
Enhancement of the ESSENZ Method and Application in a Case Study on Batteries

Supplementary Material

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S1. Scaling of Indicators to Characterization Factors

The scaling approach of the underlying indicators to characterization factors (CFs) is slightly adjusted compared to ESSENZ and SCARCE [1,2] as outlined in this section.

In order to be able to fill data gaps of country-based (sub-)indicators, the indicators have to be scaled to the same range: The respective indicators are scaled from 0 to 1 over all countries x with a min-max approach (see Equation (S1)), before they are (if intended) complemented with suitable indicators, followed by (if intended) aggregation and country-wise multiplication with the share of global production of a raw material.

$$indicator\ value_{x,scaled_{0-1}} = \frac{value_x - value_{min}}{value_{max} - value_{min}} \quad (S1)$$

Exceptions are the sub-indicators *Forced labor* and *Freedom of association, collective bargaining and right to strike* which show a very uneven distribution with an accumulation at the minimum value. Therefore, these sub-indicators are scaled from 0.1 to 1 (see Equation (S2)) to avoid zero values for many countries implying “no residual risk” even though this implication would not be justified.

$$indicator\ value_{x,scaled_{0.1-1}} = (1 - 0.1) \frac{value_x - value_{min}}{value_{max} - value_{min}} + 0.1 \quad (S2)$$

To complement indicators with several data gaps, i.e., missing values for certain countries, correlation analyses are conducted. An example for an indicator for which the complementing indicator is changed compared to the original ESSENZ method is given in Figure S1: The Enabling Trade Index (ETI) is examined for correlation with the per capita gross domestic product (GDP) at purchasing power parity (PPP) and with the Worldwide Governance Indicator (WGI) “Regulatory Quality” multiplied by 1.16. The latter shows a better fit with an R value (root of R^2) of 0.947.

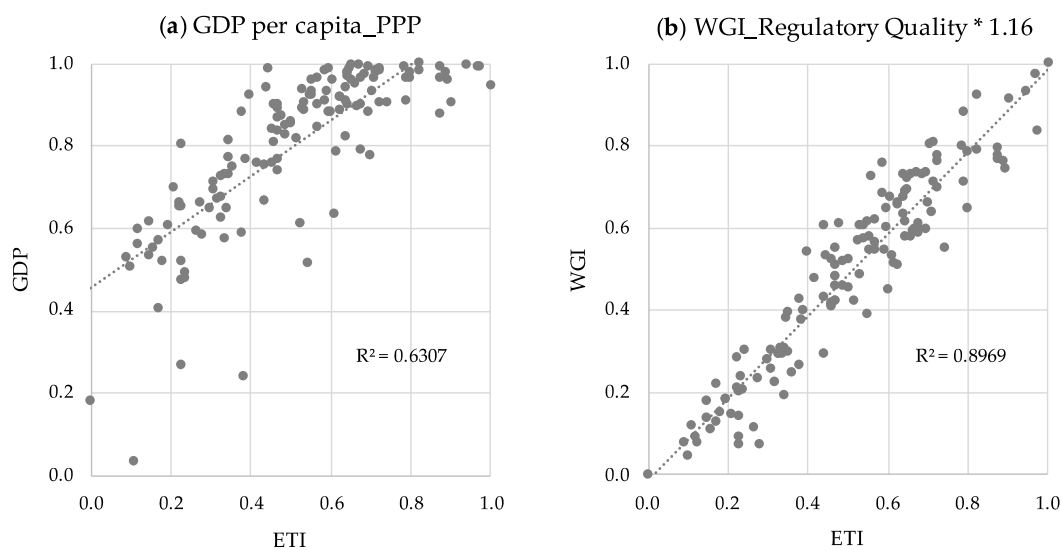


Figure S1. Correlation analysis regarding ETI and GDP vs. WGI. ETI set into correlation with: (a) GDP per capita (Purchasing Power Parity); (b) WGI “Regulatory Quality” multiplied with 1.16.

