Supplementary materials

LCA and C-LCC indicator as tools for Sodium-ion batteries eco-design

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Summary: This supporting information contains a full inventory of the different batteries' components and results.

Cathode

Cathode Inventory

Table S1 - Inventory data for the cathodic active material production process, at the laboratory scale, considering two different synthesis processes: Sol-Gel (SG) and Solid-State (SS). For sol-gel synthesis, two scenarios were considered: From nitrates (SG_N) and from acetates (SG_A).

Production process	**SG_N**	**SG_A**	**SS**
	Amount	**Amount**	**Amount**
Input			
Materials			
Sodium nitrate $NaNO_3$ [g]	1.2086	-	-
Manganese nitrate $Mn(NO_3)_2.4H_2O$ [g]	4.9165	-	-
Sodium acetate $C_2H_3NaO_2$ [g] (Carlo Erba, CAS 127-09-3)	-	1.1665	-
Manganese acetate tetrahydrate $(CH_3COO)_2Mn \cdot 4H_2O$ [g] (Acros Organic, CAS 6156-78-1)	-	4.8005	-
Citric acid $C_6H_8O_7$ [g] (Carlo Erba, CAS 5949-29-1)	12.8999	6.2466	-
Deionized water [ml]	100	100	5
Manganese carbonate $MnCO_3$ [g] (Sigma-Aldrich, CAS 598-62-9)	-		2.25149
Sodium carbonate Na_2CO_3 [g] (Sigma-Aldrich, CAS 497-19-8)	-		0.68508
Energy/Heat			
Stirring and heat at 80°C [kWh]	0.1300	0.1300	-
Heat treatment [kWh]	12	12	10.56
Milling [kWh]	-	-	0.25
Output			
$Na_{0.66}MnO_2$ [g]	2	2	2
Emissions			
CO_2 [g]	-	2.5749	0.93657
H_2O [ml]	101.4258	101.3921	5
NO_2 [g]	2.6992	-	-
$C_6H_8O_7$ [g]	12.9899	6.2466	-

Table S2 shows the inventory data sources for modelling background processes. The processes have been modelled through specific datasets available on Ecoinvent 3.8 or, when not available in Database, literature data have been used.

Table S2 - Background processes modelling for the cathodic active material $Na_{0.66}MnO_2$ production.

