Supplementary Information

S1. Methodology—Matrix Formulation

As presented in Section 2.2 of the article, one can express a life cycle (LCI) inventory problem with the following matrix representation and further characterise the corresponding life cycle impacts assessment (LCIA) [1,2]:

$$q = B \cdot A^{-1} \cdot f \tag{1}$$

$$r = C \cdot B \cdot A^{-1} \cdot f \tag{2}$$

where we have:

- Functional vector (*f*) of processes × FU (1 functional unit);
- Technology matrix (*A*) of processes × processes;
- Intervention matrix (*B*) of elementary flows × processes;
- LCI vector (*q*) of elementary flows × FU (1 functional unit), *i.e.* a vector representing the inventory of elementary flows from and to the environment activated by the service unit;
- Characterization matrix (*C*) of impact categories × elementary flows;
- LCIA result vector (*r*) of impact categories × FU (1 functional unit), *i.e.*, a vector representing the life cycle assessment results for all environmental impact categories associated with one service unit.

Figure S1 gives a graphical overview of the matrix system. Figure S2 in Section S2 gives more detail regarding the content and structure of the matrices.

S2. MI Abiotic Characterisation Factors

For a beta version of the MIT abiotic characterisation factors in EcoSpold format, see attached file "SuppMat_S2.xml". It should be noted that this is a beta release, fit for testing but not for production since bugs may remain. Future versions will be made available through the WI website. The EcoSpoldImpact xml file can be imported into the LCA software of your choice after you have imported the ecoinvent database and, optionally, other impact assessment methods. This approach has been tested with the software openLCA and version 2.2 of the ecoinvent database.

For a beta version (same restrictions as above apply) of the MIT abiotic characterisation factors in tab-separated text format, see attached file "SuppMat_S2.txt". The file can be imported into a numerical computation software (e.g., Scilab) along with the ecoinvent database.

Figure S2 graphically shows how the content and structure of the matrices are linked.

In the $n \times n$ technology matrix A, any given column represents a process and the elements in this column are the inflows (negative numbers) and outflows (positive numbers) of commodities necessary for the execution of this process. Any given row of B represents an elementary flow (natural resource, pollutant, *etc.*) and each element in this row corresponds to the amount extracted from or emitted to the environment by the corresponding process in column. Any given row in C represents a characterisation method and each element in this row is a weight (characterisation factor) applied to the corresponding elementary flow (resource extraction, emission, *etc.*) in column. The imported MI abiotic characterisation factors appear at the bottom of matrix C.

Figure S1. Matrix formulation of LCI and LCIA/MIPS calculations.