Furthermore, the Distance-to-Target (DtT) approach is slightly adjusted. The step of setting DtT results below one to zero [1] is changed by setting the threshold from one to 0.8. That way, indicator values that are below but close to the target are still included in the following process instead of being omitted by zeroing. Thus, the identified shortcoming regarding the DtT approach (see Section 2.1 in the paper) is addressed. However, this does not eliminate the necessity to deal with the step "Set DtT results below X to zero" as such in future research (see Section 2.2 in the paper).

Moreover, as the indicator scaling is partly different to the original ESSENZ method, some targets for the DtT approach have to be adjusted accordingly. All targets for the categories of the *Socio-economic availability* dimension are listed in Table S1.

Table S1. Targets for DtT approach. Partly adjusted due to different scaling of indicators.

Category	Target
Company concentration	0.15
Concentration of reserves	0.15
Concentration of production	0.15
Mining capacity	50 [years]
Feasibility of exploration projects	0.55
Occurrence of co-production	0.25
Trade barriers	0.41 ¹
Political instability	0.45 ²
Demand growth	0.05
Primary material use	0.75
Price fluctuations	0.20

Original target divided by max of original indicator range to obtain respective target between 0 and 1:

¹ $3.15/7.6 = 0.414$

² $1.9/4.26 = 0.446$

The relations and order of the different scaling steps are displayed in Figure S2. Please note that there are differences in scaling of CFs of the *Socio-economic availability* and the *Societal acceptance* dimension, since the categories of the *Societal acceptance* dimension do not undergo the DtT approach and are not multiplied with the bill of material in the end due to reasons given in Bach et al. [3].