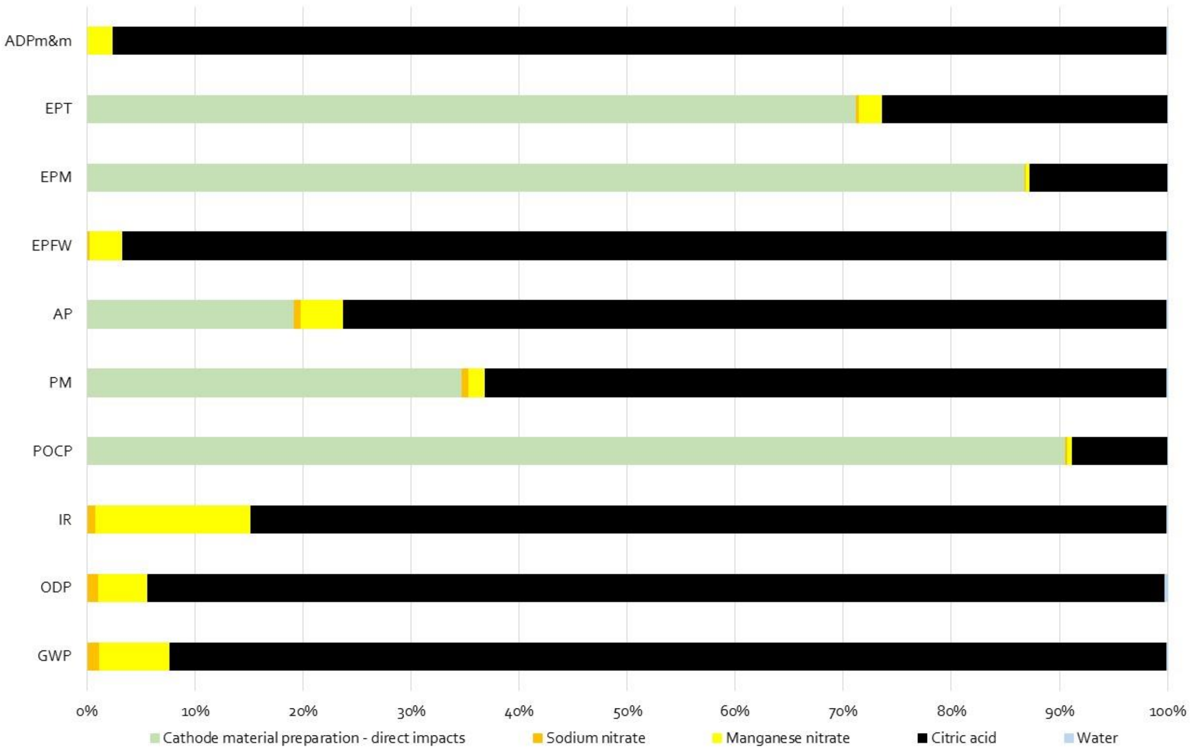
Procut flow	**Data source**	**Dataset/ Reference**
Manganese carbonate $MnCO_3$	Literature	Dai [1]
Sodium carbonate Na_2CO_3	*Ecoinvent* 3.8 dataset	Soda ash, dense {GLO}∣ market for ∣ Cut-off, U
Sodium acetate $C_2H_3NaO_2$	Literature	Jungbluth [2]
Manganese acetate tetrahydrate $(H_3CCOO)_2Mn{\cdot}4H_2O$	Literature	Dai [1]
Energy	Literature	Carvalho [3]
Citric acid $C_6H_8O_7$	*Ecoinvent* 3.8 dataset	Citric acid {GLO}∣ market for ∣ Cut-off, U
Manganese nitrate $Mn(NO_3)_2.4H_2O$	Literature	Johansson and Norrman [4]
Sodium nitrate $NaNO_3$	*Ecoinvent* 3.8 dataset	Sodium nitrate, technical grade {GLO}∣ market for sodium nitrate, technical grade ∣ Cut-off, U
Deionized water	*Ecoinvent* 3.8 dataset	Water, deionized {Europe without Switzerland} ∣ market for water, deionized ∣ Cut-off, U

Table S3 – Average work potentials and capacities (SG_N: Sol-gel synthesis from nitrates; SG_A: Sol-gel synthesis from acetates; SS: Solid state synthesis).

	Potential (V)	Capacity (mAh/g)	Potential (V)	Theoretic capacity (mAh/g)
SG_N	3.08	160	4.4	175
SG_A*	3.08	160		
SS	2.96	137.5		

* The same as SG_N

Cathode results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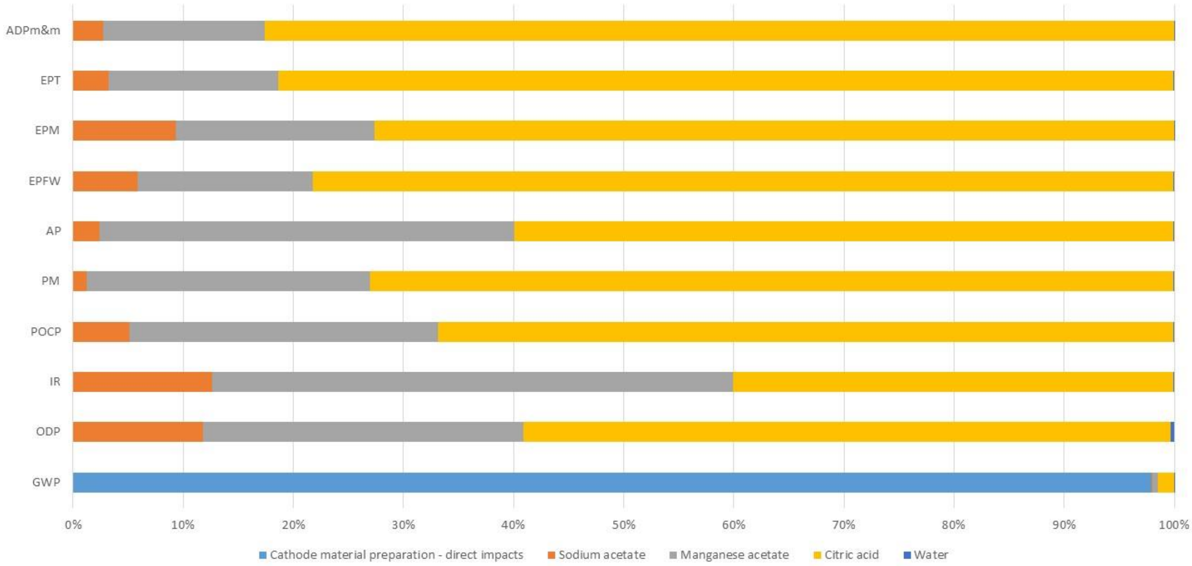
80%
90%
100%
Cathode material preparation - direct impacts
Sodium nitrate
Manganese nitrate
Citric acid
Water

