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Integrated Hybrid Life Cycle Assessment and Supply Chain Environmental Profile Evaluations of Lead-based (Lead Zirconate Titanate) versus Lead-free (Potassium Sodium Niobate) Piezoelectric Ceramics

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Supporting Information Document

This document includes:

- Supplementary Data and Methods
- Supplementary Results and Discussion
- Supplementary References

This Supplementary Information document includes:

(1) Unit process exchanges (materials and energy) representing the process analysis data for 1 kg of PZT and 1 kg of KNN; (2) Breakdown of electrical and thermal energy consumption for the production of 1 kg of PZT and 1 kg of KNN (3) Life cycle inventory analysis of materials whose emissions intensity data are not directly available in Ecoinvent database, detailing the steps involved in deriving new emissions intensity data; (4) Life cycle impact assessment results of PZT and KNN across a number of sustainability metrics; (5) Life cycle impact assessment results of PZT and KNN based on Eco-indicator 99; (6) Derivation of environmental intensities of other indicators (excluding GHG and toxicology) for Input-Output analysis; (7) Supplementary research methodology; (8) Derivation of environmental intensities of toxicology for Input-Output analysis; (9) Disaggregated economic sectors; (10) Risk assessment summary of piezoelectric materials; (11) Sensitivity analysis of emissions intensity of electricity based on different countries (Climate change impact category)

1.0 Supplementary data

1.1 Materials and energy inventory

Table S1a: Unit process exchanges (materials and energy) representing the process analysis data for 1 kg of PZT

Process input	Value	Unit
Titanium dioxide (TiO_2)	0.113	kg
Zirconium dioxide (ZrO_2)	0.190	kg
Lead oxide (PbO)	0.687	kg
Cumulative thermal energy consumption	1145.2	MJ
Cumulative electrical energy consumption	285.14	MJ
Products	**Value**	**Unit**
Lead zirconate titanate (PZT)	1.00	kg
waste	0.29	kg

Table S1b: Unit process exchanges (materials and energy) representing the process analysis data for 1 kg of KNN

Process input	Value	Unit
Potassium carbonate (K_2CO_3)	0.201	kg
Sodium carbonate (Na_2CO_3)	0.154	kg
Niobium pentoxide (Nb_2O_5)	0.773	kg
Cumulative thermal energy consumption	1353.24	MJ
Cumulative electrical energy consumption	295.94	MJ
Products	**Value**	**Unit**
Potassium sodium niobate (KNN)	1.00	kg
Carbon dioxide (CO_2)	0.128	kg
waste	0.310	kg

The quantities of raw materials for PZT and KNN fabrication were derived based on laboratory compositions. Detailed manufacturing routes as well as inventory tables, and life cycle impact assessment data derived from Ecoinvent database[1] and stoichiometry guidelines for LCA[2] is applied where necessary.

1.2 Electrical and thermal energy demand calculations for the fabrication of laboratory-based PZT

Table S2a: Breakdown of electrical energy consumption for the production of 1 kg of PZT

Process	Equipment power rating (W)	Time (s)	Electrical energy (J)	Electrical energy (MJ)
Batch weighing	13.5	1800	24300	0.0243
Ball milling-stage 1	1800	86400	155520000	155.52
Drying-stage 1	50	86400	4320000	4.32
Calcining	1500	14400	21600000	21.6
Ball milling- stage 2	1800	43200	77760000	77.76
Drying-stage 2	50	86400	4320000	4.32
Sintering	2000	10800	21600000	21.60

All energy data in the table above are a function of power of the equipment under consideration and their corresponding operating time. This is then converted into kWh as indicated.

Table S2b: Breakdown of thermal energy consumption for the production of 1 kg of PZT

Mass (kg)		Process	Specific heat capacity (J/kg·K)	Change in temperature (oC)	Change in temperature (K)	Thermal energy (MJ)
1		Drying-stage 1	350	90	363	127.05
1		Calcination	350	800	1073	375.55
1		Drying-stage 2	350	90	363	127.05
1		Sintering	350	1200	1473	515.55
					Total	**1145.2**

1.3 Electrical and thermal energy demand calculations for the fabrication of laboratory-based KNN

Table S3a: Breakdown of electrical energy consumption for the production of 1 kg of KNN

Process	**Equipment power rating (W)**	**Time (s)**	**Electrical energy (J)**	**Electrical energy (MJ)**
Batch weighing	13.5	1800	24300	0.0243
Ball milling-stage 1	1800	86400	155520000	155.52
Drying-stage 1	50	86400	4320000	4.32
Calcining	1500	21600	32400000	32.40
Ball milling- stage 2	1800	43200	77760000	77.76
Drying-stage 2	50	86400	4320000	4.32
Sintering	2000	10800	21600000	21.60

Table S3b: Breakdown of thermal energy consumption for the production of 1 kg of KNN

Mass (kg)	Process	Specific heat capacity (J/kg·K)	Change in temperature (oC)	Change in temperature (K)	Thermal energy (J)	Thermal energy (MJ)
1	Drying-stage 1	420	90	363	152460	152.46
1	Calcination	420	850	1123	471660	471.66
1	Drying-stage 2	420	90	363	152460	152.46
1	Sintering	420	1100	1373	576660	576.66
					Total	**1353.24**

1.4 Life cycle inventory analysis of materials whose emissions intensity data are not directly available in Ecoinvent database

Given that emissions intensity datasets of some of the materials involved for the LCA are not available within the Ecoinvent Database, it follows that their emissions intensity data have to be derived using well established guidelines based on stoichiometry. A simple illustration is given below. As shown, assuming CO_2 is the new material and we know it is produced based on the chemical equation shown.

12 kg of C + 32kg of O_2 = 44kg of CO_2

$$EI\ of\ C = \frac{12}{44}A + \frac{32}{44}B$$

Where A and B represents the emissions intensity, EI ($KgCO_2e$, for example) of carbon oxygen respectively taken from Ecoinvent or other LCA database. With such relationship established, the EI for 1kg of carbon dioxide can then be derived.

1.4.1 Preparation of lead oxide

The environmental sustainability metrics of lead oxide is not available in the Ecoinvent database which was the secondary data sources used for conducting this study. As such, the emissions intensity datasets across a number of indicators were derived on the basis of stoichiometric reactions (i.e. materials) involved in producing lead oxide. The procedure for preparing lead oxide was based on the work of Kwestroo and Huizing[3] as described below:

Precipitation of PbO

The first step involved the preparation of pure ammonia from NH_3 gas (stored in a cylinder) and deionised water, yielding about 15 N ammonia when the solution was saturated at room temperature. This is then followed by the introduction of a purified solution of 120 g of lead acetate in 250 g of water into a 2000 ml silica vessel. 1500 ml concentrated ammonia (15 N) were added while vigorously stirring, yielding a white gelatinous precipitate of basic lead acetate, 2Pb $(OH)_2$. Pb $(CH_3COO)_2$. After stirring for 1 - 2 hours, the white precipitate was found to have transformed into a greenish crystalline mass. X-ray investigations then revealed that orthorhombic (yellow) PbO was formed. Sometimes the transformation did not occur until the precipitate had been washed several times by decanting with concentrated ammonia, thus removing CH_3COO^- ions and adding OH^- ions:

$$2Pb\,(OH)_2 .\ Pb\,(CH_3COO)_2 + 2\,OH^- = 3\,PbO + CH_3COO^- + 3\,H_2O$$

White **green**

The greenish precipitate was washed by decantation with 2N ammonia and the moist precipitate collected in a shallow silica vessel. After first drying at 70 - 95°C the precipitate was heated at 150°C, yielding about 60 g of canary yellow PbO were obtained which is reasonably pure with the main impurity being silica. We refer readers to Kwestroo and Huizing[3] for further details on the procedure for preparing pure PbO. Based on these preparation steps, the emissions intensity of lead oxide was then derived. Given that lead acetate is needed to produce lead oxide with its emissions intensity data also not available in Ecoinvent database, its emissions intensity data were first derived based on its preparation from hydrogen peroxide, lead and acetic acid (Table S4, process input-stage 1) whose emissions intensity data is available. Lead acetate with its newly derived emissions intensity data is now used with emissions intensity data of water, ammonia gas and silica as shown in Table S4 (process input stage 2)