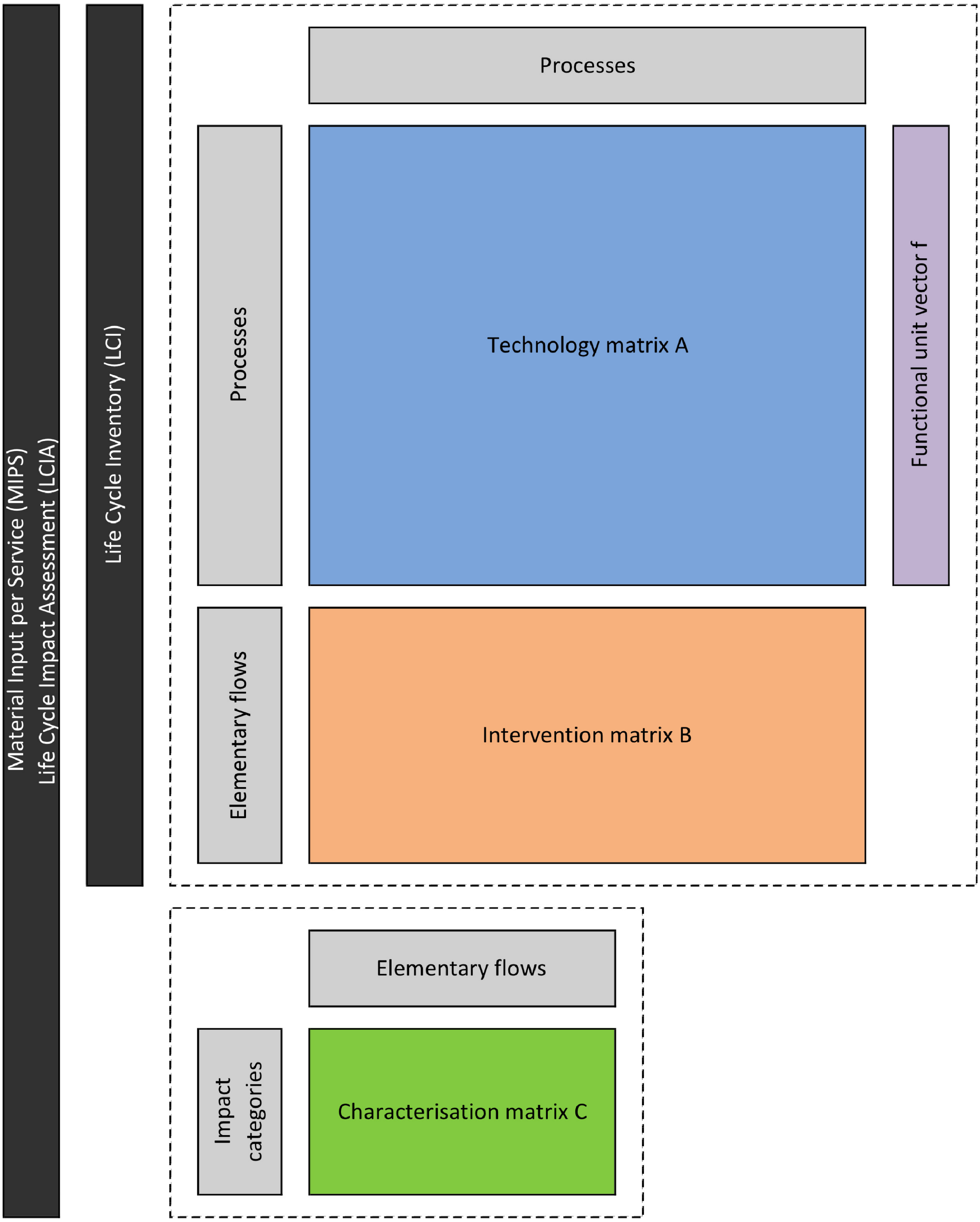
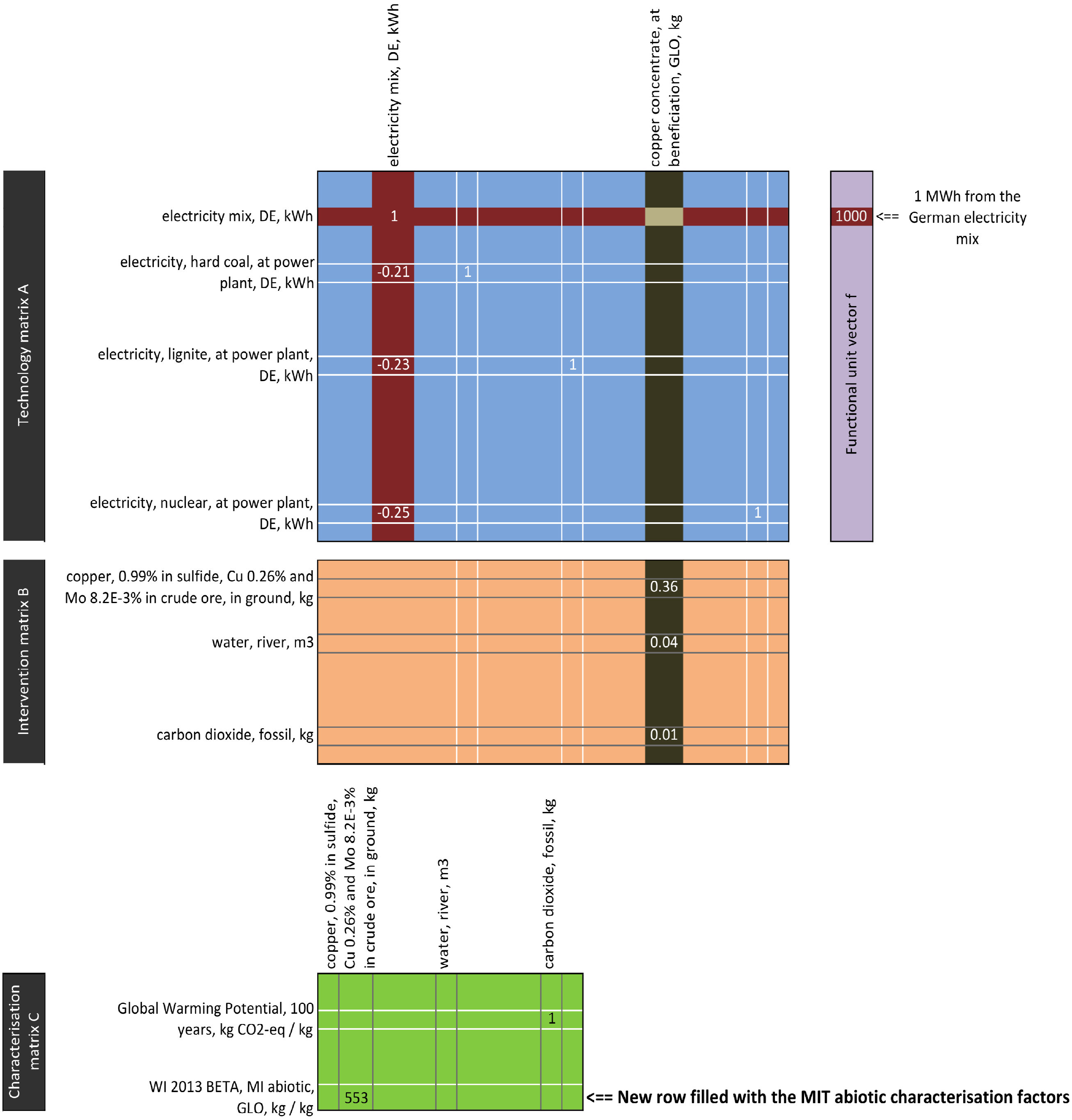