(a)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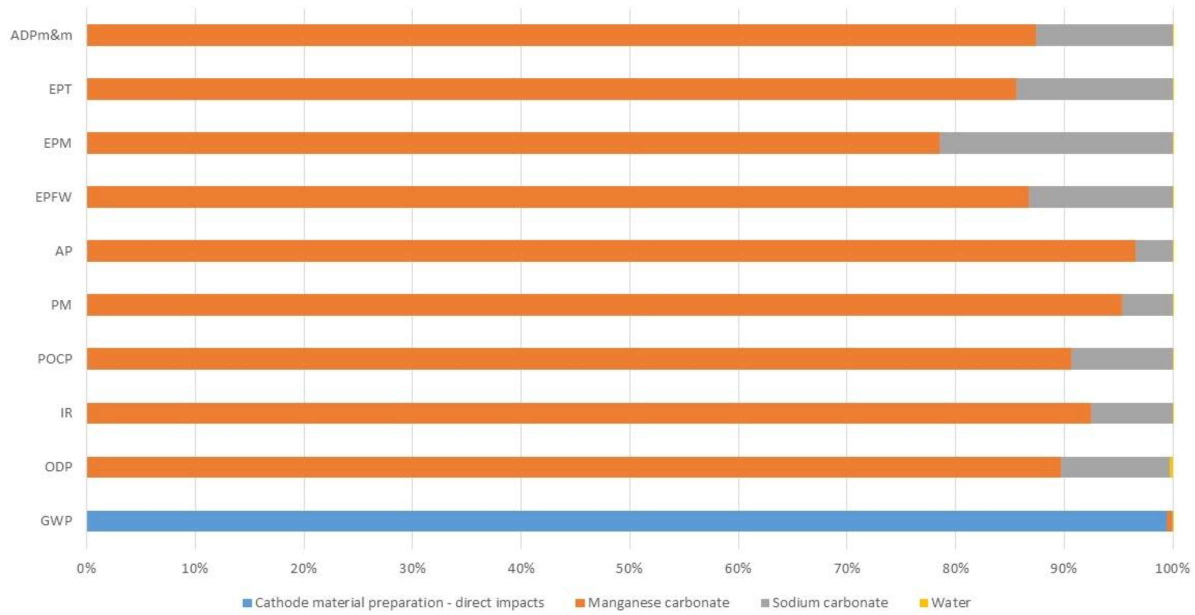
100%
Cathode material preparation - direct impacts
Sodium acetate
Manganese acetate
Citric acid
Water

(b)



(c)

Figure S1. Impact assessment results for 1 Wh of cathodic active material capacity, broken down different components/phases of the production proces, excluding energy consumption: (a) SG_N: sol-gel synthesis, nitrate precursors; (b) SG_A: sol-gel synthesis, acetate precursors and (c) SS: solid state synthesis (GWP: Global warming Potential, ODP: Ozone depletion potential, IR: Ionizing radiation, POCP: Photochemical ozone formation, PM: Particulate matter, AP: Acidification, EPFW: Eutrophication freshwater, EPM: Eutrophication marine, EPT: Eutrophication terrestrial, ADPm&m: Resource use, minerals and metals).

Anode

Anode Inventory

Table S1 – Inventory data for anode materials production process, at laboratory scale.