1.4.2 Material and energy inventory of a lead oxide manufacturing route

Table S 4: Material and energy inventory of a lead oxide manufacturing route

Material	Value	Unit
Process input- stage 1		
Hydrogen peroxide	0.11	kg
Lead (at regional storage)	0.64	kg
Acetic acid (in water)	0.37	kg
Product		
Lead acetate (subtotal)	1.46	kg
Process input -stage 2		
Lead acetate	1.46	kg
Water	0.08	kg
Ammonia gas	0.08	kg
Silica	0.27	kg
Final product		
Lead oxide (PbO)	1	kg

Table S5 shows the impact categories/endpoint indicators for lead acetate which was later used as an input to derive the impact categories/ endpoint indicators for lead oxide as shown in Table S6

Table S5: impact categories/ endpoint indicators for lead acetate

Impact categories/ Endpoint indicators	Unit	Hydrogen peroxide	Lead (at regional storage)	Acetic acid (in water)	Lead acetate (subtotal)
Climate change	kgCO2-eq	0.118	0.678	0.574	1.371
Acidification potential	kg SO2-eq	0.000	0.015	0.002	0.017
Eutrophication potential	kg NOx-eq	0.000	0.004	0.001	0.005
Land use	m2a	0.002	0.029	0.013	0.044
Material use	MJ-eq	2.392	10.116	19.685	32.193
Freshwater aquatic ecotoxicity (FAETP 100a)	kg 1, 4-DCB-eq.	0.048	0.709	0.195	0.953
Freshwater sediment ecotoxicity (FSETP 100a)	kg 1, 4-DCB-eq.	0.109	1.453	0.404	1.965
Human toxicity (HTP 100a)	kg 1, 4-DCB-eq.	0.379	0.558	0.195	1.132
Marine aquatic ecotoxicity (MAETP 100a)	kg 1, 4-DCB-eq.	0.185	2.525	0.737	3.447
Marine sediment ecotoxicity (MSETP 100a)	kg 1, 4-DCB-eq.	0.209	2.568	0.763	3.540
Terrestrial ecotoxicity (TAETP 100a)	kg 1, 4-DCB-eq.	0.000	0.000	0.000	0.001
Ionising radiation	DALYs	0.000	0.000	0.000	0.000
Malodours air	m3 air	1600.095	6972.160	38660.130	47232.385
Ecosystem quality	points	0.001	0.025	0.003	0.029
Human health	points	0.002	0.112	0.011	0.125
Resources	points	0.005	0.063	0.045	0.113

Table S6: impact categories/ endpoint indicators for lead oxide

Impact categories/ Endpoint indicators	**Unit**	**Lead acetate (subtotal)**	**Water**	**Ammonia gas**	**Silica**	**Lead oxide (PbO) (Total)**
Climate change	kgCO2-eq	1.371	0.004	0.159	0.661	2.196
Acidification potential	kg SO2-eq	0.017	0.000	0.000	0.003	0.021
Eutrophication potential	kg NOx-eq	0.005	0.000	0.000	0.004	0.010
Land use	m2a	0.044	0.000	0.001	0.071	0.116
Material use	MJ-eq	32.193	0.143	3.188	11.162	46.685
Freshwater aquatic ecotoxicity (FAETP 100a)	kg 1, 4-DCB-eq.	0.953	0.002	0.013	0.208	1.176
Freshwater sediment ecotoxicity (FSETP 100a)	kg 1, 4-DCB-eq.	1.965	0.005	0.027	0.452	2.449
Human toxicity (HTP 100a)	kg 1, 4-DCB-eq.	1.132	0.001	0.064	0.136	1.334
Marine aquatic ecotoxicity (MAETP 100a)	kg 1, 4-DCB-eq.	3.447	0.008	0.155	0.770	4.380
Marine sediment ecotoxicity (MSETP 100a)	kg 1, 4-DCB-eq.	3.540	0.008	0.167	0.814	4.528
Terrestrial ecotoxicity (TAETP 100a)	kg 1, 4-DCB-eq.	0.001	0.000	0.000	0.000	0.001
Ionising radiation	DALYs	0.000	0.000	0.000	0.000	0.000
Malodours air	m3 air	47232.385	28.206	3342.784	8902.555	59505.930
Ecosystem quality	points	0.029	0.000	0.001	0.008	0.037
Human health	points	0.125	0.000	0.002	0.015	0.142
Resources	points	0.113	0.000	0.008	0.025	0.146

1.4.3 Preparation of Niobium pentoxide

The impact categories/endpoint indicators for niobium pentoxide were derived based on the stoichiometric relationship as highlighted in the chemical equation below:

$$6Nb + 10HNO_3 + 42HF + 42NH_3 \cdot H_2O = 10NO + 3Nb_2O_5 + 42NH_4F + 47H_2O$$

Table S 7: Material and energy inventory of a Niobium pentoxide manufacturing route

Material	**Value**	**Unit**
Process input		
Niobium (Nb)	0.699	kg
Nitric acid (HNO_3)	0.790	kg
Hydrogen fluoride (HF)	1.054	kg
Ammonium hydroxide ($NH_3.H_2O$)	1.846	kg
Product	**Value**	**Unit**
Niobium pentoxide (Nb_2O_5)	1.000	kg
Nitrogen monoxide (NO)	0.376	kg
Water (H_2O)	1.062	kg
Ammonium fluoride (NH_4F)	1.951	kg

The material inventory shown in Table S7 was then used as the basis for deriving impact categories/endpoint indicators for niobium pentoxide as shown in Table S8.

Table S8: Life cycle impact assessment results for 1 kg Niobium pentoxide

Impact categories/ Endpoint indicators	Unit	Niobium (Nb)	Nitric acid (HNO3)	Hydrogen fluoride (HF)	Ammonium hydroxide (NH3.H2O)	**Niobium pentoxide (Total)**
Climate change	kgCO_2-eq	181.884	2.508	2.830	3.529	**190.752**
Acidification potential	kg SO_2-eq	1.319	0.008	0.089	0.007	**1.422**
Eutrophication potential	kg NO_x-eq	1.212	0.014	0.011	0.005	**1.242**
Land use	m^2a	54.976	0.015	0.131	0.030	**55.152**
Material use	MJ-eq	3046.751	10.578	55.164	73.672	**3186.165**
Freshwater aquatic ecotoxicity (FAETP 100a)	kg 1, 4-DCB-eq.	70.715	0.103	1.512	0.270	**72.600**
Freshwater sediment ecotoxicity (FSETP 100a)	kg 1, 4-DCB-eq.	147.261	0.216	3.185	0.572	**151.233**
Human toxicity (HTP 100a)	kg 1, 4-DCB-eq.	118.411	0.360	1.930	1.282	**121.984**
Marine aquatic ecotoxicity (MAETP 100a)	kg 1, 4-DCB-eq.	265.630	0.709	5.742	2.809	**274.890**
Marine sediment ecotoxicity (MSETP 100a)	kg 1, 4-DCB-eq.	272.893	0.751	5.923	3.008	**282.575**
Terrestrial ecotoxicity (TAETP 100a)	kg 1, 4-DCB-eq.	0.036	0.000	0.001	0.002	**0.040**
Ionising radiation	DALYs	0.000	0.000	0.000	0.000	**0.000**
Malodours air	m^3 air	901906.638	12637.883	20724.115	86549.387	**1021818.023**
Ecosystem quality	points	5.015	0.009	0.037	0.017	**5.078**
Human health	points	9.166	0.029	0.191	0.045	**9.431**
Resources	points	5.923	0.028	0.100	0.195	**6.247**

1.4.4 Life cycle impact assessment of PZT across a number of sustainability metrics

Table S9: Life cycle impact assessment results of PZT across a number of sustainability metrics