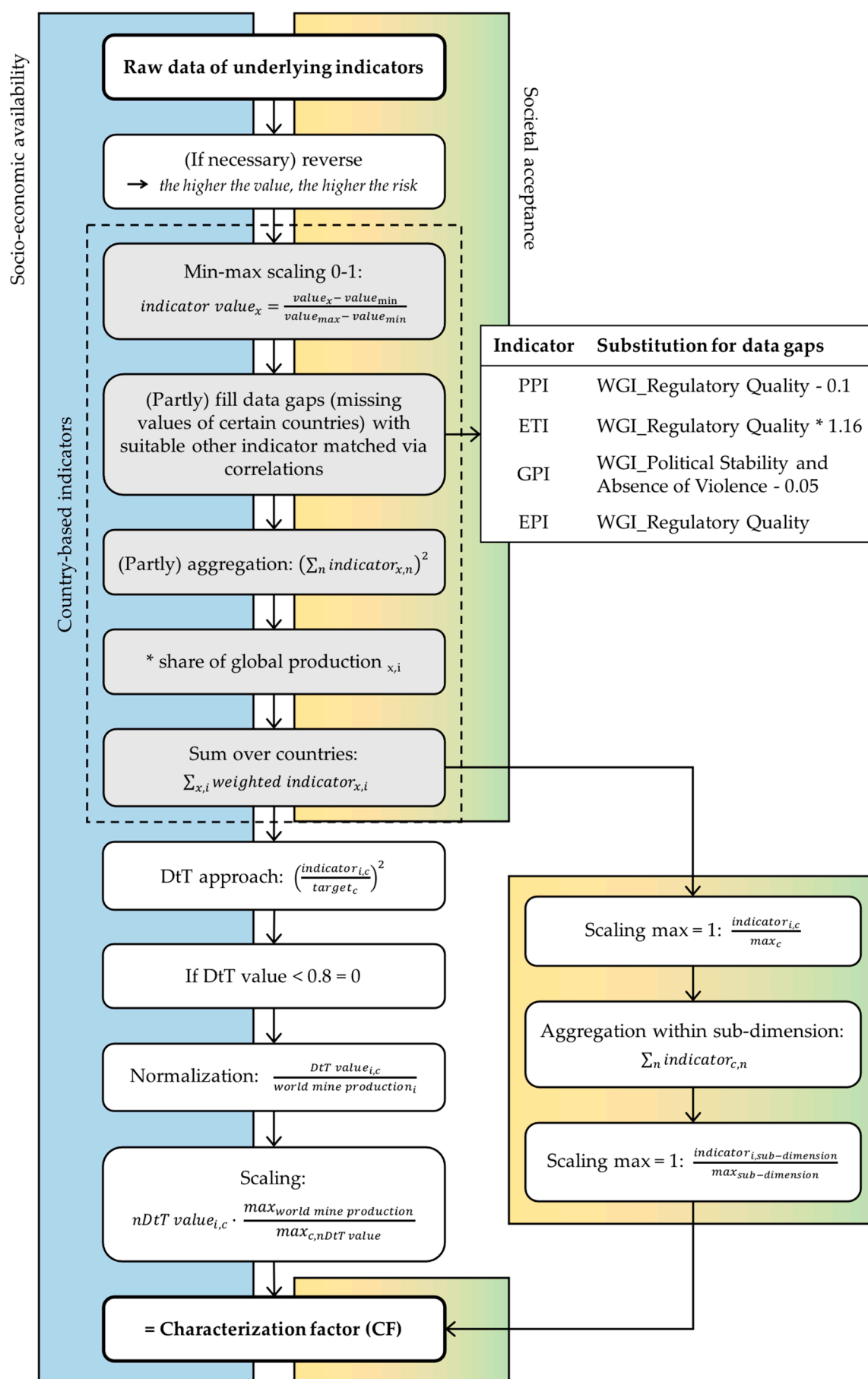


Figure S2. Scaling steps from raw data of indicators to characterization factors. Subscripts: x = country, n = number of indicators, i = raw material, c = category.

S2. Update of Characterization Factors

Regular data updates are necessary to adequately reflect changing supply risks [4]. Hence, for the raw materials and categories considered in the case study, the underlying indicators are updated if possible. An overview is given in Table S2. The updated CFs are provided in the Electronic Supplementary Material.

Table S2. Data update of underlying indicators of considered categories. Indicators with a grey background are country-based. Red marked indicators are not updated.

Category	Indicator	Data update	Year	Reference
<i>Socio-economic availability</i>				
Company concentration	Herfindahl-Hirschman Index (HHI) → SNL Metals & Mining dataset	not accessible ¹	-	-
Concentration of reserves	Herfindahl-Hirschman Index (HHI) → Mineral Commodity Summaries of USGS	yes	2019	[5]
Concentration of production	Herfindahl-Hirschman Index (HHI) → Mineral Commodity Summaries of USGS	yes	2019	[5]
Mining capacity	Static lifetime → Mineral Commodity Summaries of USGS	yes	2019	[5]
Feasibility of exploration projects	Policy Perception Index (PPI)	yes ²	2020	[6]
Occurrence of co-production	Percentage of production as companion metal	not available	-	-
Trade barriers	Enabling Trade Index (ETI)	not available ³	-	-
Political instability	Worldwide Governance Indicators (WGI)	yes ²	2019	[7]
Demand growth	Compound annual growth rate (CAGR)	yes ²	2021	own research ⁴
Primary material use	Share of primary material	not available	-	-
Price fluctuations	Volatility → “Volatilitätsmonitor” of BGR	yes ²	2020	[8]
<i>Societal acceptance</i>				
Artisanal and small-scale mining	Share of material extracted in an ASM operation	small changes compared to SCARCE	diverse	[2], own research
Risk of labor rights violation	Social Hotspots Database (SHDB) risk indicators	yes ²	2011/ 2012	[9]
Geopolitical risk	Global Peace Index (GPI)	yes ²	2020	[10]
	Worldwide Governance Indicators (WGI)	yes ²	2019	[7]
Sensitivity of local biodiversity	Ecoregion factor (EF)	yes ²	2019	[11] (adjusted)
Environmental policy	Environmental Performance Index (EPI)	yes ²	2020	[12]

¹ Own calculation only for CFs for recyclates (see Section S3.3). ² Not only a simple data update but a new version of the indicator/category (see Section 3.1 in main paper). ³ No data update of underlying indicator available, but further processing of existing raw data is changed (see explanation below table). ⁴ See Table S4.