Production process	**Sn-NC_PVDF**	**Sn-NC_CMC**	**Sn**
Anodic active material production	**Amount**	**Amount**	**Amount**
Input			
Materials			
Sn powder [g] (Atlantic equipment engineers, CAS 7440-31-5)	0.67	0.58	0.7
Carbon nanofibers [g] (Sigma-Aldrich, CAS 308063-67-4)	0.13	0.12	
Energy/Heat			
Milling [kWh]	0.40	0.35	0.42
Output			
Sn and Carbon nanofibers	0.8	0.7	0.7
Anodic material production	**Amount**	**Amount**	**Amount**
Input			
Materials			
Anodic active material [g]	0.8	0.7	0.7
Binder_ PVDF [g] (Solef, Solvay)	0.1		0.1

Binder_ CMC [g] (Sigma-Aldrich, CAS 9004-32-4)		0.15	
Additive_ Black carbon (C65) [g] (Imerys, CAS 1333-86-4)	0.1	0.15	0.2
Solvent_ acetone[g]	5.91		
Solvent_ demi water [g]		8.33	
Solvent_ NMP[g]			6.85
Energy/Heat			
Energy drying [kWh]	4.08	4.08	3.27
Energy calendering [kWh]	1	1	1
Output			
Materials			
Anodic material [g]	1	1	1
Emissions			
Acetone [g]	5.91		
Demi water [g]		8.33	
NMP [g]			6.85

Table S2 – Average work potentials and capacities.

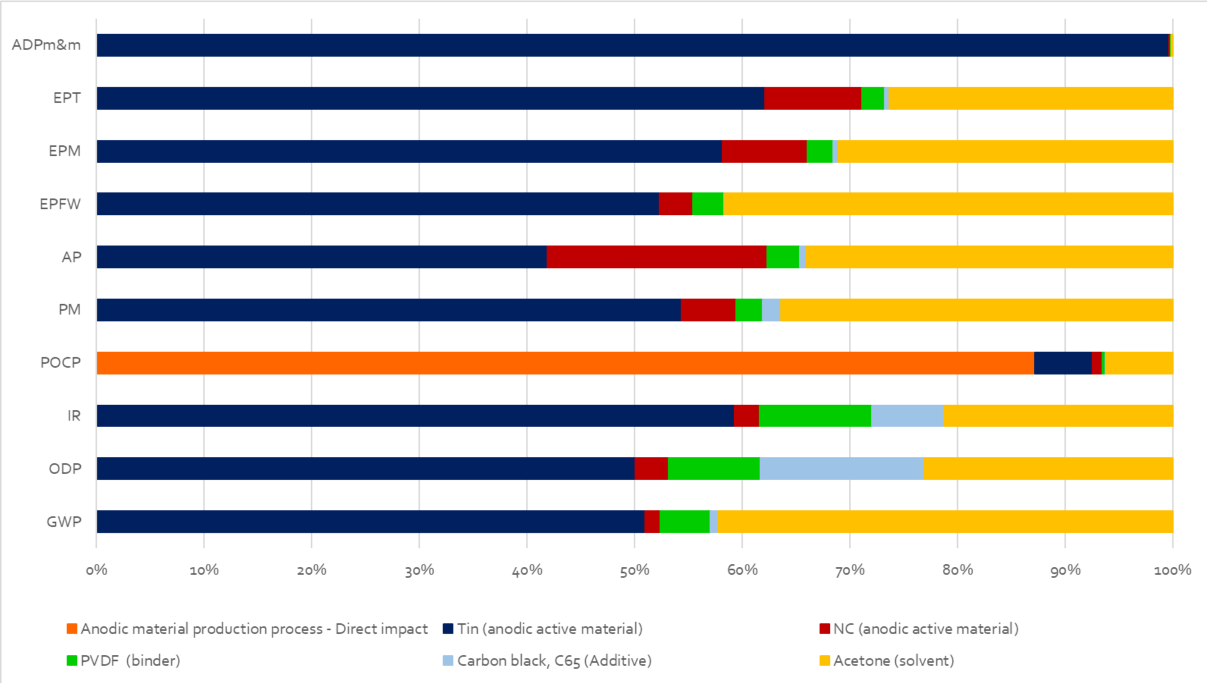
Anodic material	Potential (V)	Capacity (mAh/g)	Sn theoretical capacity (mAh/g)
Sn-NC_PVDF	0.64	85.5	847
Sn-NC_CMC	0.56	89	
Sn	0.58	222	

Table S6 shows the inventory data sources for modeling background processes. The processes have been modeled through specific datasets available on Ecoinvent 3.8 or, when not available in Database, literature data have been used.