Impact category	Lead oxide	Titanium dioxide	Zirconium dioxide	Electricity	Gas (thermal energy)	Waste disposal	Total
Climate change	1.508	0.565	0.756	41.552	2.282	0.002	46.665
Acidification potential	0.015	0.005	0.004	0.166	0.006	0.000	0.196
Eutrophication potential	0.007	0.002	0.003	0.105	0.008	0.000	0.125
Land use	0.080	0.009	0.044	1.108	0.014	0.001	1.257
Material use	32.073	9.254	13.718	865.612	1148.523	0.074	2069.254
Freshwater aquatic ecotoxicity (FAETP 100a)	0.808	0.083	0.331	8.608	0.163	0.238	10.231
Freshwater sediment ecotoxicity (FSETP 100a)	1.682	0.178	0.705	18.035	0.372	0.571	21.544
Human toxicity (HTP 100a)	0.916	0.114	0.311	6.328	0.232	0.042	7.944
Marine aquatic ecotoxicity (MAETP 100a)	3.009	0.349	1.238	34.818	14.334	0.816	54.564
Marine sediment ecotoxicity (MSETP 100a)	3.111	0.375	1.284	35.763	16.010	0.956	57.498
Terrestrial ecotoxicity (TAETP 100a)	0.001	0.000	0.001	0.006	0.000	0.000	0.008
Ionising radiation	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Malodours air	40880.574	9985.358	5073.760	34958.719	15432.715	51.612	106382.739

Table S 10: Life cycle impact assessment results of PZT based on Eco-indicator 99

	Ecosystem quality	Human health	Resources
Lead oxide	0.025	0.098	0.101
Titanium dioxide	0.003	0.019	0.023
Zirconium dioxide	0.008	0.020	0.024
Electricity	0.140	0.721	1.599
Gas (thermal energy)	0.012	0.035	3.085
Waste disposal	0.189	0.892	4.831
Total	0.377	1.784	9.661

1.4.5 Life cycle impact assessment of KNN across a number of sustainability metrics

Table S11: Life cycle impact assessment results of KNN across a number of sustainability metrics

	Potassium carbonate	Sodium carbonate	Niobium pentoxide	Electricity	Gas (thermal energy)	Waste disposal	Total
Climate change	0.469	0.162	147.451	43.126	2.697	0.543	194.447
Acidification potential	0.002	0.001	1.100	0.172	0.007	0.001	1.282
Eutrophication potential	0.001	0.001	0.960	0.109	0.010	0.000	1.080
Land use	0.015	0.005	42.632	1.150	0.017	0.003	43.822
Material use	8.598	2.963	2462.905	898.398	1357.167	5.231	4735.261
Freshwater aquatic ecotoxicity (FAETP 100a)	0.175	0.051	56.120	8.934	0.192	0.675	66.148
Freshwater sediment ecotoxicity (FSETP 100a)	0.369	0.108	116.903	18.718	0.439	1.594	138.131
Human toxicity (HTP 100a)	0.219	0.109	94.293	6.568	0.274	0.063	101.527
Marine aquatic ecotoxicity (MAETP 100a)	0.654	0.229	212.490	36.136	16.939	2.329	268.776
Marine sediment ecotoxicity (MSETP 100a)	0.673	0.238	218.430	37.117	18.918	2.782	278.158
Terrestrial ecotoxicity (TAETP 100a)	0.000	0.000	0.031	0.006	0.001	0.000	0.038
Ionising radiation	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Malodours air	5371.524	2475.704	789865.332	36282.800	18236.262	991.408	853223.030

Table S 12: Life cycle impact assessment results of KNN based on Eco-indicator 99

	Ecosystem quality	Human health	Resources
Potassium carbonate	0.003	0.009	0.016
Sodium carbonate	0.001	0.003	0.007
Niobium pentoxide	3.925	7.290	4.829
Electricity	0.145	0.748	1.659
Gas (thermal energy)	0.014	0.041	3.645
Waste disposal	0.000	0.007	0.013
Total	4.089	8.099	10.170

Table S 13: Comparison between KNN and PZT across all indicators based on Process LCA

	PZT	**KNN**	**Total impact**	**% contribution KNN**	**% contribution PZT**
Climate change	46.67	194.45	241.11	81%	19%
Acidification potential	0.20	1.28	1.48	87%	13%
Eutrophication potential	0.12	1.08	1.20	90%	10%
Land use	1.26	43.82	45.08	97%	3%
Material use	2069.25	4735.26	6804.51	70%	30%
Freshwater aquatic ecotoxicity (FAETP 100a)	10.23	66.15	76.38	87%	13%
Freshwater sediment ecotoxicity (FSETP 100a)	21.54	138.13	159.68	87%	13%
Human toxicity (HTP 100a)	7.94	101.53	109.47	93%	7%

Marine aquatic ecotoxicity (MAETP 100a)	54.56	268.78	323.34	83%	17%
Marine sediment ecotoxicity (MSETP 100a)	57.50	278.16	335.66	83%	17%
Terrestrial ecotoxicity (TAETP 100a)	0.01	0.04	0.05	83%	17%
Ionising radiation	0.00	0.00	0.00	78%	22%
Malodours air	106382.74	853223.03	959605.77	89%	11%

1.5 Supplementary Research methodology (detailed mathematical model of integrated hybrid LCA)

1.5.1 Process-based LCA framework

The process LCA entails the unit process exchange and supply chain inputs that are employed directly in the fabrication of the product or material under consideration. It evaluates the amount of supply chain inputs required to produce a given functional unit (i.e. 1kg of PZT vs. KNN in this study). Using life cycle inventories, the process LCA can be expressed mathematically as:

$$Process\ LCA = \sum_{i=1}^{n} A_{p(i)} * E_{p(i)} \qquad (1)$$

where: A_p is the inputs (i) into a product's (i.e. PZT vs. KNN piezoelectric materials) supply chain including raw material extraction, energy consumption, material production and manufacturing processes, etc.; n is the total number of process input (i) into the product's supply chain and E_p is the emissions intensity across a number of environmental and sustainability metrics (e.g. GHG emissions, land use etc.), for each input (i) into a product's supply chain emissions.

The entity $\mathrm{A_p}$ in Equation 1 above is characterised based on the process production system and it is the matrix representing the Process LCA framework. For n different types of supply chain inputs into the Process LCA system, A_p is a matrix of dimension $(n+1)\ x\ (n+1)$;

where there are n supply chain product inputs and 1 main product output. Let q_n denotes the quantity of supply chain inputs used for any given input, n and $k_{r,c}$ the elements of A_p so that $A_p = [k_{r,c}]$ where r (rows) represents inputs and c (columns) processes of those inputs in the process system matrix. In mathematical form, the entity A_p can be expressed as follows:

$$\boldsymbol{A_p} = [k_{r,c}] = \begin{cases} k_{r,c} = q_n & if\ r = c\ (and\ r \neq n+1, c \neq n+1) \\ k_{r,c} = 1 & if\ r = c = n+1 \\ k_{r,c} = -q_n & \forall\ r\ when\ r = c\ except\ if\ r = c = n+1 \\ k_{r,c} = 0 & if\ r \neq c \end{cases} \qquad (2)$$

The process-based approach used for the characterisation of the initial production system as described above offers an advantage in that the environmental impacts of those inputs can be determined with some degree of accuracy and accounted for within the defined system boundary.[4] However, due to truncation of some of the process inputs within the system boundary under consideration given that it may not be possible to account for all the inputs of very complex product supply chains which transcends different countries, the process-based approach has been described as incomplete.[5, 6] This drawback is addressed by using the IO framework as discussed in section 4.2.

1.5.2 Environmental Input Output LCA framework

The EIO LCA is carried out by linking national IO tables with direct industrial emissions intensities to produce results that can be adopted in the LCA of a product. [7, 8] The general IO model is a quantitative technique[9] which details how products and services flow from one economic sector (i.e. producer) to other economic sectors (consumers).[7] It is adopted as the methodological basis to compute the upstream indirect emissions associated with the inputs into the supply chain for the production of the final product. The process entails the conversion of economic flows into physical flows (in this case $CO_{2\text{-eq}}$ emission within the overall IO framework, using well-established assumptions of IO analysis.

For a given economy, the basic IO relationship can be written as:

$$\underline{x} = A\underline{x} + \underline{y} \qquad (3)$$

Where: A is mxm matrix of which each column in A describes the domestic and imported intermediate requirements (including raw materials, energy, good and services, machinery, transport, etc.) in monetary values which are required to produce one unit output of the sector; $\underline{x}$ is the total economic output of each industry; $\underline{y}$ is the final demand matrix of each industry which is further subdivided into government, household, capital investment and export based on final consumption.