The HHI for the category *Company concentration* is not updated for primary raw materials due to non-affordability of access to the SNL Metals & Mining dataset [13]. For recyclates, the HHI is calculated for battery recycling companies considering their recycling capacities [t/a] and number of plants worldwide (see Section S3.3).

For the indicators of the categories *Occurrence of co-production*, *Trade barriers* and *Primary material use*, there is no comprehensive data update available. However, the ETI used for the *Trade barriers* category is scaled differently. Furthermore, data gaps of certain countries are complemented by extrapolation based on the WGI instead of the gross domestic product (GDP) as before (see correlation analysis in Figure S1).

The country-based indicators (marked with a grey background in Table S2) are multiplied with the global production shares based on USGS data. In the course of the data update, USGS data from 2019 is used [5]. For recyclates, the country shares regarding the global Li-ion battery recycling are compiled doing product-specific research (see Section S3.3). These country shares serve the same purpose as the USGS data for primary raw materials.

S3. Additional Information regarding the Case Study

Regarding the case study on batteries in the automotive sector, some additional information is given in this section.

S3.1. Inventory Data

In Table S3 the data on the bill of material of the five assessed NMC battery cell chemistries with regard to the functional unit of 1 kg/kWh is provided. Compared to the original data from Mathieu & Mattea [14], the data given for steel are assumed to be the same for iron as a simplification.

Table S3. Inventory data regarding NMC batteries. Data from [14] with simplification: steel = iron.

Raw material	Bill of material [kg/kWh]				
	NMC 111	NMC 532	NMC 622	NMC811	NMC 9.5.5
Aluminum	0.62	0.58	0.55	0.50	0.46
Cobalt	0.34	0.19	0.18	0.08	0.04
Copper	0.36	0.34	0.32	0.29	0.27
Graphite	0.94	0.88	0.83	0.76	0.69
Iron	0.36	0.34	0.32	0.29	0.27
Lithium	0.12	0.11	0.11	0.08	0.07
Manganese	0.32	0.27	0.17	0.08	0.03
Nickel	0.34	0.47	0.53	0.64	0.66

S3.2. Demand Growth

For the raw material portfolio assessed in the case study, the compound annual growth rate (CAGR), the underlying indicator of the *Demand growth* category, is given in Table S4.

Table S4. Demand growth indicator for case study specific raw material portfolio.

Raw material	Compound annual growth rate [%]	References as basis for calculation
Aluminum	2.8	[15–17]
Cobalt	10.6	[16,18]
Copper	2.2	[15,16,19]
Graphite	10.2	[20–23]
Iron	1.1	[15,24–27]
Lithium	17.3	[15,16,28]
Manganese	3.1	[29,30]
Nickel	6.4	[15,16,31–33]

S3.3. Adjustment regarding Recyclates

For country-based indicators, country shares regarding the global recycling activities replace the global production shares derived from USGS data (see Section 3.2.2 in the paper). To compile the list of country shares regarding the global Li-ion battery recycling, several conditions are collected and assumptions are made: Battery production is and will be “located close to vehicle production to fit into the ‘just in time’ manufacturing model of the automotive industry” [14] (p. 20). This adjacent production “helps minimize supply-chain risk and enables improved collaboration between battery and automakers, while reducing logistics costs and improving safety” [34]. As a further consequence, the battery recycling is and will be mainly located close to battery production, alone already to manage production scraps [35]. This leads to the conclusion that the recycled cobalt, lithium and nickel used in new batteries will mainly come from Li-ion battery recycling activities.

Based on these conditions, research is conducted not only focusing on battery recycling locations and capacities but also on battery and (electric) vehicle production to complement the research results. The research is furthermore not limited to current battery production and recycling capacities but includes announcements and forecasts to obtain a valid picture of how the battery recycling industry will look like in the near future considering the booming e-mobility. That way, a comprehensive list of country shares is prepared including the following aspects listed in Table S5.

Table S5. Aspects of research regarding country shares for recyclates in the case study.