Figure S2. Matrix formulation of LCI and LCIA problems, extended with MI abiotic characterisation factors for MIPS calculations.



S3. Allocation in MI Abiotic Characterisation Factors

In case of coupled production, the unused extraction coefficients used in the article were built as follows:

1. Allocation of total used extraction to each of the co-products, using a mass-based allocation method as described in [3];
2. Allocation of total unused extraction to each co-product, using the same mass-based allocation (same allocation coefficients as in step 1);

3. The unused extraction coefficient of a given co-product is the ratio of the unused and used extraction allocated to it.

So we have [*unused extraction coeff. for product i*] = [*unused extraction allocated to product i*]/[*used extraction allocated to product i*], which in the end gives the same unused extraction coefficient for each product of the coupled production, because [*unused extraction coeff. for product i*] = [*total unused extraction* × *allocation coeff. product i*]/[*total used extraction* × *allocation coeff. product i*] = [*total unused extraction*]/[*total used extraction*].

Interestingly, this also shows that the unused extraction coefficients are independent from the allocation method. The allocation method only plays a role when calculating the absolute unused extraction: [*unused extraction for product i*] = [*used extraction allocated to product i*] × [*unused extraction coeff. for product i*].

S4. Application of Structural Path Analysis

The ecoinvent report on metals states that an "overall 57.5% yield [is] assumed" in ferronickel mining [4] (p. 278). As shown in Table S1, ecoinvent assumes that about 1.7 kg nickel is required per kilogram ferronickel. It would indeed correspond to a 57.5% yield (1/0.575 = 1.7) if ferronickel were made of 100% nickel. It is, however, a ferroalloy containing 25% nickel. This explanation is consistent with the fact that no iron elementary flow into the ferronickel process is inventoried in ecoinvent. We were not capable of exactly reconstructing where the problem may have come from and what the assumed "overall yield" actually represents.