Table S3 – Background processes modelling for the anodic materials.

Product flow	Data source	Dataset/ Reference
Sn powder	*Ecoinvent* 3.8 dataset	Tin {GLO}, market for ǀ Cut-off, U
Carbon nanofibers	Literature	Khanna et al. [5]
Energy	Literature	Carvalho et al. [3]
Binder_ PVDF	*Ecoinvent* 3.8 dataset	Polyvinylfluoride {GLO}ǀ market for ǀ Cut-off, U (proxy for PVDF)
Binder_ CMC	*Ecoinvent* 3.8 dataset	Carboxymethyl cellulose, powder {GLO}ǀ market for ǀ Cut-off, U
Additive – Carbon black (C65)	*Ecoinvent* 3.8 dataset	Carbon black {GLO}ǀ market for ǀ Cut-off, U RSE
Solvent_ Acetone	*Ecoinvent* 3.8 dataset	Acetone, liquid {RER}ǀ market for acetone, liquid ǀ Cut-off, U
Solvent_ Demi water	*Ecoinvent* 3.8 dataset	Water, deionised {Europe without Switzerland} ǀ market for water, deionised ǀ Cut-off, U
Solvent_ N-metil-2-pirrolidone	*Ecoinvent* 3.8 dataset	N-methyl-2-pyrrolidone {GLO}ǀ market for ǀ Cut-off, U

Anode Results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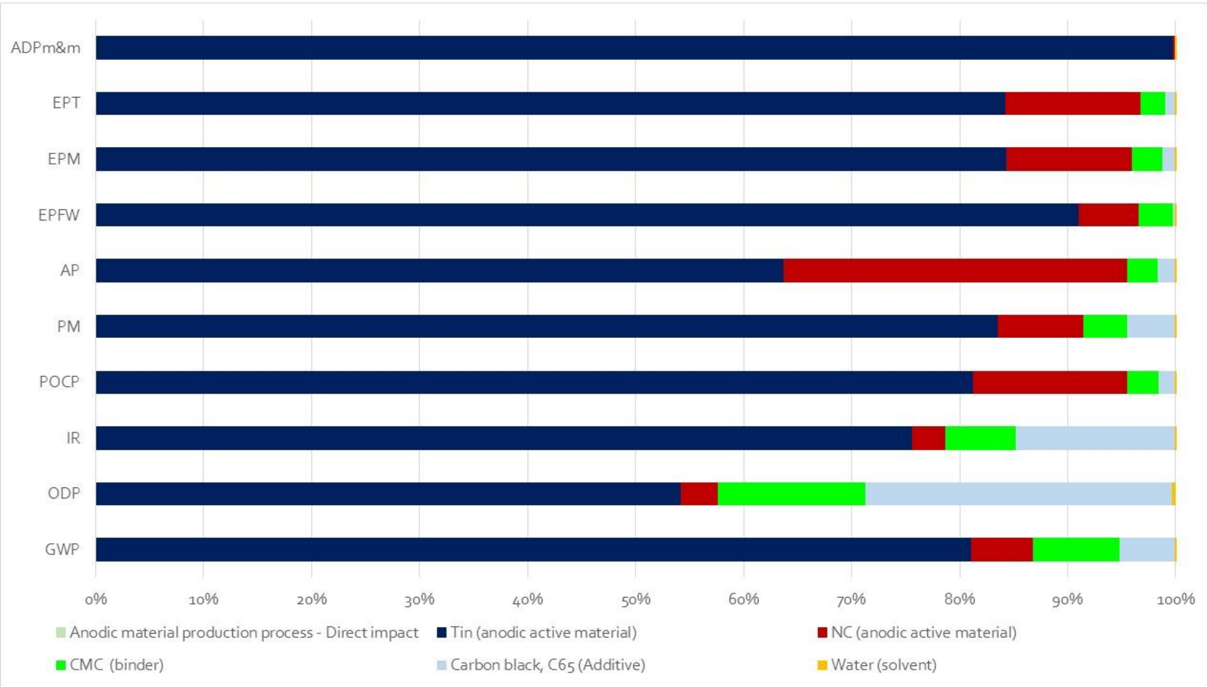
ODP
GWP
0%
10%
20%
30%
40%
50%
60%
70%
80%
90%
100%
Anodic material production process - Direct impact
Tin (anodic active material)
NC (anodic active material)
PVDF (binder)
Carbon black, C65 (Additive)
Acetone (solvent)