Equation 3 indicates the linearity assumption of the economy[7] wherein total production is equal to total consumption; that is, it is assumed that the total output of goods and services produced by industries in an economy ($\underline{x}$) is equal to the total goods and services used by all other industries for their own need ($A\underline{x}$) plus the total goods and services used up by the final demand (eg: government, households, exports)y. The total output of an economy, x can therefore be expressed as the sum of intermediate consumption,Ax, and final consumption, y:

$$\underline{x} = (\boldsymbol{I} - \boldsymbol{A})^{-1} \cdot \underline{y} \tag{4}$$

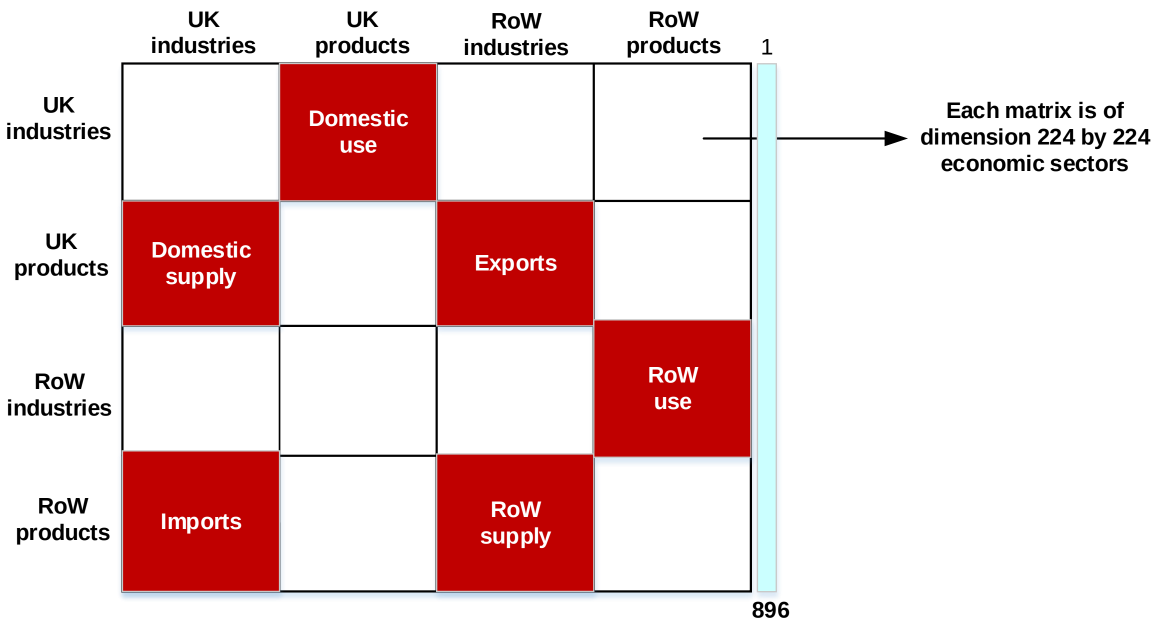
Where: $(I - A)^{-1}$ represents the Leontief Inverse matrix and $(I - A)^{-1} \cdot \underline{y}$ describes the total (direct and indirect) requirements needed to produce the total output, $\underline{x}$,for a given final demand $\underline{y}$.[10] I denotes an identity matrix of dimension mxm. This distinguishing feature of capturing direct and indirect industrial requirements ensures a supply chain that is completely visible which is a fundamental requirement in environmental modelling across supply chains. [11, 12] Equation 4 represents the basic IO relationship and can be generalised for an open economy to include imports from other countries or regions [13-15]as detailed in Section 4.2.1, from which further developments in the methodology are applied in this study.

1.5.3 Multi-Region Input-Output (MRIO) model

The distinguishing characteristics of Multi-Region Input-Output (MRIO) framework is that it enables the tracking of the production of a given product in a given economic sector, quantifying the contributions to the value of the product from different economic sectors in various countries or regions captured in the model.[16, 17] The model which is in tune with current United Nations Accounting Standards,[18] therefore provides an account of the global supply chains of products consumed given it is globally closed and sectorally highly disaggregated thereby facilitating international supply chains tracking and produce more accurate results.[19, 20] MRIO framework combines, in a robust way, the matrices of domestic or local technical coefficient with the matrices of import from numerous countries or regions into one big coefficient matrix. This has the overall influence of capturing the supply chains associated with trade between all the participating trading partners as well as provide feedback pathways and effects.[20]

The MRIO framework adopted in EIO analysis can be represented as a model based on two regions. For instance, Ibn-Mohammed *et al.*[15] adopted a MRIO model based on two regions namely UK and Rest of the World (ROW) to evaluate the CO_2 emissions embodied in international trade flows of a number of building energy retrofit options.. By extension, the Supply and Use (S&U) format within a two-region (UK and ROW) IO framework is adopted in the current work. The benefits of S&U tables as an essential part of the national emissions accounting system pertains to the fact that it exhibit details that are robust and guarantees a higher degree of homogeneity of the individual product. As such, it offers a better and improved possibilities for determining categories of uses and consequently the environmental impacts[21], allowing the split of emissions based on supply chain inputs which are sourced from either the ROW or the UK.

As shown in Figure 2, the basic entities in the MRIO Supply and Use table are industries and commodities (i.e. products). The basic assumption is that Domestic (or UK) and ROW products are supplied to both UK and ROW industries as supply chain inputs and Domestic and ROW industries also produce products for use in the UK and in the ROW. The framework is interpreted as follows. Consider, for instance, the first column in Figure 2 which consists of 4 segments with each containing 224×224 disaggregated economic sectors. Segment 1 in column 1 is empty as the intersection is UK industries by UK industries. Segment 2 is labelled Domestic Supply; implying products from the UK are supplied to UK industries. Segment 3 is also blank as the intersection is UK industries by ROW industries. Segment 4 is named Imports; which indicates, the UK industry use imported products from the ROW. Overall, the entire S&U table is a 896×896 matrix.



Supplementary Figure 1: Framework for MRIO in the Supply and Use format

The methodology which entails the MRIO approach and constructed within the EIO methodology is presented below. Following on from defining the technical coefficient matrix $\boldsymbol{A}$, the I-O system in this study is setup as a MRIO system $(\mathrm{A_{io}})$ presented in the S&U format as shown in Figure 2.

In matrix form, Figure 2 becomes:

$$\mathrm{A_{io}} = \begin{bmatrix} 0 & \boldsymbol{A}_{(UK),U} & 0 & 0 \\ \boldsymbol{A}_{(UK),S} & 0 & \boldsymbol{A}_{(UK),EXP} & 0 \\ 0 & 0 & 0 & \boldsymbol{A}_{(ROW),U} \\ \boldsymbol{A}_{(UK),IMP} & 0 & \boldsymbol{A}_{(ROW),S} & 0 \end{bmatrix} \quad (5)$$

Where $\mathrm{A_{io}}$ becomes the 2-region (UK and ROW) MRIO technical coefficient matrix. This includes the respective technical coefficient matrices for UK Domestic Use, $\boldsymbol{A}_{(UK)U}$, UK Domestic Supply, $\boldsymbol{A}_{(UK)S}$, UK Export to ROW, $\boldsymbol{A}_{(UK)EXP}$, ROW Use, $\boldsymbol{A}_{(ROW)U}$, UK Imports from ROW, $\boldsymbol{A}_{(UK)IMP}$ and ROW Supply to ROW, $\boldsymbol{A}_{(ROW)S}$. All of the individual $\boldsymbol{A}$ matrices are of dimensions $224\ x\ 224$; hence, both $\mathrm{A_{io}}$ and $\boldsymbol{I}$ (the Identity Matrix) have a dimension $896\ x\ 896$.

The Technical Coefficient Matrix for UK Imports from ROW, $\boldsymbol{A}_{(UK)IMP}$, for example, is defined as:

$$\boldsymbol{A}_{(UK)IMP} = \left[\frac{q_{ij}^{(ROW,UK)}}{x_j}\right] \quad (6)$$

Where: $q_{ij}^{(ROW,UK)}$ represents elements of UK imports IO table from the ROW region representing the input of product (i) from ROW into the industry (j) of the UK while x_j represents the total output of UK industry, (j).