We nevertheless propose a simple tentative correction shown in Table S1. We assumed 75%–25% Fe-Ni in ferronickel and the same "overall yield" of 57.5% for both nickel and iron (0.25/0.575 = 0.4 and 0.75/0.575 = 1.3). This correction has a large impact on the MI abiotic value of ferronickel, now at about 100 kg/kg down from 291 kg/kg.

This in turn drastically changes the MI abiotic value of stainless steel, now at 45 kg/kg down from 107 kg/kg. The new value is still higher than past MIPS calculations have shown, but the difference is in a range not incompatible with differences due to background system modelling, cut-off criteria, *etc*. Figure S3 is the result of a structural path analysis applied to ecoinvent's stainless steel after the ferronickel process has been corrected (processes contributing at least 5% to the overall NI abiotic are represented). The contribution of nickel to the overall MI abiotic is now down to 47%. One can also notice that the disaggregation (threshold also set at 5%) went one level deeper into the process chain (tier 4).

Table S1 also shows that the correction has no impact on impact categories such as climate change and terrestrial acidification, which may partly explain why the issue went unnoticed so far. It may become relevant, however, for studies looking at demand for single metals, e.g., for a criticality assessment, and using ecoinvent for their modelling.

Figure S3. Structural path analysis for MI abiotic of stainless steel calculated with ecoinvent 2.2, after correction of the ferronickel process (% of MI abiotic of "chromium steel 18/8, at plant, RER").