Research aspect	References
Motor vehicle production (2019)	[36]
Electric vehicle (EV) sales (2020)	[37]
EV sales 2030 forecast	[37]
EV exports	[38]
Key player companies in EV supply chain	[35]
Battery production plants (existing and announced)	among others [38,39]
Battery production capacity [GWh/a]	
Battery recycling plants (existing and announced)	among others [14,35,38,40,41]
Battery recycling capacity [t/a]	

Out of this information regarding the respective country shares, an average is built, neglecting countries in the column of motor vehicle production that are not mentioned neither in the column of EV sales nor in the battery production or recycling. In a final step, these averaged country shares are scaled so that they account for 100% in total. The resulting list is given in Table S6.

Table S6. Country shares regarding global recycling activities of Li-ion batteries.

Rank	Country	Share [%]
1	China	32.5
2	Germany	10.5
3	USA	9.5
4	India	5.4
5	Japan	4.9
6	South Korea	4.7
7	Canada	3.4
8	France	3.4
9	Hungary	3.2
10	UK	2.4
11	Norway	2.0
12	Netherlands	1.8
13	Mexico	1.5
14	Belgium	1.4
15	Sweden	1.3
16	Finland	1.3
17	Italy	1.3
18	Thailand	1.2
19	Spain	1.0
20	Poland	0.9
21	Brazil	0.8
22	Turkey	0.8
23	Indonesia	0.7
24	Czech Republic	0.6
25	Slovakia	0.6
26	Singapore	0.5
27	Australia	0.5
28	Switzerland	0.5
29	Malaysia	0.4
30	Taiwan	0.4
31	Vietnam	0.4
32	Austria	0.3

For the category *Company concentration*, the Herfindahl-Hirschman Index (HHI) is calculated for battery recycling companies using Equation (S3).

$$HHI_{company\ concentration} = \sum s_{company}^2 \quad (S3)$$

The share of each company $s_{company}$ is calculated by taking the average of the share regarding the recycling capacity [t/a] and the share regarding the number of plants of the respective company worldwide. In principle, the global recycling capacity of a company is the parameter with more significance. However, since data is often lacking for this parameter, the number of plants is also taken into account. Data on both aspects are collected from literature [14,35,38,40–44]. If a recycling plant is a joint venture, the share is assumed to be split 50-50 between the two companies.

S3.4. Supplementary Results

To enable a valid comparison of the categories of the *Societal acceptance* dimension between the adjusted CFs regarding certified mine sites and recycle use, the results of the sensitivity analysis regarding certified mine sites are shown in Figure S3 also for the raw material subset used for the sensitivity analysis regarding recycle use. Part (a) of the figure corresponds to Figure 10 in the paper to demonstrate that the difference between the whole raw material portfolio and the subset is marginal for the displayed categories. Thus, the comparison made in Section 4.2.3 in the paper is justifiable.

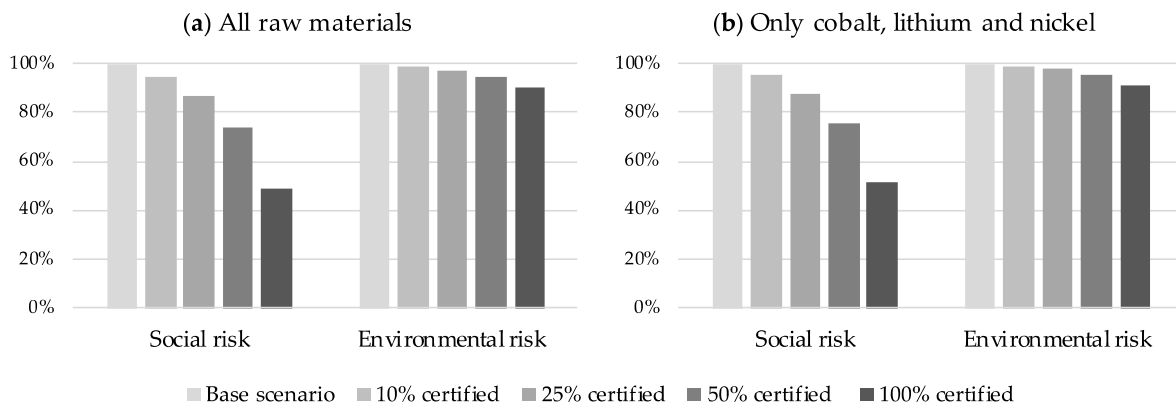


Figure S3. Comparison of results for the sensitivity analysis regarding certified mine sites. Considered raw materials: (a) All raw materials considered in the case study; (b) Only cobalt, lithium and nickel.