Given that requirements of supply chain inputs needed for the production of a given product or material can be as a result of domestic (or UK) supplies or ROW supplies, the final demand matrix can be presented as shown below:

$$\boldsymbol{y} = \begin{bmatrix} \underline{y}_{(UK,UK)} & \underline{y}_{(UK,ROW)} \\ \underline{y}_{(ROW,UK)} & \underline{y}_{(ROW,ROW)} \end{bmatrix} \quad (7)$$

Where: $\underline{y}_{(UK,UK)}$ and $\underline{y}_{(ROW,ROW)}$ represents UK final demand for UK products and ROW final demand for ROW products respectively. Similarly, $\underline{y}_{(UK,ROW)}$ and $\underline{y}_{(ROW,UK)}$ represents ROW final demand for UK products and UK final demand for ROW products respectively. Indeed, by linking the domestic with the ROW IO tables to form a 2-region MRIO table, the model is able to capture all indirect upstream requirement that are required for the production of all the individual supply chain inputs either from resources from the UK or from outside the UK (i.e. ROW). In this study, it is assumed that the UK demand for products produced in the UK or from the rest of the world, hence $\underline{y}_{(UK,ROW)}$ and $\underline{y}_{(ROW,ROW)}$ are set to zero and the final demand matrix becomes a column matrix (dimension $896\ x\ 1$):

$$\underline{y} = \begin{bmatrix} \underline{y}_{(UK,UK)} \\ \underline{y}_{(ROW,UK)} \end{bmatrix} \quad (8)$$

Following on from the basic IO Equation (4), the total (direct and indirect) requirements needed by an industry to produce a given final demand using the MRIO model become:

$$\underline{x} = \left([I] - \begin{bmatrix} 0 & \boldsymbol{A}_{(UK),U} & 0 & 0 \\ \boldsymbol{A}_{(UK),S} & 0 & \boldsymbol{A}_{(UK),EXP} & 0 \\ 0 & 0 & 0 & \boldsymbol{A}_{(ROW),U} \\ \boldsymbol{A}_{(UK),IMP} & 0 & \boldsymbol{A}_{(ROW),S} & 0 \end{bmatrix} \right)^{-1} \cdot \begin{bmatrix} \underline{y}_{(UK,UK)} \\ \underline{y}_{(ROW,UK)} \end{bmatrix} \quad (9)$$

1.5.4 Environmentally extended MRIO Model

IO framework can be extended to an EIO methodology to generate results which can be used in the embodied emissions calculations of products. By adding environmental information, such as GHG emissions, to each sector, an environmental burden (a "footprint") can be assigned to the financial transactions associated with the purchase of a product. This characterises the environmental impact of an additional unit cost of output from each industry.

Let $\mathbf{E} = \{\mathbf{e_{kj}}\}$ be the vector of environmental effect or environmental extension matrix; **X** be the total output. The EIO methodology can therefore be defined in a generalised form as:

$$\underline{E} = \boldsymbol{E}_{io} \cdot \underline{x} = \boldsymbol{E}_{io} \cdot (\boldsymbol{I} - \boldsymbol{A})^{-1} \cdot \underline{y} \tag{10}$$

Where $\boldsymbol{E}_{io}$ is the direct emissions intensity (e.g. kg NO_x-eq/£) of the I-O industries.

By extending the principles described above within a MRIO framework, the matrix $\boldsymbol{E}_{io}$ expressed in terms of the MRIO Supply and Use structure becomes:

$$\boldsymbol{E}_{io} = \begin{bmatrix} \hat{E}_{UK} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{E}_{ROW} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{11}$$

Where $\hat{E}_{UK}$ and $\hat{E}_{ROW}$ are respectively the diagonalised direct emissions intensity (Sector emissions in kg NO_x-eq per total output in £, for example) of each industrial sector in the UK and the ROW.

Hence, the environmental-extended MRIO methodology takes the following form, where the matrix $(\underline{EE})$ describes the total embodied emissions:

$$\begin{bmatrix} \hat{E}_{UK} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{E}_{ROW} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \cdot \left([I] - \begin{bmatrix} 0 & \boldsymbol{A}_{(UK),U} & 0 & 0 \\ \boldsymbol{A}_{(UK),S} & 0 & \boldsymbol{A}_{(UK),EXP} & 0 \\ 0 & 0 & 0 & \boldsymbol{A}_{(ROW),U} \\ \boldsymbol{A}_{(UK),IMP} & 0 & \boldsymbol{A}_{(ROW),S} & 0 \end{bmatrix} \right)^{-1} \cdot \begin{bmatrix} \underline{y}_{UK,UK} \\ \underline{y}_{ROW,UK} \end{bmatrix} \tag{12}$$

In the same vein, the environmental extended component for the process LCA system $\boldsymbol{E}_p$ in the hybrid model (see Equation 1) is defined as a diagonalised matrix of the respective environmental values e_n of each input n into the process LCA system obtained by multiplying product input quantities q and emissions intensities e_{int} of the respective sustainability metrics under consideration. Accordingly, $\boldsymbol{E}_p$ is defined as:

$$\boldsymbol{E}_p = [\hat{e}_n] \tag{13}$$

Where $\forall\, n$ into the process lCA system;

$$e_n = q_n \cdot e_{(int)_n} \tag{14}$$

As described earlier, $\underline{y}$ represents the final demand; in this instance, the output of the LCA system. This final demand matrix is represented as a column matrix. The generic matrix dimension or size of $\underline{y}$ has already been ascertained to be $(\mathrm{s} + \mathrm{m}, 1)$. With respect to this study, this dimension equals $((n + 1 + 896), 1\ )$; where n is the number of supply chain product inputs of the process LCA system and 896, the dimension of the MRIO matrix.

1.6 Derivation of environmental intensities of other indicators (excluding GHG and toxicology) for Input-Output analysis

In this paper, we expanded upon an existing integrated hybrid (Process + EIO) LCA framework for the systematic quantifications of impacts in supply chain of PZT versus KNN across a number of sustainability metrics namely greenhouse gas (GHG) emissions, land use, material use, toxicity and pollution (i.e. acidification and eutrophication potentials) . The process LCA offers some level of accuracy and specificity albeit incomplete due to boundary truncation, the input-output approach provides system boundary completeness. Process data fed into the hybrid framework were obtained from three main sources namely: laboratory data, Ecoinvent database, study assumptions and well established literatures. On the other hand, only the IO environmental intensities of GHG were available in the 896 × 896 format.

As such, the IO environmental intensities of other metrics have to be derived. For metrics such as land use, material use and pollution (i.e. acidification and eutrophication potentials), the sectoral direct emissions per country were collected from World Input-Output Database (WIOD) database[22]. The WIOD database consist of national IO tables, MRIO tables, environmental accounts for 40 countries and one Rest of World (ROW) category comprising all other regions. These 40 countries include all European Union (EU) member countries, Non-EU OECD countries (e.g. the USA, Canada, Japan), and some large emerging economies (e.g. Brazil, India, China). Most of countries in the ROW region are developing countries in Africa, Asia, and Latin America. The IO table in each country includes 35 × 35 economic sectors. These economic sectors are listed in Table S14.

Table S14: Economic sectors within the WIOD database

Economic sectors within the WIOD database	
1	Agriculture, Hunting, Forestry and Fishing
2	Mining and Quarrying
3	Food, Beverages and Tobacco
4	Textiles and Textile Products
5	Leather, Leather and Footwear
6	Wood and Products of Wood and Cork
7	Pulp, Paper, Printing and Publishing
8	Coke, Refined Petroleum and Nuclear Fuel
9	Chemicals and Chemical Products
10	Rubber and Plastics
11	Other Non-Metallic Mineral
12	Basic Metals and Fabricated Metal
13	Machinery, Nec
14	Electrical and Optical Equipment
15	Transport Equipment
16	Manufacturing, Nec; Recycling
17	Electricity, Gas and Water Supply
18	Construction
19	Sale, Maintenance and Repair of Motor Vehicles and Motorcycles; Retail Sale of Fuel
20	Wholesale Trade and Commission Trade, Except of Motor Vehicles and Motorcycles
21	Retail Trade, Except of Motor Vehicles and Motorcycles; Repair of Household Goods
22	Hotels and Restaurants
23	Inland Transport
24	Water Transport
25	Air Transport
26	Other Supporting and Auxiliary Transport Activities; Activities of Travel Agencies
27	Post and Telecommunications
28	Financial Intermediation
29	Real Estate Activities
30	Renting of M&Eq and Other Business Activities

31	Public Admin and Defence; Compulsory Social Security
32	Education
33	Health and Social Work
34	Other Community, Social and Personal Services
35	Private Households with Employed Persons

Given that the technology matrix A_{i-o} in this study is a (896 × 896) multi regional input-output (MRIO) technology matrix and describes input and output coefficients requirements from one sector to another within the UK vs. Rest of the World (ROW) Supply and Use MRIO framework, it is important to make the IO environmental intensities of other indicators to conform with the same framework. As such, 39 countries (i.e. excluding the UK) and one Rest of World (ROW) were aggregated to become an "integrated" ROW.