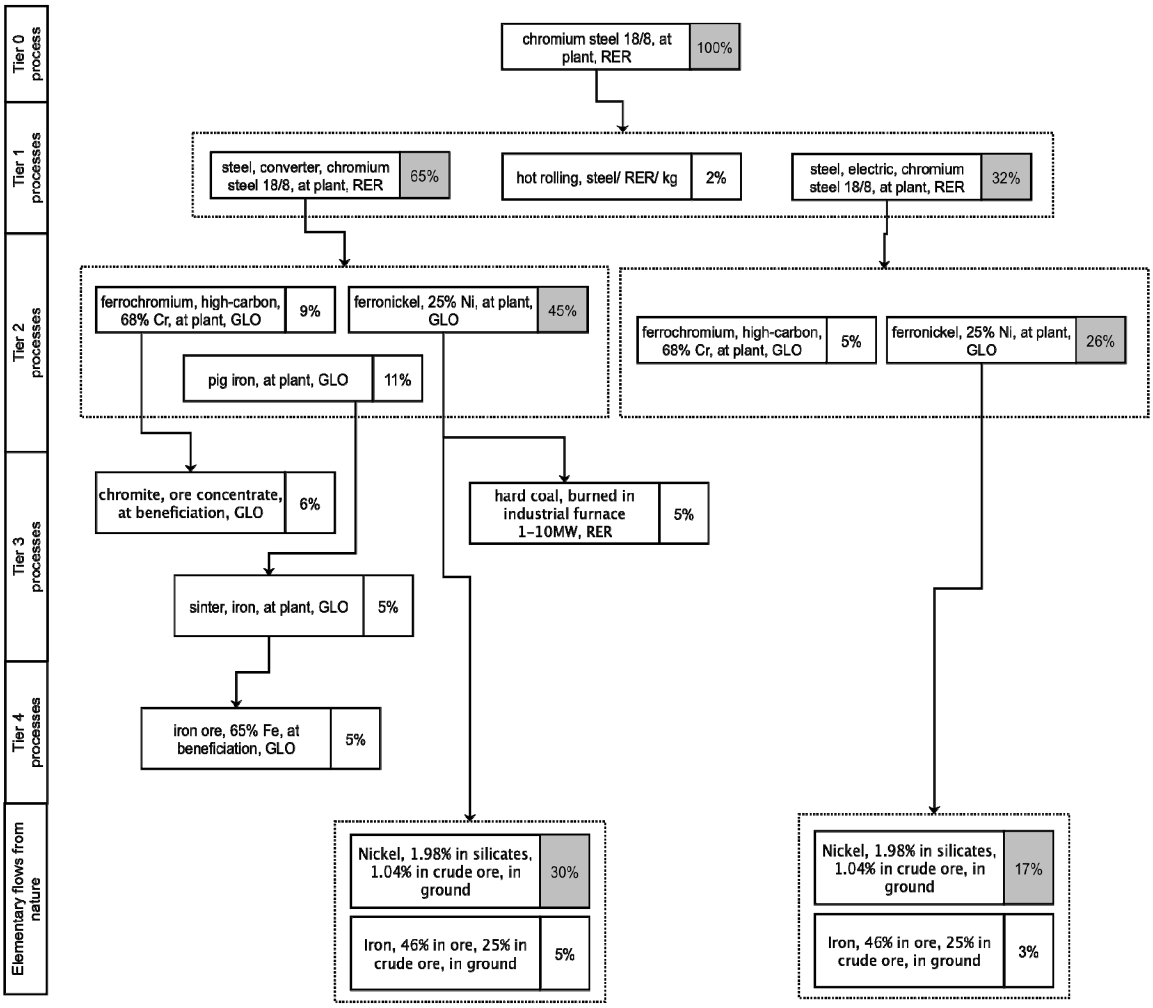


Table S1. Selected elementary flows and environmental indicators of ferronickel process in ecoinvent, and suggested corrections.

Ferronickel, 25% Ni, at plant, GLO	**Unit**	**Original ecoinvent 2.2**	**Suggested correction**
Elementary flows from nature			
Nickel, 1.98% in silicates, 1.04% in crude ore, in ground	[kg]	1.7404	0.4348
Iron, 46% in ore, 25% in crude ore, in ground	[kg]	N.A.	1.3043
Environmental indicators			
MI abiotic	[kg]	291.53	100.41
MI water	[kg]	101.96	101.96
Climate change	[kg CO_2-eq]	9.23	9.23
Terrestrial acidification	[kg SO_2-eq]	0.04	0.04

S5. Application of MI Abiotic Characterisation Method

Table S2 starting on the next page presents the data used in Figure 2 of the article.

Table S2. Data used in Figure 2 of the article (MIT values from MIPS online and values calculated with our MI characterization method applied to ecoinvent 2.2).

Materials	MIPS online	Ecoinvent processes											
METALS													
	aluminium, primary, Europe	aluminium, primary, at plant/ RER/ kg											
aluminum, primary	37.00	32.65											
	gold, estimated, world	gold, primary, at refinery/GLO/kg	gold, at refinery/ CA/kg	gold, at refinery/ US/kg	gold, at refinery/ ZA/kg	gold, at refinery/ TZ/kg	gold, at refinery/AU/kg	gold, at regional storage/ RER/kg	gold, from combined gold-silver production, at refinery/PG/kg	gold, from combined gold-silver production, at refinery/CL/kg	gold, from combined gold-silver production, at refinery/ PE/kg	gold, from combined metal production, at beneficiation/ SE/kg	gold, from combined metal production, at refinery/ SE/kg
gold, primary	540,000.00	1,686,339.30	526,816.13	2,528,902.00	515,244.19	792,986.44	6,862,009.50	1,163,345.90	851,509.63	206,158.33	2,066,321.80	9,256.17	23,428.00
	copper, primary, world	copper, primary, at refinery/GLO/kg			copper, primary, at refinery/RER/kg			copper, primary, at refinery/RAS/kg			copper, primary, at refinery/ID/kg		
copper, primary	348.47	717.59			123.67			585.88			230.30		
	steel, hot rolled, blast furnace route, world	steel, converter, unalloyed, at plant/RER/kg											
steel, blast furnace, unalloyed	7.63	15.03											
	zinc, electrolytic, Germany	zinc, primary, at regional storage/RER/kg			zinc, from combined metal production, at refinery/SE/kg								
zinc, primary	22.18	15.00			132.99								