(a)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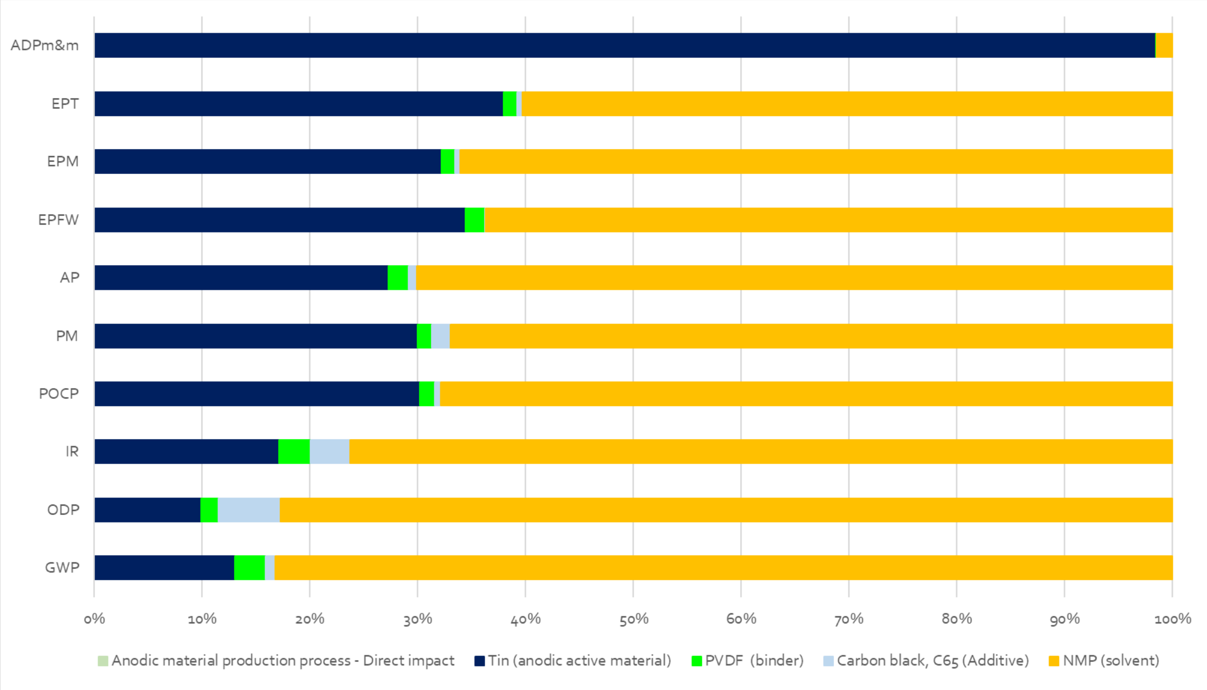
80%
90%
100%
Anodic material production process - Direct impact
Tin (anodic active material)
NC (anodic active material)
CMC (binder)
Carbon black, C65 (Additive)
Water (solvent)

(b)



(c)

Figure S2. Impact assessment results for 1 Wh of anode material capacity, broken down different components/phases of the production proces, excluding energy consumption: (a) Sn-NC_PVDF ; (b) Sn-NC_CMC and Sn (c) (GWP: Global warming Potential, ODP: Ozone depletion potential, IR: Ionizing radiation, POCP: Photochemical ozone formation, PM: Particulate matter, AP: Acidification, EPFW: Eutrophication freshwater, EPM: Eutrophication marine, EPT: Eutrophication terrestrial, ADPm&m: Resource use, minerals and metals).