The direct intensity matrix, DIM (i.e. the sectoral direct emissions intensities derived for metric k across j industries) is given by:

$$D_{IM} = \frac{\text{Environmental Extension Matrix}}{\text{Total output}} = \frac{\text{E}}{\text{X}} \qquad (S1)$$

As such the direct intensity matrix for the integrated ROW is given by:

$$\frac{\sum_i^n DIM_i T_i}{\sum_i^n T_i} \qquad (S2)$$

Where DIM_i is the sectoral direct emissions intensities of individual country (i) within the WIOD; T_i is total sectoral outputs (£) from individual country(i); n is the total number of countries represented in the ROW within the WIOD database.

For the UK, the direct intensity matrix is derived using:

$$\frac{\sum DIM_{UK} T_{UK}}{\sum T_{UK}} \qquad (S3)$$

Where DIM_{UK} is the sectoral direct emissions intensities from the UK; T_i is total sectoral outputs (£) from the UK. The IO table in each country within the WIOD database includes 35 × 35 economic sectors. Therefore, the derived DIMs are also in 35 × 35 economic sectors. These sectors are therefore, disaggregated to conform to the 896 × 896 technology matrix based on Table S4.

Table S15: Economic Input-Output Sub-Sectors

Sector Number	Disaggregated Sector	Aggregated Sectors
1	Growing of cereals and other crops n.e.c. (except wheat)	Agriculture (1-28)
2	Organic: Growing of cereals and other crops n.e.c. (except wheat)	
3	Growing of wheat	
4	Organic: Growing of wheat	
5	Growing of oil seeds	
6	Growing of rice	
7	Growing of sugar beet and sugar cane	
8	Growing of fibre crops	
9	Growing of crops and plants for biofuels	
10	Growing of crops nec	
11	Conventional Growing of vegetables, fruits and other crops	
12	Organic Growing of vegetables, fruits and other crops	
13	Growing of horticulture specialities and nursery products	
14	Raising of dairy cattle and production of raw cow milk	
15	Organic: Raising of dairy cattle and production of raw cow milk	
16	Farming of cattle for meat	
17	Organic: Farming of cattle for meat	
18	Raising of horses, equines and other animals; animal hair	
19	Raising of sheep and goats; Production of raw wool, sheep or goat milk	
20	Organic: Raising of sheep and goats; Production of raw wool, sheep or goat milk	
21	Farming of swine	
22	Organic: Farming of swine	
23	Farming of poultry	
24	Organic: Farming of poultry	

25	Other farming of animals	
26	Growing of crops combined with farming of animals (mixed farming)	
27	Agricultural service activities; landscape gardening	
28	Animal husbandry service activities, except veterinary activities	
29	Forestry, logging and related service activities (conventional)	**Forestry (29-30)**
30	Forestry, logging and related service activities ('sustainable' / FSC)	
31	Fishing	**Fishing (31-33)**
32	Fish farming (non-organic)	
33	Fish farming (organic/sustainable)	
34	Mining of coal and lignite; extraction of peat	**Mining (34-42)**
35	Oil: Crude petroleum and services related to crude oil extraction, excluding surveying	
36	Gas: Natural gas and services related to natural gas extraction, excluding surveying	
37	Mining of uranium and thorium ores	
38	Mining of iron ores	
39	Mining of non-ferrous metal ores and concentrates	
40	Stone	
41	Sand and clay	
42	Chemical and fertilizer minerals, salt and other mining and quarrying products n.e.c.	
43	Processing and preserving of meat from cattle (beef)	**Food (43-66)**
44	Organic: Processing and preserving of meat from cattle (beef)	
45	Processing and preserving of meat from pigs	
46	Organic: Processing and preserving of meat from pigs	
47	Conventional poultry meat and poultry meat products	
48	Organic poultry meat and poultry meat products	
49	Meat products nec	
50	Organic: Meat products nec	

51	Fish and fish products	
52	Conventional Fruit and vegetables	
53	Organic Fruit and vegetables	
54	Vegetable and animal oils and fats	
55	Dairy products (conventional)	
56	Organic dairy products	
57	Grain mill products, starches and starch products	
58	Prepared animal feeds	
59	Bread, rusks and biscuits; manufacture of pastry goods and cakes (conventional)	
60	Organic bread, rusks and biscuits; manufacture of pastry goods and cakes	
61	Sugar	
62	Cocoa, chocolate and sugar confectionery	
63	Other food products	
64	Alcoholic beverages	
65	Production of mineral waters and soft drinks	
66	Tobacco products	
67	Preparation and spinning of textile fibres	**Textile (67-76)**
68	Textile weaving	
69	Finishing of textiles	
70	Made-up textile articles, except apparel	
71	Carpets and rugs	
72	Other textiles	
73	Knitted and crocheted fabrics and articles	
74	Wearing apparel; dressing and dying of fur	
75	Tanning and dressing of leather; manufacture of luggage, handbags, saddlery and harness	
76	Footwear	

77	Wood and wood products, except furniture	**Wood & Paper (77-83)**
78	Pulp	
79	Paper and paperboard	
80	Articles of paper and paperboard (except paper stationary)	
81	Paper stationary	
82	Paper-based publishing, printing and reproduction	
83	Non paper-based publishing and reproduction of recorded media	
84	Coke oven products	**Fuel (84-91)**
85	Motor spirit (gasoline)	
86	Kerosene, including kerosene type jet fuel	
87	Gas oils	
88	Fuel oils n.e.c.	
89	Petroleum gases and other gaseous hydrocarbons, except natural gas	
90	Other petroleum products	
91	Processing of nuclear fuel	
92	Industrial gases	**Chemicals (92-102)**
93	Dyes and pigments	
94	Inorganic basic chemicals	
95	Organic basic chemicals	
96	Fertilisers and nitrogen compounds	
97	Plastics and synthetic rubber in primary forms	
98	Pesticides and other agro-chemical products	
99	Paints, varnishes and similar coatings, printing ink and mastics	
100	Pharmaceuticals, medicinal chemicals and botanical products	
101	Soap and detergents, cleaning and polishing preparations, perfumes and toilet preparations	
102	Other chemical products	
103	Man-made fibres	**Minerals (103-113)**
104	Rubber products	

105	Plastic plates, sheets, tubes and profiles, builders' ware of plastic and other plastic products (excl. plastic packing goods)	
106	Plastic packing goods	
107	Glass and glass products	
108	Ceramic goods	
109	Bricks, tiles and other structural clay products for construction	
110	Manufacture of cement	
111	Manufacture of lime	
112	Manufacture of plaster	
113	Articles of concrete, plaster and cement; cutting, shaping and finishing of stone; manufacture of other non-metallic products	
114	Basic iron and steel and of ferro-alloys; manufacture of tubes and other first processing of iron and steel	**Metals (114-121)**
115	Precious metals production	
116	Aluminium production	
117	Lead, zinc and tin production	
118	Copper production	
119	Other non-ferrous metal production	
120	Casting of metals	
121	Structural metal products	
122	Tanks, reservoirs and containers of metal; manufacture of central heating radiators and boilers; manufacture of steam generators	**Equipment (122-150)**
123	Forging, pressing, stamping and roll forming of metal; powder metallurgy; treatment and coating of metals	
124	Cutlery, tools and general hardware	
125	Other fabricated metal products	
126	Machinery for the production and use of mechanical power, except aircraft, vehicle and cycle engines	
127	Other general purpose machinery	
128	Agricultural and forestry machinery	
129	Machine tools	