Table S2. *Cont.*

Materials	MIPS online	Ecoinvent processes			
BASIC MATERIALS					
	alumina, Al_2O_3, Bayer-process, Germany	aluminium oxide, at plant/RER/kg			
alumina	7.43	6.83			
	lime, calcium hydroxide, Germany	quicklime, in pieces, loose, at plant/CH/kg	quicklime, milled, loose, at plant/CH/kg	quicklime, milled, packed, at plant/CH/kg	
lime	2.46	1.92	1.93	1.95	
	soda, heavy, synthetic, Na_2CO_3, Germany	soda, powder, at plant/RER/kg			
soda	4.46	2.32			
ENERGY AND FUELS					
	electricity, electrical power (public network), Germany (2008)	electricity, low voltage, at grid/DE/kWh			
electricity, Germany	3.15	2.62			
	hard coal, Hu: 23.25 MJ/kg, world	hard coal mix, at regional storage/UCTE/kg			
hard coal	5.06	7.52			
CHEMICALS					
	ammonia, Europe	ammonia, liquid, at regional storehouse/RER/kg			
ammonia	1.85	1.96			
	formaldehyde, Germany	formaldehyde, production mix, at plant/RER/kg			
formaldehyde	1.11	2.11			
	methanol, Europe	methanol, at plant/GLO/kg	methanol, from biomass, at regional storage/CH/kg	methanol, from synthetic gas, at plant/CH/kg	methanol, at regional storage/CH/kg
methanol	1.67	1.12	1.21	1.12	1.24
	hydrochloric acid, 37%, Germany	hydrochloric acid, 30% in H2O, at plant/RER/kg			
hydrochloric acid	3.03	3.89			