Uncertainty analysis: Monte Carlo

The C-LCC indicator is based on market prices: therefore, price fluctuations might have an impact on the indicator values. Market price volatility might be factored-in with an uncertainty assessment carried out with the Monte Carlo method.

Since the probability distribution of price series in unknown (and cannot be estimated with distribution fitting techniques due to the low number of observations), it is assumed that all price series follow a triangular distribution. The parameters used to describe the triangular distribution are the maximum and minimum values of each price series during a ten-year period and the mean (used to compute the baseline indicator) over the same period.

Starting from triangular distributions, for each series, 10,000 casual values have been generated, in turn used to compute the C-LCC indicator for 10,000 times. Given the high number of simulations, the empirical distribution function is used to calculate the probability that the C-LCC falls above or under the baseline value and the probability that – given price volatility – the C-LCC calculated for an anode (cathode) is higher or lower that calculated for the other alternatives.

The Monte Carlo analysis, therefore, is an effective tool to assess the robustness of the baseline values and the ordering of the alternatives based on the C-LCC indicator. Figure S3 and figure S4 illustrate the simulation results, while figures S5 and S6 show the probabilities that, given price fluctuations, the indicator falls below baseline values. Such likelihood is high in all cases, meaning that the baseline values are relatively "optimistic".

Finally, the Monte Carlo analysis shows that, even taking price volatility into account, the ordering of the anodes and cathodic active materials considered do not change, highlighting the high robustness of the indicator in identifying the less natural resource-intensive alternatives.

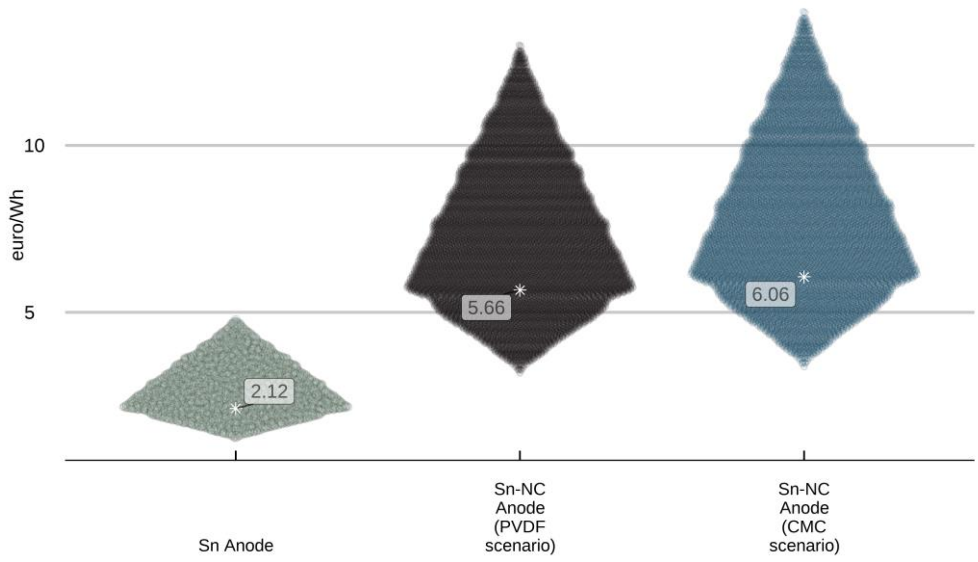


Figure S3. Anode: Monte Carlo simulations and comparison with baseline values.

