109768

Hermansson, F., Edgren, F., Xu, J., Asp, L. E., Janssen, M., & Svanström, M. (2023). Climate impact and energy use of structural battery composites in electrical vehicles—a comparative prospective life cycle assessment. *The International Journal of Life Cycle Assessment*. doi:https://doi.org/10.1007/s11367-023-02202-9

International Organization of Standardization. (2006). *Environmental management-Life cycle assessment-Principles and framework (ISO 14040)*. Retrieved from https://www.iso.org/obp/ui/#iso:std:iso:14040:ed-2:v1:en

Karlsmo, M., & Johansson, P. (2022). Sustainability and Technical Performance of An All-Organic Aqueous Sodium-Ion Hybrid Supercapacitor. *Batteries & Supercaps, 5*(11), e202200306. doi:https://doi.org/10.1002/batt.202200306

Lamb, J. J., & Burheim, O. S. (2021). Lithium-ion capacitors: A review of design and active materials. *Energies, 14*(4), 979. doi:https://doi.org/10.3390/en14040979

Liu, H., Zhang, M., Song, Z., Ma, T., Huang, Z., Wang, A., & Shao, S. (2021). A super hybrid supercapacitor with high energy density based on the construction of CoMoO4/MoO2 decorated 3D sulfur-doped graphene and porous lotus leaves carbon. *Journal of Alloys and Compounds, 881*, 160660. doi:https://doi.org/10.1016/j.jallcom.2021.160660

Piccinno, F., Hischier, R., Seeger, S., & Som, C. (2016). From laboratory to industrial scale: a scale-up framework for chemical processes in life cycle assessment studies. *Journal of Cleaner Production, 135*, 1085-1097. doi:https://doi.org/10.1016/j.jclepro.2016.06.164

Prior, T., Wäger, P. A., Stamp, A., Widmer, R., & Giurco, D. (2013). Sustainable governance of scarce metals: The case of lithium. *Science of The Total Environment, 461-462*, 785-791. doi:https://doi.org/10.1016/j.scitotenv.2013.05.042

Rudnick, R. L., & Gao, S. (2003). 3.01 - Composition of the Continental Crust. In H. D. Holland & K. K. Turekian (Eds.), *Treatise on Geochemistry* (pp. 1-64). Oxford: Pergamon.

Shanmugam, K., Chandrasekar, N., & Balaji, R. (2023). Barrier Performance of Spray Coated Cellulose Nanofibre Film. *Micro, 3*(1), 192-207. Retrieved from https://www.mdpi.com/2673-8023/3/1/14

Soudani, N., Souissi-najar, S., & Ouederni, A. (2013). Influence of Nitric Acid Concentration on Characteristics of Olive Stone Based Activated Carbon. *Chinese Journal of Chemical Engineering, 21*(12), 1425-1430. doi:https://doi.org/10.1016/S1004-9541(13)60638-2

Wickerts, S., Arvidsson, R., Nordelöf, A., Svanström, M., & Johansson, P. (2024). Prospective life cycle assessment of sodium-ion batteries made from abundant elements. *Journal of Industrial Ecology, 28*(1), 116-129. doi:https://doi.org/10.1111/jiec.13452

Appendix

Table S1: Parameters to calculate the volume of the cell.

Cell component		Density (g/cm^3)	Mass (g)	Volume (cm^3)
PTCDA electrode	PTCDA	1.7	6.1	3.6
	Carbon black	1.95	1.2	0.63
	CMC	1.6	0.8	0.51
	Graphite foil	1.8 (assumed the same as for graphite)	140	78
Activated carbon electrode	Activated carbon	2	20	10
	Carbon black	1.95	4	2.0
	CMC	1.6	3	1.7
	Graphite foil	1.8	140	78
Electrolyte		1.4	515	368
Separator	Cellulose	1.5 (assumed the same as for cellulose)	68	39
Total			888	581

Procedure for changing the electricity mixes

All electricity providers in the foreground system were changed from *"market group for electricity, medium voltage | electricity, medium voltage | Cutoff, U – RER"* to *"market for electricity, medium voltage | electricity, medium voltage | Cutoff, U – SE"*. Subsequently, the providers of all flows in the background system now contributing to more than 5% of the climate impact were also changed.

Activated carbon electrode

<u>market for water, deionised | water, deionised | Cutoff, U -Europe without Switzerland:</u>
The input provider *"Water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland"* was changed.[2] The electricity providers were changed to *"market for electricity, medium voltage | electricity, medium voltage | Cutoff, U – SE"*. The process *"market for sewage sludge |sewage sludge |Cutoff, U – RoW"* was changed such that the provider for the output flow *"Treatment of sewage sludge by anaerobic digestion | sewage sludge | Cutoff, U – RoW"* in turn was altered in terms of the input of electricity and set to the corresponding Swedish market provider.

<u>treatment of wastewater, average, wastewater treatment | wastewater, average | Cutoff, U – Europe without Switzerland:</u>
The electricity provider was changed to the corresponding Swedish market provider.

[2] Deionized water used in the foreground systems of this study was also changed in line with this

activated carbon production, granular from hard coal | activated carbon, granular | Cutoff, U – RER:
The electricity provider was changed to the corresponding Swedish market provider.

Cellulose film production

steam production, in chemical industry | steam, in chemical industry | Cutoff, U – RER:
The process *"market for heat, from steam, in chemical industry | heat, from steam, in chemical industry | Cutoff, U"* has a singular input: *"steam production, as energy carrier, in chemical industry | heat, from steam, in chemical industry | Cutoff, U".* This latter process was changed, and its electricity provider was changed to the corresponding Swedish provider[3].

market for urea | urea | Cutoff, U – RER:
The input providers to *"urea production | urea | Cutoff, U – RER"* was altered in terms of electricity provider, to the corresponding Swedish market, and the provider for steam, *"market for steam, in chemical industry | steam, in chemical industry | Cutoff, U – RER"*, was changed to the steam process altered above in this section.

Current collectors

Market for aluminium collector foil, for Li-ion battery | aluminium collector foil, for Li-ion battery | Cutoff, U – GLO:
The process *"market for aluminium, wrought alloy | aluminium, wrought alloy | Cutoff, U – GLO"* is responsible for 14% of total HSC climate impact, where the process *"market for aluminium, primary, ingot | aluminium, primary, ingot | Cutoff, U – RoW"* is responsible for the majority (12 % of total HSC climate impact). The main contributor to this process is *"aluminium production, primary, ingot | aluminium, primary, ingot | Cutoff, U – CN*" (9% of total HSC climate impact). Here, the provider *"market for electricity, medium voltage, aluminium industry | electricity, medium voltage, aluminium industry | Cutoff, U – CN"* was changed to *"market for electricity, medium voltage | electricity, medium voltage | Cutoff, U – SE"* as there was no specific process available for electricity to the aluminium industry in Sweden.

Casing

market for steel, low-alloyed | steel, low-alloyed | Cutoff, U – GLO:
The process *"steel production, converter, low-alloyed | steel, low-alloyed | Cutoff, U – RoW"* is changed so all electricity inputs are from a Swedish provider.

[3] Steam used in the foreground system of the study was also modelled with this process as the provider.

DEPARTMENT OF TECHNOLOGY
MANAGEMENT AND ECONOMICS
CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden
www.chalmers.se