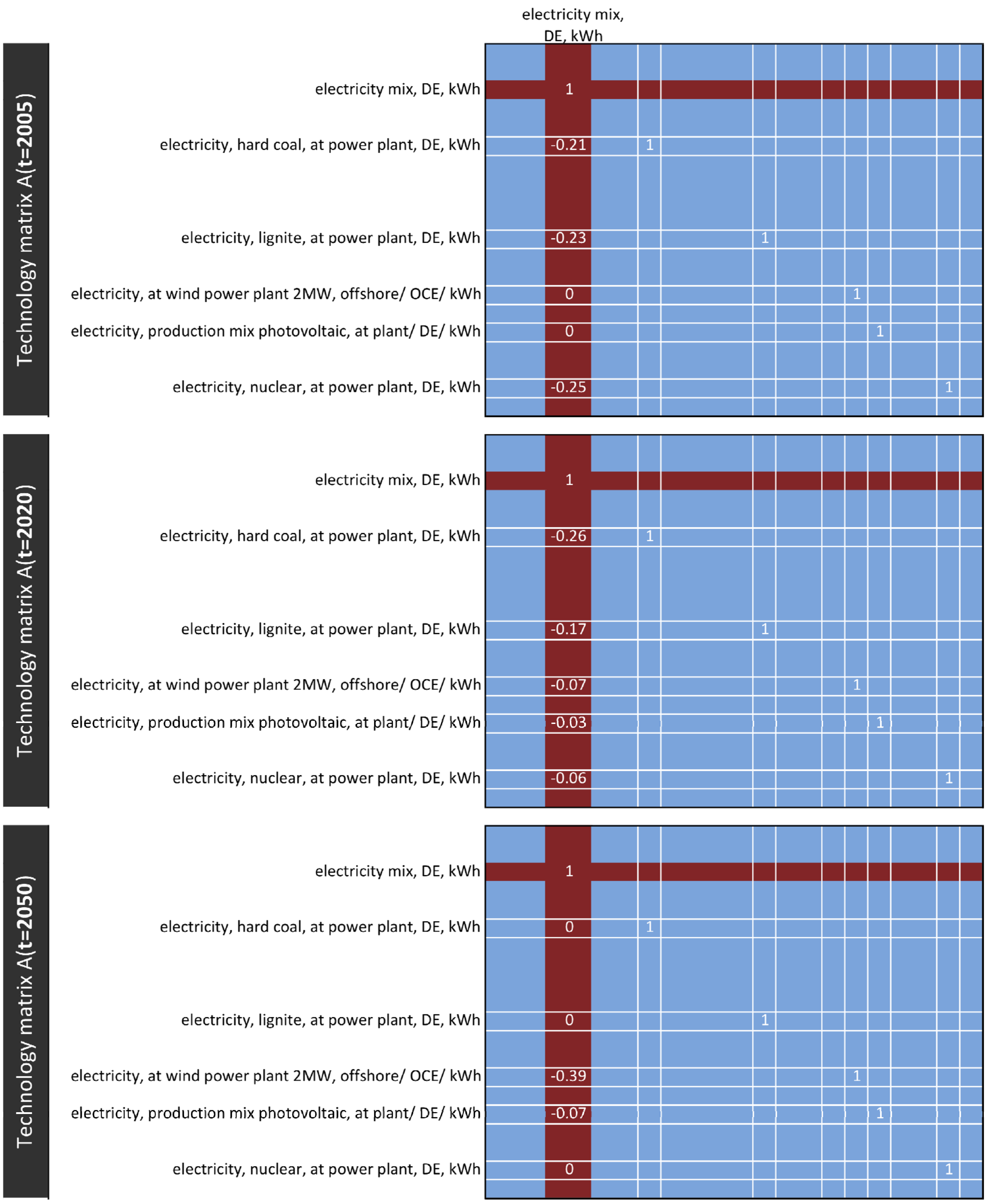
Table S2. *Cont.*

Materials	**MIPS online**	**Ecoinvent processes**			
PLASTICS					
polyamid (nylon)	polyamid, Nylon, PA 6.6, Europe 5.51	nylon 66, at plant/RER/kg 6.84	nylon 6, at plant/RER/kg 5.97	nylon 6, glass-filled, at plant/RER/kg 6.23	nylon 66, glass-filled, at plant/RER/kg 6.63
polyethylene high density HD	polyethylene HD, Europe 2.52	polyethylene, HDPE, granulate, at plant/RER/kg 2.44			
polyethylene linear low density LLD	polyethylene LLD, Europe 2.12	polyethylene, LLDPE, granulate, at plant/RER/kg 2.20			
polyethylene terephtalat (PET)	PET, Europe 6.45	polyethylene terephthalate, granulate, bottle grade, at plant/RER/kg 5.98	polyethylene terephthalate, granulate, amorphous, at plant/RER/kg 5.16		
CONSTRUCTION MATERIALS					
roofing tile	roofing tile, Germany 2.11	roof tile, at plant/RER/kg 3.40			
Portland cement	Portland cement, Germany 3.22	portland cement, strength class Z 42.5, at plant/CH/kg 2.44	portland cement, strength class Z 52.5, at plant/CH/kg 2.47	portland calcareous cement, at plant/CH/kg 2.13	
brick	brick, lightweight clay brick (PS)/solid clay brick, Germany 2.11	light clay brick, at plant/DE/kg 2.48	brick, at plant/RER/kg 3.33		
OTHERS					
container glass	container glass, 53% cullets, Germany 1.72	packaging glass, white, at plant/DE/kg 1.47	packaging glass, white, at plant/CH/kg 1.47	packaging glass, white, at plant/RER/kg 1.86	packaging glass, white, at regional storage/CH/kg 1.69
corrugated cardboard	corrugated cardboard, Europe 1.86	corrugated board base paper, kraftliner, at plant/RER/kg 1.88	corrugated board base paper, semichemical fluting, at plant/RER/kg 3.22	corrugated board base paper, testliner, at plant/RER/kg 1.03	

S6. Application of Dynamic MIPS

See attached the text file "SuppMat_S5.txt" listing the input processes (and quantities) for 1 kWh German electricity mix in the WWF scenario "Innovation without CCS" 2005–2050. We imported this file into Scilab together with the ecoinvent 2.2 database and the MI abiotic characterisation method. We then processed it as described in the algorithm in Section 2.4.2 of the article. In practice, the technology matrix A (see Figures S1 and S2) is duplicated for each time step of the time series. The column corresponding to the process "electricity mix, DE, kWh" is then modified for each time step following the scenario information in the input file "SuppMat_S5.txt", thus constructing a simplified dynamic electricity mix for Germany. Figure S4 illustrates this procedure.

Figure S4. Matrix formulation of LCI and LCIA problems, extended with MI abiotic characterisation factors for MIPS calculations.



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