S4. Additional Aspects of Discussion

S4.1. Mine Site Certification

The question arises whether recyclates could also be certified, not by certification of a mine site but of a recycling plant. Both risk reducing aspects could be merged that way, leading to a chance to countervail the residual risk regarding recyclates in the categories of the *Societal acceptance* dimension due to the high share of recycling activities in China (see Figure 12 in the main paper and description below). Whereas the IRMA standard only applies to mining, the SA8000 standard is suitable for all kind of organizations and covers important aspects of the *Social risk* category, namely child labor, forced labor and freedom of association and the right to collective bargaining [45]. However, the *Environmental risk* category is not covered by this standard. An integration of a risk reduction regarding certified recyclates could be the subject of future research.

Besides the IRMA standard, there are other standards like the mentioned SA8000 or further mining-specific standards like the Responsible Minerals Initiative [46] and the Certified Trading Chains [47]. If a different standard would be used as a reference for ESSENZ+, the results might vary.

Concerning the quantification of the influence of certifications, it has to be noted that the used risk multipliers represent an estimated average risk reduction. In practice, the influence of mine site certification is heterogeneous: In countries with strong existing policies, the enhancement due to a certification might be only incremental, whereas in countries with weak policies or poor implementation of regulations a certification can imply, in relative terms, substantial improvements [48]. Besides, it should be noted that the values of the risk multipliers are estimations based on qualitative information in the literature and consultation of an IRMA expert. The validity should be verified in future research.

An alternative to the relative approach using risk multipliers, if raw materials are procured from certified mine sites, would be to set the risk in the affected categories to a fixed value corresponding to a well performing country. However, this approach would not reflect reality, considering the example of a certified mine site in the Democratic Republic of the Congo that certainly does not have the same social standards in practice like a mine site in Finland (one of the best performing countries in the *Risk of labor rights violation* category, see [9]).

Another aspect related to mine site certification is the validity of the certificates. Depending on the auditing organization, issues like corruption, insufficient training of auditors and checklist mentality can pose a problem [49]. Especially external audits can be a weak point [50]. In general, “audits should only be carried out by experienced auditors who are familiar with local conditions” and at the same time “adequate resources and time [should be] available to ensure an effective inspection” [50] (p. 20).

S4.2. Data Update for the Case Study

Regarding the data update, it has to be noted that the raw data of the SHDB accessed in 2021 differ to the raw data obtained for the initial CFs of the original ESSENZ method, but in the documentation on the website of the database, the reference years are still mostly indicated as 2011 and 2012 [9]. In the

“Supporting documentation”, however, more recent data sources are stated, e.g., for forced labor, references from 2016 to 2018 [51]. This presumably outdated data situation should be taken into account when interpreting the results regarding the social risk.

A complete set of baseline CFs for eight raw materials is compiled to carry out the introduced case study. The same applies to CFs intended for certified mine sites whereas the CFs for recyclates are only available in a product-specific context for the three raw materials cobalt, lithium and nickel. The transferability of the case study results is differently complex for several aspects of ESSENZ+: Regarding the country-based indicators, the extension on other raw materials can be accomplished with little effort by incorporation of the respective USGS data. On the contrary, underlying indicators of the other categories require more individual research if databases or overviews of several resources in the literature are missing like in the case of the future based *Demand growth* category. Once the baseline CFs for all raw materials exist, the extension of the CF set for certified mine sites is rather easy due to the relative approach using the risk multipliers for the respective indicators (see Section 3.2.1 in the main paper). Concerning the CFs for recyclates, the greatest effort occurs since an extension on other raw materials and products is just not possible. Instead, individual research is necessary for the new product to be assessed along with the affected raw materials.

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