130	Other special purpose machinery	
131	Weapons and ammunition	
132	Domestic appliances (e.g. white goods)	
133	Computers and other office machinery and equipment	
134	Electric motors, generators and transformers; manufacture of electricity distribution and control apparatus	
135	Insulated wire and cable	
136	Electrical equipment not elsewhere classified	
137	Electronic valves and tubes and other electronic components	
138	Television and radio transmitters and line for telephony and line telegraphy	
139	Television and radio receivers, sound or video recording or reproducing apparatus and associated goods	
140	Medical, precision and optical instruments, watches and clocks	
141	Motor vehicles, trailers and semi-trailers	
142	Building and repairing of ships and boats	
143	Railway transport equipment, motorcycles, bicycles and transport equipment n.e.c.	
144	Aircraft and spacecraft	
145	Furniture	
146	Jewellery and related articles; manufacture of musical instruments	
147	Sports goods, games and toys	
148	Miscellaneous manufacturing not elsewhere classified; recycling	
149	Recycling of metal waste and scrap	
150	Recycling of non-metal waste	
151	Electricity production - coal	**Utilities (151-164)**
152	Electricity production - gas	
153	Electricity production - oil	
154	Electricity production - nuclear	
155	Electricity by hydro power (inland)	

156	Electricity by wind power	
157	Electricity by biomass	
158	Electricity by geothermal, solar, tidal or wave power	
159	Electricity by waste incineration	
160	Transmission of electricity	
161	Distribution and trade in electricity	
162	Gas distribution	
163	Steam and hot water supply	
164	Collection, purification and distribution of water	
165	Construction (other than commercial and domestic buildings)	**Construction (165-167)**
166	Construction of commercial buildings	
167	Construction of domestic buildings	
168	Sale, maintenance and repair of motor vehicles, and motor cycles; retail sale of automotive fuel	**Trade (168-174)**
169	Retail sale of automotive fuel	
170	Wholesale trade and commission trade, except of motor vehicles and motor cycles	
171	Retail trade, except of motor vehicles and motor cycles	
172	Repair of personal and household goods	
173	Hotels and accommodation	
174	Restaurants, cafes, bars etc.	
175	Passenger transport by railways	**Transport & Telecommunication (175-190)**
176	Freight transport by inter-urban railways	
177	Inter-city coach service	
178	Urban and suburban passenger railway transportation by underground, metro and similar systems	
179	Other scheduled passenger land transport n.e.c.	
180	Taxi operation	
181	Other passenger land transport	

182	Freight transport by road	
183	Transport via pipeline	
184	Sea and coastal water transportation services	
185	Inland water transportation services	
186	Passenger air transport	
187	Freight and other air transport	
188	Supporting and auxiliary transport activities: travel agencies, cargo handling, storage, etc.	
189	Postal and courier services	
190	Telecommunications	
191	Banking and financial intermediation, except insurance and pension funding	**Business Services** (191-223)
192	Insurance and pension funding, except compulsory social security	
193	Auxiliary financial services	
194	Real estate activities with own property; letting of own property, except dwellings	
195	Letting of dwellings, including imputed rent	
196	Real estate agencies or activities on a fee or contract basis	
197	Renting of cars and other transport equipment	
198	Renting of machinery and equipment, excl. office machinery and computers	
199	Renting of office machinery and equipment including computers	
200	Renting of personal and household goods	
201	Computer services and related activities	
202	Research and development	
203	Legal activities	
204	Accounting, book-keeping and auditing activities; tax consultancy	
205	Business and management consultancy activities; management activities; market research and public opinion polling	
206	Technical consultancy; technical testing and analysis; architectural and engineering related activities	

207	Advertising	
208	Other business services	
209	Public administration (not defence); compulsory social security	
210	Public administration - defence	
211	Primary, secondary and other education	
212	Higher-level education	
213	Human health and veterinary activities	
214	Social work activities	
215	Collection and treatment of sewage and liquid waste	
216	Collection of waste	
217	Incineration of waste	
218	Landfill of waste	
219	Sanitation, remediation and similar activities	
220	Activities of membership organisations	
221	Recreational and cultural activities	
222	Sporting and other activities	
223	Dry cleaning, hair dressing, funeral parlours and other service activities	
224	Private households as employers of domestic staff	**Personal Services**

Table S16: 2008 WIOD Input-Output data for land use indicator

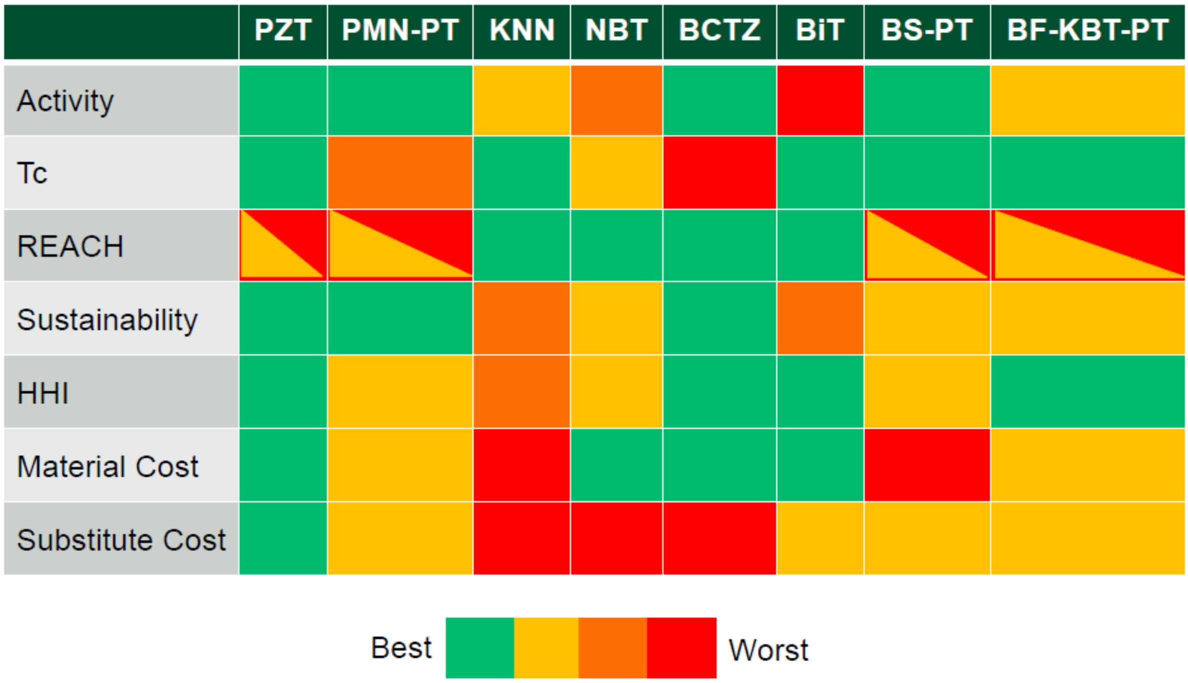
1000 ha		Arable_Area	PermanentCrops_Area	Pastures_area	Forest_area	Total
secAtB	Agriculture, Hunting, Forestry and Fishing	6005	46	11633	2549.878277	20233.88
secC	Mining and Quarrying					0
sec15t16	Food, Beverages and Tobacco					0
sec17t18	Textiles and Textile Products					0
sec19	Leather, Leather and Footwear					0
sec20	Wood and Products of Wood and Cork					0
sec21t22	Pulp, Paper, Paper , Printing and Publishing					0
sec23	Coke, Refined Petroleum and Nuclear Fuel					0
sec24	Chemicals and Chemical Products					0
sec25	Rubber and Plastics					0
sec26	Other Non-Metallic Mineral					0
sec27t28	Basic Metals and Fabricated Metal					0
sec29	Machinery, Nec					0
sec30t33	Electrical and Optical Equipment					0
sec34t35	Transport Equipment					0
sec36t37	Manufacturing, Nec; Recycling					0
secE	Electricity, Gas and Water Supply					0
secF	Construction					0
sec50	Sale, Maintenance and Repair of Motor Vehicles and Motorcycles; Retail Sale of Fuel					0
sec51	Wholesale Trade and Commission Trade, Except of Motor Vehicles and Motorcycles					0
sec52	Retail Trade, Except of Motor Vehicles and Motorcycles; Repair of Household Goods					0
secH	Hotels and Restaurants					0
sec60	Inland Transport					0
sec61	Water Transport					0
sec62	Air Transport					0
sec63	Other Supporting and Auxiliary Transport Activities; Activities of Travel Agencies					0
sec64	Post and Telecommunications					0
secJ	Financial Intermediation					0
sec70	Real Estate Activities					0
sec71t74	Renting of M&Eq and Other Business Activities					0
secL	Public Admin and Defence; Compulsory Social Security					0
secM	Education					0
secN	Health and Social Work					0
secO	Other Community, Social and Personal Services					0
secP	Private Households with Employed Persons					0
secQ						0
FC_HH						
total		6005	46	11633	2549.878277	**20233.88**