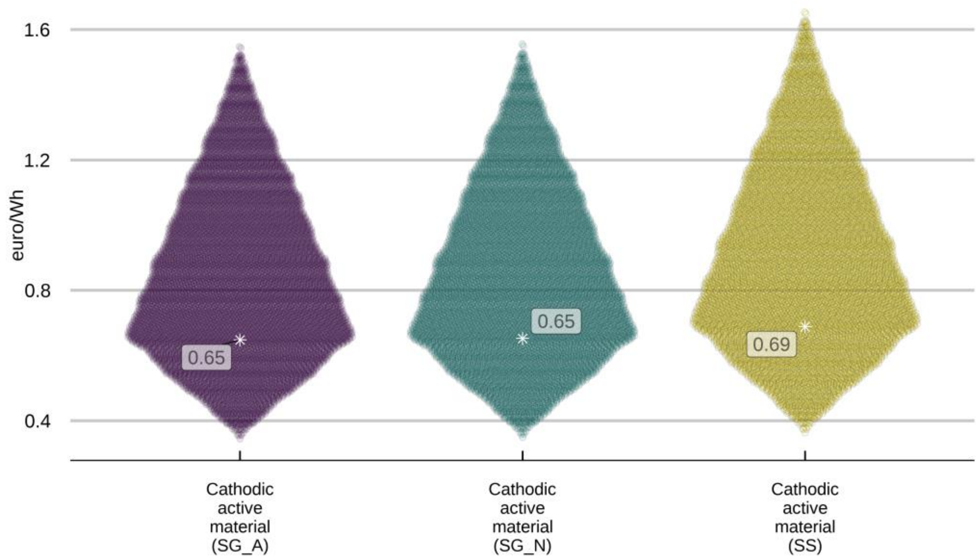


Figure S4. Cathodic material: Monte Carlo simulations and comparison with baseline values.

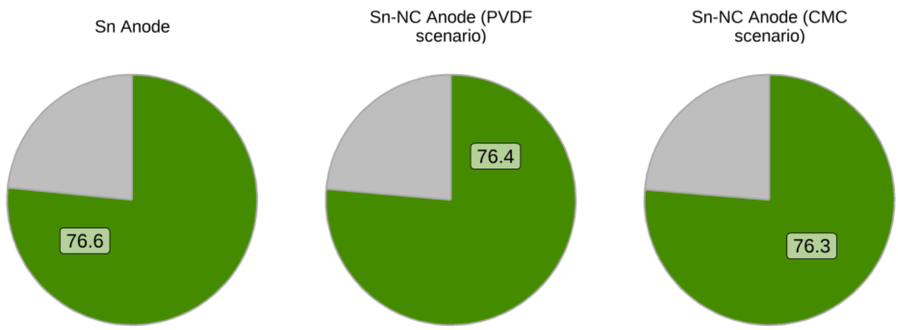


Figure S5. Anode: probabilities that the C-LCC indicator falls below the baseline value, given price fluctuations.

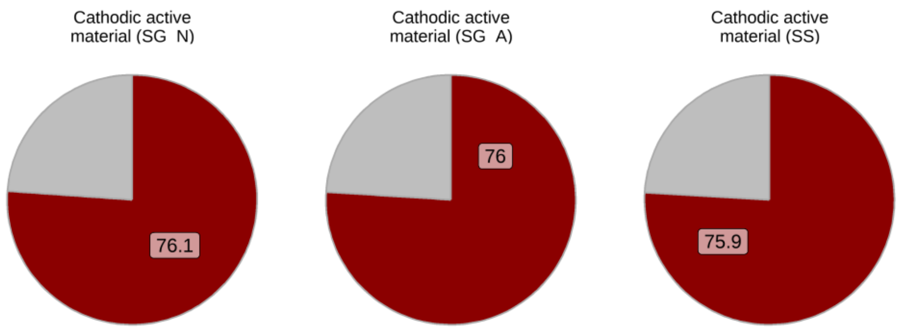


Figure S6. Cathod material: probabilities that the C-LCC indicator falls below the baseline value, given price fluctuations.

References

[1] Q. Dai, "Life Cycle Assessment of Natural Gas Utilization in Light-duty Passenger Vehicles," Civil and Environmental Engineering Ann Arbor,University of Michigan, MI (USA), 2014.

[2] N. Jungbluth, "Life Cycle Inventory of Sodium Acetate and Expanded Graphite," ESU-servives Ltd., 2008.

[3] M. L. Carvalho, B. Marmiroli, G. Mela and A. Molocchi, "LCA ed esternalità del kWh italiano: 2020 e scenari futuri," RSE SpA, Milano, 2022.

[4] E. Johansson and F. Norrman, "Life cycle analysis on phase change materials for thermal energy storage," Royal institute of technology (KTH), Stockholm, 2019.

[5] V. Khanna, B. Bakshi and L. Lee, "Carbon Nanofiber Production. Life Cycle Energy Consumption and Environmental Impact," *Journal of Industrial Ecology*, vol. 12, no. 3, pp. 394-410, 2008.