1.7 Derivation of environmental intensities of toxicology for Input-Output analysis

An environmental extension matrix for toxicology does not exist. Therefore, in this paper, a newly developed set of data were derived from the toxic release inventory database[23] for the US. This newly developed data on sectoral toxic intensities (i.e. a measure of the efficiencies of the economic sectors in terms of toxicity) were then used within the hybrid framework to investigate trends in the distribution of industrial toxic discharge. The classifications of economic sectors in the US are based on North American Industry Classification System (NAICS).[24] So, for consistency, the NAICS, which exists in a disaggregated form were mapped to conform to the 35 × 35 economic sectors of WIOD.

To obtain the direct intensity matrices of the ROW, we multiplied their respective Leontief inverse matrix by the US sectoral toxic intensities which was estimated as total kilogram of toxic release per dollars' worth of output. The sectoral intensities were derived using the toxic release inventory (TRI) database which provides toxic release estimates, including air, water, land and underground, for a number of toxic chemicals; and the US national economic input-output table which provides information on economic activities. Our derivations of the direct toxic intensity matrices of the ROW based on sectoral intensities of the US can only be defended as the best possible approach since actual toxic release data for the ROW are not available. The same steps as discussed in Section 1.1 were used to make the 35 × 35 economic sectors conform to 896 × 896 as used within the Supply and Use table.

1.8 Risk assessment summary of piezoelectric materials



Supplementary Figure 2: Risk assessment summary of potential piezoelectric materials[25]

1.9 Sensitivity analysis of emissions intensity of electricity based on different countries (Climate change impact category)

Here we show the sensitivity of emissions intensity factors for electricity consumption based on sample countries. This was performed for climate change impact category for the PZT manufacturing route given that it impact outweighs that of lead which is the main component of the material composition of PZT.

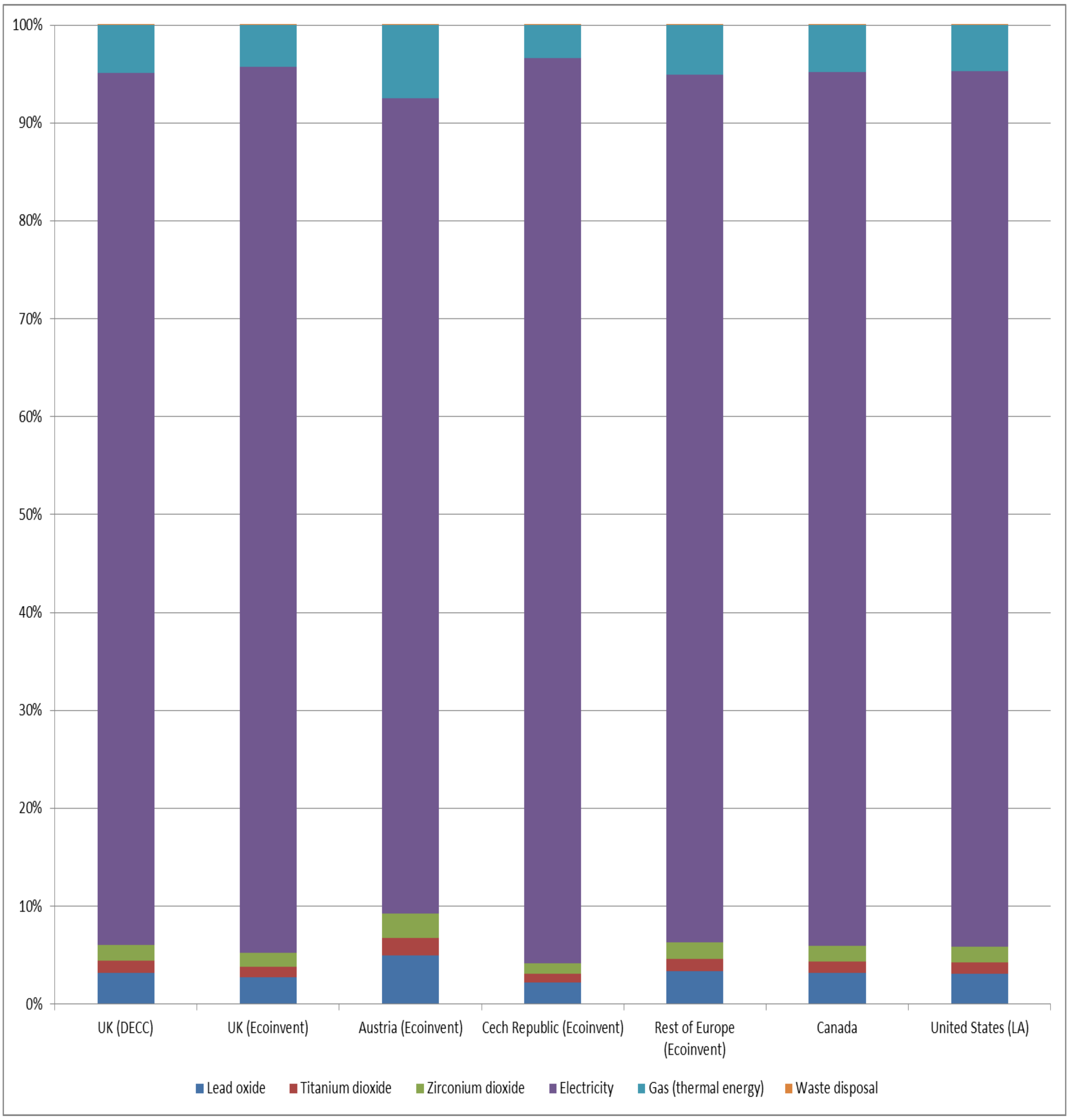
Table S17: Emissions intensity factor for electricity for selected countries

	Electrical energy consumption (kWh)	Emissions intensity ($kgCO_2$-eq/kWh)	Impact ($kgCO_2$-eq)
UK (DECC)	79.21	0.52	41.55
UK (Ecoinvent)	79.21	0.62	48.92
Austria (Ecoinvent)	79.21	0.32	25.39
Czech Republic (Ecoinvent)	79.21	0.78	61.92
Rest of Europe (Ecoinvent)	79.21	0.50	39.78
Canada	79.21	0.53	42.09

United States (LA)	79.21	0.54	43.15

Table S18: Effect of emissions intensity factor of electricity on environmental profile of PZT

Climate change						
	Lead oxide	**Titanium dioxide**	**Zirconium dioxide**	**Electricity**	**Gas (thermal energy)**	**Waste disposal**
UK (DECC)	1.51	0.57	0.76	41.55	2.28	0.00
UK (Ecoinvent)	1.51	0.57	0.76	48.92	2.28	0.00
Austria (Ecoinvent)	1.51	0.57	0.76	25.39	2.28	0.00
Cech Republic (Ecoinvent)	1.51	0.57	0.76	61.92	2.28	0.00
Rest of Europe (Ecoinvent)	1.51	0.57	0.76	39.78	2.28	0.00
Canada	1.51	0.57	0.76	42.09	2.28	0.00
United States (LA)	1.51	0.57	0.76	43.15	2.28	0.00



Supplementary Figure 3: Environmental profile of 1 kg of laboratory-based PZT ceramic showing relative proportions contributing processes based on climate change impact category using emissions intensity factor for selected countries

As shown in Supplementary Figure 3 above, the effect of location does not affect the influence of electricity in the environmental impact assessment. It boils down to the fact that the quantity of electricity required to produce 1kg of PZT is higher and hence its corresponding higher impact in comparison with PbO.

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